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Generalized nonlinear impurity in a linear chain

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We study the problem of one nonlinear impurity embedded in a linear tight-binding host. The impurity is of the type found in the generalized discrete nonlinear Schrödinger equation. We obtain analytically a phase diagram that describes the presence of bound states for different nonlinearity parameter values and nonlinearity exponents. We find that two impurity states are possible in some parameter regimes. From the numerical solution of the complete dynamical problem we obtain information on the nonlinear site survival probability that shows a dynamical self-trapping that is compatible with the findings of the stationary-state analysis.

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Phenomena associated with the simultaneous presence of nonlinearity and disorder are of much current interest, especially in the context of models associated with various dynamical processes in materials (see, for instance, [1,2]). In most of these models nonlinearity enters either through the coupling of two independent types of degrees of freedom (for instance, electron-phonon coupling) or through on-site potentials that arise from chemical bonds. A typical example of the first category, which is of interest here, is that of the cubic nonlinearity term of the discrete nonlinear Schrödinger equation (DNLS) [3]. Disorder can arise through various mechanisms in these systems such as through the presence of substitutional nonlinear impurities in a linear host. These impurities are a result of doping of materials with atoms or molecules that have strong local couplings. It is of interest to understand the role that nonlinearity plays in these disordered materials. In this context, analytical solutions can provide exact information for the role of nonlinearity and disorder when found together.

We consider an electron (or in general an excitation) moving in a one-dimensional periodic lattice. The dynamics is described by a discrete nonlinear Schrödinger equation:

$$i\frac{dc_n}{dt}=V(c_{n+1}+c_{n-1})-\chi|c_n|^d c_n\delta_{n,0}\ , \tag{1}$$

with c_n being the probability amplitude of the electron to be at site n, V is nearest-neighbor transfer matrix element, and χ representing the nonlinearity parameter describing strong interaction of the electron with the local vibrations on the impurity site. This type of generalized nonlinearity with arbitrary exponent d was introduced by Christiansen and Scott in the context of the generalized discrete self-trapping equation [4–6].

In the following we consider stationary solutions for the case of a nonlinear impurity of arbitrary exponent embedded on a linear lattice. The case $d=2$ has been discussed in Ref. [7].

Bound states. For determination of the bound states we present a simple analytical approach compatible with the Green's function formalism [7,8]. The stationary solutions are of the form $c_n(t)=\exp(iE_0t)\phi_n$, with ϕ_n being time independent, and the corresponding stationary equation becomes

$$E_0\phi_n=V(\phi_{n+1}+\phi_{n-1})-\chi|\phi_n|^d\phi_n\delta_{n,0}\ . \tag{2}$$

For bound state solutions we make the ansatz [8,9]

$$\phi_n=A\eta^{|n|}\ , \tag{3}$$

with $0<|\eta|<1$. The normalization factor A follows from $\sum_n|\phi_n|^2=1$ and is given by

$$A=\left[\frac{1-\eta^2}{1+\eta^2}\right]^{1/2}. \tag{4}$$

Taking into account the different solution behavior of the impurity site and the remaining linear chain, we obtain the set of equations

$$E_0=\begin{cases}2V\eta-\chi A^d, & n=0 \qquad (5)\\ V\left[\eta+\dfrac{1}{\eta}\right], & n\neq 0\ . \qquad (6)\end{cases}$$

Combining these two equations, we get a nonlinear equation in η:

$$\eta-\frac{1}{\eta}-\beta A^d=0\ , \tag{7}$$

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where we introduced the dimensionless parameter $\beta=\chi/V$. Utilizing the normalization factor of Eqs. (4) and (7), we obtain after some algebra a polynomial equation for the amplitude:

$$\beta^2 A^{2d}-\frac{4A^4}{1-A^4}=0 . \tag{8}$$

The number of possible roots of this equation in the range $0\leq A\leq 1$ depends on the values of the exponent d and the nonlinearity parameter β. For a discussion of the solution behavior it is convenient to rewrite Eq. (8) in the following form:

$$A^{2(d-2)}-A^{2d}=\frac{4}{\beta^2} . \tag{9}$$

Simple analysis reveals the existence of one bound state (one solution) for all $d<2$ *regardless of the value of the nonlinearity parameter* β. At $d=2$ we recover the results of Ref. [7] showing a bifurcation in the stationary-state space: for $d=2$ and $\beta<\beta_{\rm crit}=2$, there is no bound state, whereas for $\beta\geq\beta_{\rm crit}=2$, there is one unique bound state. For nonlinearity exponents larger than 2 i.e., for $d>2$, we obtain a much richer behavior, viz. we observe the existence of a *critical line* $\beta_{\rm crit}=\beta_{\rm crit}(d)$ that has the following functional form:

