Absence of Localization in a Nonlinear Random Binary Alloy

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We investigate electronic propagation in a one-dimensional nonlinear random binary alloy modeled by a discrete nonlinear Schrödinger equation. We find absence of electronic localization except for large nonlinearity parameter values. The presence of disorder is completely overcome by the nonlinear terms leading to ballistic propagation of the untrapped electronic fraction. The existence of disorder in the model is manifested in the power-law decay of the transmissivity of plane waves through the medium as a function of the system size.

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The theory of Anderson localization predicts that the wave function of a free electron moving in a one-dimensional lattice with on-site energetic disorder is localized even for an infinitesimal amount of disorder [1]. This effect leads to the absence of transport in one-dimensional infinite disordered lattices. On the other hand, if the interaction of the particle with lattice vibrational modes is taken into account, the resulting polaron dynamics becomes more complicated, leading in some cases to the possibility for occurrence of a mobility edge [2]. Furthermore, this interaction with the lattice can lead, in other instances, to an effective correlation between the local lattice site energies and the nearest-neighbor overlap integrals resulting in possible particle delocalization even in one dimension [3]. Particular forms of the electron-phonon interaction can be eliminated and effectively taken into account as a nonlinear term in the electronic equation [4]. In these cases, the dynamics of an electron in the disordered medium can be addressed as a problem of the combined effects of disorder and nonlinearity in transport in quasi-one-dimensional media. As with disorder, nonlinearity in a discrete lattice leads effectively to the creation of localized wavelike modes, that, nevertheless, have the ability for efficient propagation in an ordered medium. When nonlinearity and disorder coexist in a one-dimensional model, their combined effects lead in some cases to suppression of propagation of these modes, whereas in others to partial propagation [5–8]. To address the issue of propagation in a disordered nonlinear lattice, we study a model based on the discrete nonlinear Schrödinger equation (DNLS) where the disorder resides completely in the nonlinearity.

Consider an electron (or, more generally, an excitation) moving in an infinite one-dimensional (host) lattice that contains random impurity molecules. The two species of impurity (type A) and host (type B) molecules form a random binary alloy and each have an identical, unique electronic state accessible to the electron. The existence of strong local couplings between the electronic and vibrational modes in each species results in a random binary distribution of cubic nonlinearity type terms in the tight-binding equation for c_n, the electronic probability amplitude at site n,

$$i\frac{dc_n}{dt} = V(c_{n+1} + c_{n-1}) - \chi_n |c_n|^2 c_n , \qquad (1)$$

where V is the nearest-neighbor electronic transfer matrix element. The nonuniform nonlinearity parameter χ_n is proportional to the local electron-phonon coupling in each species at site n under the assumption of an antiabatic approximation [4]. The probability distribution $P(\chi_n)$ for χ_n is bivalued:

$$P(\chi_n) = p\delta(\chi_n - \chi_A) + (1-p)\delta(\chi_n - \chi_B). \qquad (2)$$

We note that the system described by Eq. (1) is intrinsically nonlinear and does not reduce to a usual Anderson type problem in any limit. When $\chi_A = \chi_B = \chi$ it reduces, however, to an ordered nonlinear lattice with interesting self-trapping properties [9,10].

In order to study the localization properties of a wave packet in the nonlinear binary alloy lattice described by Eqs. (1) and (2), we place an electron initially near the middle (identified with the site $n = 0$) of a long chain and observe its time development for relatively long times. In order to quantify localization we calculate the packet mean square displacement at each instant of time; the latter is given by

$$\langle m^2 \rangle = \sum_{m=-\infty}^{\infty} m^2 |c_m(t)|^2 , \qquad (3)$$

where the normalization $\sum_{-\infty}^{\infty} |c_m(t)|^2 = 1$ has been used.