$$\beta_{\rm crit}=\frac{\sqrt{2}d^{d/4}}{(d-2)^{(1/2)(d/2-1)}} . \tag{10}$$

This line separates, for each value of the exponent d, a regime where *two bound states* are possible (for $\beta>\beta_{\rm crit}$) from the regime where no bound state is possible (for $\beta<\beta_{\rm crit}$). On the critical line itself the two bound states of the high-β regime merge into a single state. In all cases the bound state energies are determined through

$$\epsilon_0\equiv E_0/V=\frac{-2}{\sqrt{1-A^4}} . \tag{11}$$

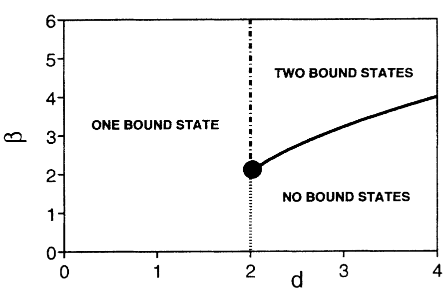

FIG. 1. Phase diagram showing the number of bound states as a function of the nonlinearity parameter β and the exponent d. We observe the following different regimes: (a) For $d<2$ there is always a bound state. (b) For $d=2$ there is no bound state for $\beta<2$ (dotted line), whereas there is a unique bound state for $\beta\geq 2$ (dot-dashed line) [7]. (c) For $d>2$ the critical line (solid line) represents Eq. (10) separating a regime where two bound states are found (larger β values) from the regime where no bound states exist (smaller β values). On the critical line itself there is a unique bound state. The circle represents a "singular point" in the sense that all possible regimes are formed around that point.

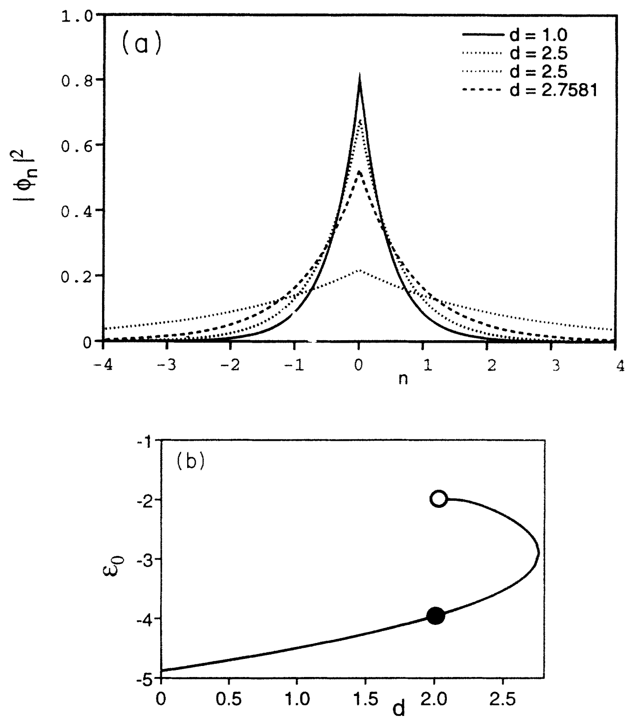

FIG. 2. (a) Probability profile for the bound states for different exponents d ($\beta=3.0$). At $d=2.7581$, the two bound states merge into a single state. (b) Bound state energy as a function of the nonlinearity exponent d ($\beta=3.0$). At $d=2$, a higher energy branch appears (open circle), whereas the solid circle marks the existence of a single state for the same d value. The two branches merge at $d=2.7581$.

In Fig. 1 we show the phase diagram in the β-d plane illustrating the different solution behavior of Eq. (9). The existence of two bound states in the high-β regime and the absence of a critical nonlinearity for the existence of a bound state mark the qualitatively different behaviors in the two regions surrounding the $d=2$ line from above and below, respectively. The bound states themselves for a given nonlinearity value ($\beta=3$) are seen in Fig. 2(a) where we plot the probability profile $|\phi_n|^2$ of possible

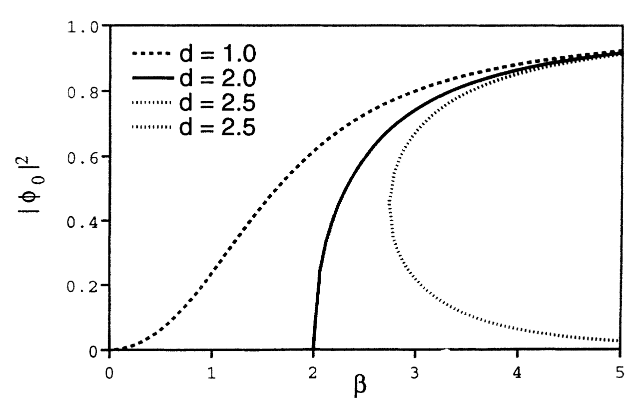

FIG. 3. The occupation probability of the nonlinear impurity site as a function of the nonlinearity parameter β for different exponents d.