Our numerical scheme is that of the fourth order Runge-Kutta; its accuracy was monitored through total probability conservation. In order to exclude any undesired boundary effects we use a self-expanding lattice [3]. The results to be presented in the present Letter involve the most disordered case, viz., $p = \frac{1}{2}$, although other binary

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fractions have also been investigated [11]. In the numerical calculations we used two distinct initial electron preparations. The simplest one (type I) involves complete initial particle localization whereas in the second (type II) the particle wave packet is spread approximately over a distance 2σ determined through a Gaussian:

$$c_n(0) = \delta_{n,0} \quad \text{type I}, \tag{4}$$

$$c_n(0) = \frac{1}{N}\exp(-n^2/4\sigma^2) \quad \text{type II}. \tag{5}$$

The normalization factor is $N^2 \equiv \sum_{-\infty}^{\infty}\exp(-m^2/2\sigma^2) = \theta_3(q)$, where the nome q of the theta function is related to the width of the Gaussian through the relation $2\sigma^2 \ln q = -1$. No phase information was added in type II initial conditions. By varying σ one can delocalize the initial spread of the electron to an arbitrary degree and also recover the initial condition of type I in the limit of $\sigma \to 0$. Since for different realizations of the lattice the central site at $n = 0$ will have different nonlinearity values, we introduce a register r_{AB} that keeps its value of χ. Thus, the $n = 0$ site coincides with the initially occupied site (in type I initial conditions) or the center of the Gaussian (in type II initial conditions). The register, defined as $r_{AB} \equiv (\chi_A, \chi_B)$, denotes that the initially occupied site (impurity or center of the Gaussian), has nonlinearity value χ_A whereas the nonlinearity value for the other type sites has value χ_B. The main results of our simulations for initial conditions of type I and type II are presented in Fig. (1). In Fig. 1(a) we plot the mean square displacement as a function of time for various χ_A for $r_{A0} \equiv (\chi_A, 0)$ whereas in Fig. 1(b) we show the corresponding case of $r_{AB} \equiv (\chi_A, \chi_B)$. The former case is that for which the host lattice is assumed to be linear, whereas in the latter case we have a genuine nonlinear binary system. In both cases we observe that, after a short initial transient, the mean square displacement becomes exactly proportional to the square of time, i.e., the motion of the packet becomes ballistic. We note, however, that the coefficient of proportionality between $\sqrt{\langle m^2 \rangle}$ and t, representing the rate (or speed) of the ballistic motion, is markedly different from that in the linear, ordered lattice. In the latter case we have $\langle m^2 \rangle = 2(Vt)^2$. Furthermore, we note that the wave packet speed changes drastically when the value of the nonlinearity parameter χ_A at the initially populated site exceeds a certain threshold critical value χ_{cr}. This behavior is directly related to the effects of the one nonlinear impurity dynamics embedded in an infinite lattice with nonlinearity value χ_B with $0 \le \chi_B < \infty$. The case for $\chi_B = 0$ is well studied and leads to a $\chi_{\mathrm{cr}} \simeq 3.2V$ [4,12]. The case with $\chi_B \neq 0$ is more complicated but it can also be shown that there is a χ_{cr} that now also depends on the value χ_B [11]. In both cases, while $\chi_A < \chi_{\mathrm{cr}}$ there is no probability for self-trapping at the initial site leading to complete particle escape. When $\chi_A \ge \chi_{\mathrm{cr}}$, on the other hand, self-trapping occurs leading to partial localization at the initial site while the rest of the probability wave escape to infinity. The results for the mean square displacement of an initial Gaussian packet with $r_{A0} \equiv (\chi_A, 0)$ show the same ballistic motion effect, although the critical value of the nonlinearity parameter χ_{cr} for occurrence of partial localization changes. An approximate analytical estimate for the modified critical nonlinearity parameter χ_{cr}^g for local self-trapping with the Gaussian initial condition for the case r_{A0} can be obtained, showing a rapid increase of χ_{cr}^g as the width of the Gaussian packet increases,

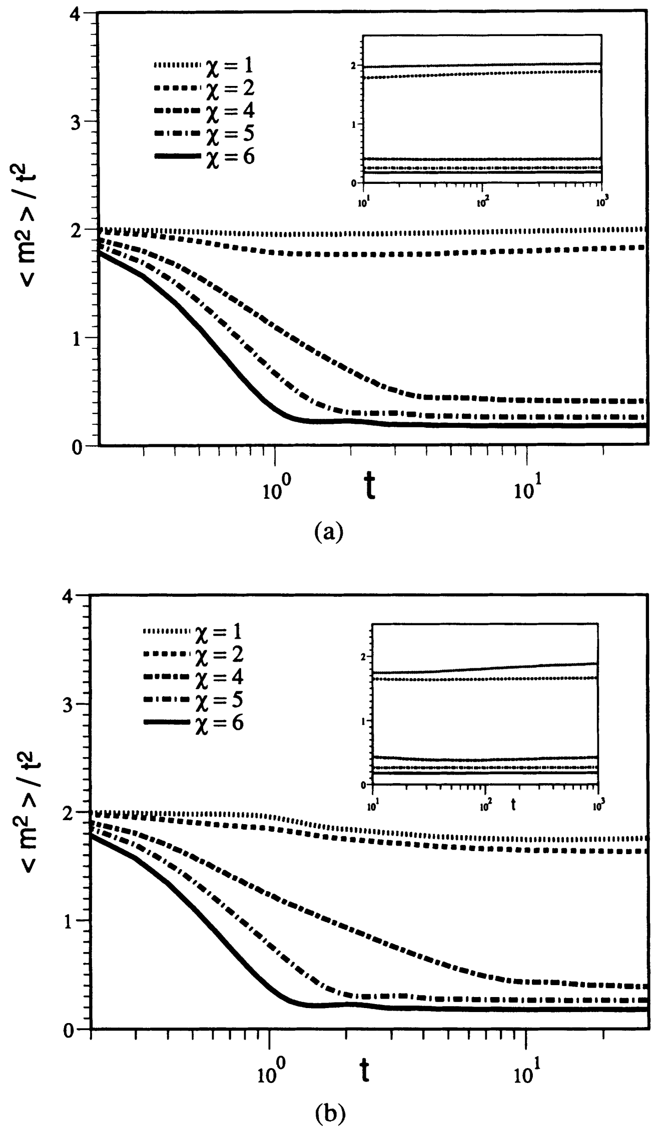

FIG. 1. Electronic mean square displacement as a function of time t for localized initial conditions ($V = 1$). In (a) nonlinear impurities are distributed randomly in a linear chain $r_{AB} = (\chi, 0)$ having several nonlinearity χ values. In (b) nonlinear impurities are distributed in the nonlinear chain $r_{AB} = (\chi, 3)$ for different nonlinearity parameter values. In the inset we plot longer time dependence of the mean square displacement showing the persistence of the ballistic nature of the notion.

especially for $\sigma \geq 0.3$ [11]. We observe that ballistic propagation prevails for all values of χ_A, although the rate of propagation is directly affected by the value of the nonlinearity parameter at the central site. For nonlinearity values in a site larger than the critical one, there is partial self-trapping, thus reducing the total probability wave that can escape to infinity. Similar effects are observed in the more general case where $\chi_B \neq 0$ [11]. In Fig. (2) we show actual particle propagation in the disordered nonlinear lattice with initial conditions of type II. We observe complete particle delocalization in Fig. 2(a) accompanied by ballistic escape to infinity while in Fig. 2(b) there is partial localization in the site at the center of the Gaussian initial condition. In both cases the mean square displacement is very similar to the one obtained with a localized initial condition.

When the previous series of numerical studies are repeated choosing an initial site (or site where the center of the Gaussian is located) without nonlinearity (r_{0B}), the ballistic propagation persists with rates close to the one of the perfect lattice. No partial localization in the vicinity of the initial site was observed except for very large nonlinearity values. In the latter cases the particle is trapped partially in the nonlinear sites adjacent to the initial one.

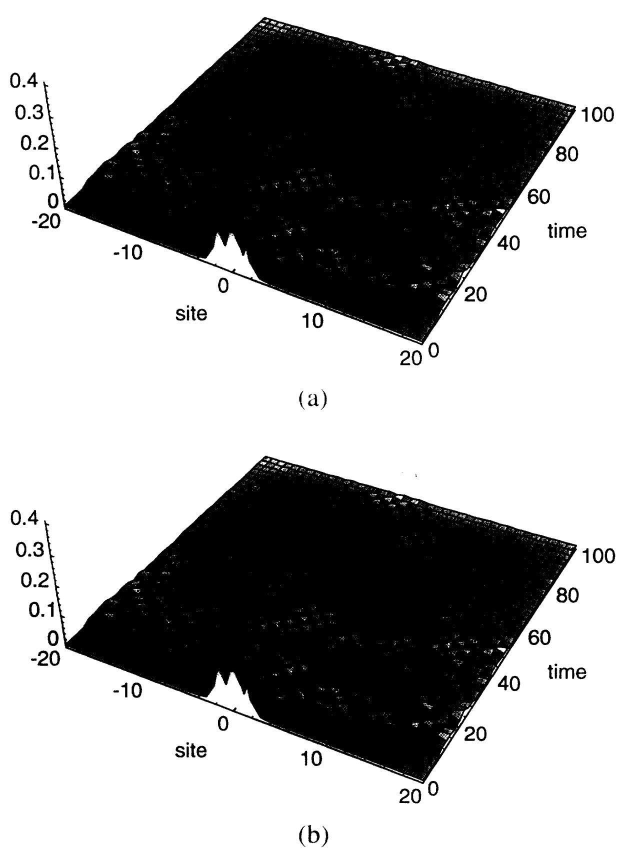

FIG. 2. Electronic probability propagation profile as a function of time for the nonlinear random binary alloy, with a Gaussian initial condition and $\sigma = 1.0$. In (a) $r_{AB} = (10, 0)$ and in (b) $r_{AB} = (20, 0)$. In (b) we observe partial localization at the central site of the Gaussian initial condition. In both cases the untrapped portion escapes ballistically.

The absence of any particle localization for nonlinearity smaller than a critical value (the actual value depends on the initial preparation of the wave packet), and the ballistic character of the electronic propagation even in the presence of genuine disorder are the most notable features of our model. These properties are consistent with the analytical results for the one impurity problem [13], but markedly different from the subdiffusive propagation occurring in the fully nonlinear lattice with on-site energetic disorder [6]. The ballistic nature of the propagation is dominated by the behavior of the model in the small nonlinearity regime. For small χ_n values we can replace the probability in the nonlinear term of Eq. (1) with the corresponding exact solution of the linear problem, viz., $|c_n(t)|^2 = |J_n(2Vt)|^2$ (for localized initial condition) and obtain $\epsilon_n = -\chi_n |c_n|^2 \approx -\chi_n J_n^2(2Vt)$, where ϵ_n plays the role of an effective local time-dependent site energy at location n, with J_n being a Bessel function of the first kind and order n. We note that in this limit the local disordered electronic site energies have an amplitude that decays in time leading to an effective asymptotic disappearance of the disorder. The large-χ_n regime, on the other hand, can be understood through the application of Aubry's anti-integrability limit [14]. The assumption of an initially localized wave function and small nearest-neighbor matrix elements leads rigorously to the existence of a breather mode that corresponds here to self-trapping [15]. The untrapped portion of the probability renormalizes χ_n in the remaining portion of the crystal to much smaller values, thus leading to ballistic propagation [16].

In addition to the dramatic departure from an anticipated Anderson type localization of the particle, "nonlinear disorder" directly affects the plane wave scattering properties. To study these effects we embed a disordered nonlinear segment of length L in an infinite linear lattice. The segment starts at site $n = 0$ and ends at site $n = L$ and has binary nonlinearity values χ_A, χ_B (with $p = \frac{1}{2}$). We then inject a plane wave with wave number k and study its transmission properties as a function of the length L [17]. We set $c_n(t) = \phi_n \exp(-iEt)$ in Eq. (1), where E is the energy of a stationary state [9,17,18] and obtain

$$E\phi_n = V(\phi_{n+1} + \phi_{n-1}) - \chi_n |\phi_n|^2 \phi_n . \qquad (6)$$

The injected (R_0), reflected (R_1), and transmitted (T) amplitudes of the waves are related though the equation

$$\phi_n = \begin{cases} R_0 e^{ikn} + R_1 e^{-ikn} & n \leq 0, \\ T e^{ikn} & n \geq L . \end{cases} \qquad (7)$$

where the energy–wave-number relation is that of the infinite linear lattice, viz., $E = 2V\cos(k)$. For a given segment of length L we obtain an averaged realization-independent transmissivity in the following way: For each wave vector k we vary T, accumulate the total number of transmitting cases through the segment characterized by $t^2 = |T|^2/|R_0|^2 > t^2_{\mathrm{cut}}$ ($t^2_{\mathrm{cut}} = 10^{-6}$), and normalize with the result of the corresponding linear ordered segment. Subsequently, we average over k (by sending waves of all wave vectors), thus obtaining a normalized estimate of the nonlinear disordered segment transmissivity. We follow this procedure for various segment lengths from $L = 20$ to 1000 [11]. In Fig. 3 we display results for several disordered segments r_{AB} and compare them with the transmissivity of the nonlinear ordered segment. We observe a power-law decay of the transmissivity with the segment size and with a seemingly nonlinearity-independent drop. This behavior is markedly different from the exponential drop of the transmissivity found in the corresponding linear disordered segment (not shown in the figure [11]) and also expected from previous investigations [19,20]. A fit to the expression $t^2 \propto L^{-\beta}$ finds $\beta \approx 0.76$, although this value depends slightly on the segment realization. Power-law decay in the transmission of plane waves has also been observed in nonlinear models with energetic on-site disorder [5,21].

The two conclusions of this study, viz., the absence of complete localization of the wave packet accompanied by ballistic propagation and the power-law decay of the transmission coefficient as a function of the segment size, present examples of the intricacies found in nonlinear disordered systems. In the present model, the initial preparation of the system plays a dramatic role in the dynamic

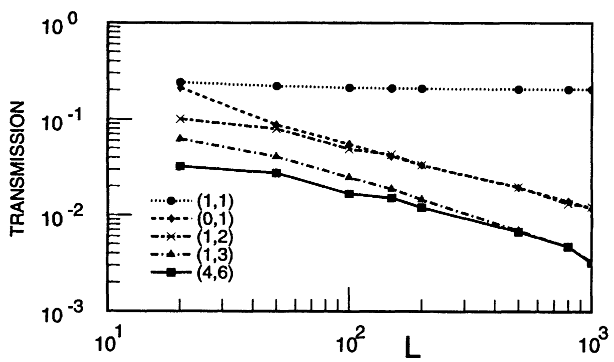

FIG. 3. The transmission coefficient for plane wave propagation across a disordered nonlinear segment of a random binary alloy $r_{AB} = (\chi_A, \chi_B)$ is plotted as a function of the segment length L, for several χ_A, χ_B values ($V = 1$). We note that the register r_{AB} does not carry any initial condition information in these cases of plane wave propagation. The curve with r_{11} corresponds to an ordered nonlinear segment studied in Refs. [17,18]. The effect of disorder in the nonlinear segment is evident.

properties of the wave propagation. The nonlinear aspect of the system effectively cancels the disorder when localized, solitonlike modes are injected, while the disorder aspect becomes more dominant when extended waves are introduced in the lattice. It is expected that this peculiar behavior has consequences in disordered quasi-one-dimensional systems with strong electron-phonon coupling.

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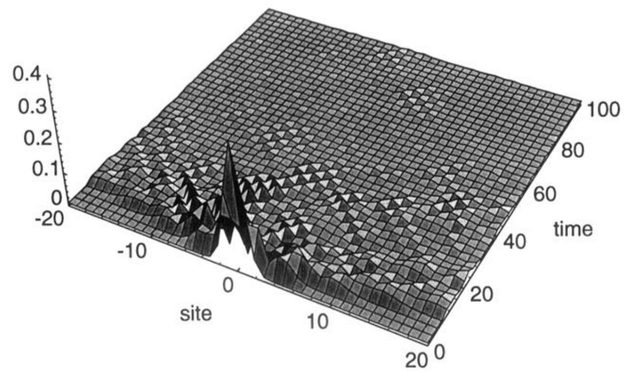
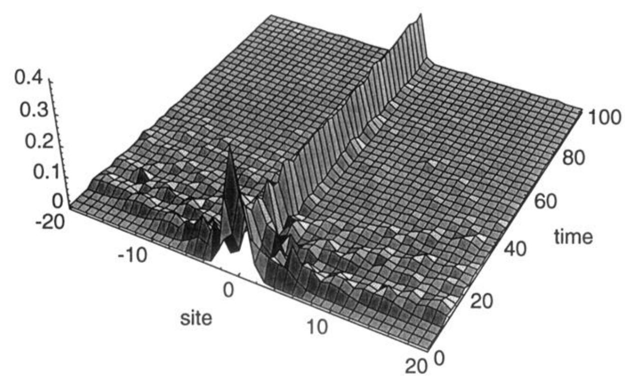


(a)



(b)

FIG. 2. Electronic probability propagation profile as a function of time for the nonlinear random binary alloy, with a Gaussian initial condition and $\sigma = 1.0$. In (a) $r_{AB} = (10, 0)$ and in (b) $r_{AB} = (20, 0)$. In (b) we observe partial localization at the central site of the Gaussian initial condition. In both cases the untrapped portion escapes ballistically.