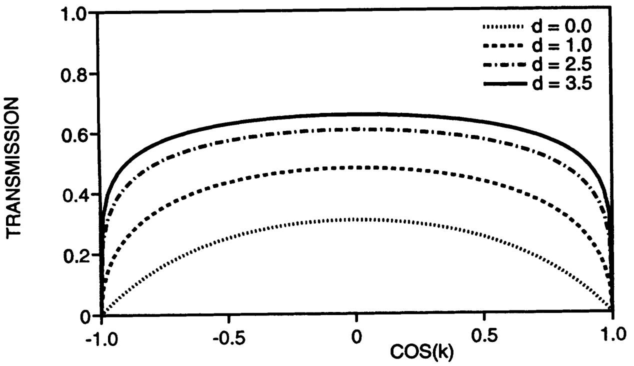

FIG. 4. Transmission coefficient t as a function of $\cos(k)$ for $\beta=3.0$ and different exponents d for an injected wave of unit amplitude. The linear case ($d=0$) is also included for comparison.

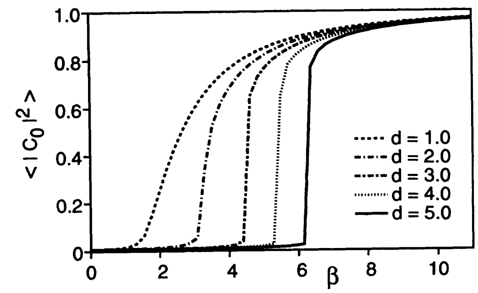

FIG. 5. Time-averaged probability at the nonlinear impurity site as a function of the nonlinearity strength β for different nonlinear exponents d.

bound states for different exponents d as a function of the lattice site n. We note the different spatial behavior of the two states corresponding to $d=2.5$ that eventually merge to a single state at $d=2.7581$. The dependence of the bound state energy on the exponent d for the same value of $\beta=3$ is shown in Fig. 2(b). We observe the gradual increase of the impurity state energy towards the lower edge of the band (occurring at energy value equal to -2). For $d>2$ a new localized state of higher energy appears (open circle). The two states coexist until their merging and subsequent disappearance. In Fig. 3 we plot the occupation probability at the impurity site as a function of the nonlinearity strength β for different exponents d. Note the gradual increase of the amplitude of the $d=1$ state in marked contrast to the $d\geq 2$ cases. In the two-bound-state regime (here for $d=2.5$), the higher energy state becomes more delocalized as nonlinearity increases, whereas the lower energy state has exactly the opposite tendency.

Extended states. We study the scattering properties of plane waves sent towards the nonlinear impurity. To obtain the transmission coefficient, we set [7]

$$\phi_n=\begin{cases} R_0 e^{ikn}+Re^{-ikn}, & n\leq 0 \qquad (12)\\ Te^{ikn}, & n\geq 1\ , \qquad (13)\end{cases}$$

with R_0, R, and T being the amplitude of the injected, reflected, and transmitted parts of the wave, respectively. After some algebra we obtain for the transmission coefficient $t=|T|^2/|R_0|^2$,

$$t=\frac{\sin^2(k)}{(\beta|R_0|^d/2)^2t^d+\sin^2(k)}\ . \qquad (14)$$

Figure 4 shows the transmission coefficient t as a function of $\cos(k)$ for different exponents d. With increasing exponent d, the transmittance of the generalized nonlinear impurity site increases. We note that the initial wave amplitude $|R_0|$ renormalizes the nonlinearity parameter β leading to an effective $\beta_{\text{eff}}=\beta|R_0|^d$. This property has been used to bridge the condensed matter and optics applications of DNLS [10].

We also studied the dynamics of the generalized nonlinear impurity embedded in the linear chain. The quantity of interest here is the time-averaged probability of the initially occupied nonlinear impurity site:

$$\langle |c_0|^2\rangle=\lim_{T\to\infty}\frac{1}{T}\int_0^T|c_0(t)|^2dt,\quad |c_0(0)|^2=1\ . \qquad (15)$$

In Fig. 5 we present the numerical results for different exponents d as a function of the nonlinearity parameter β. The case for $d=2$ has been treated in Refs. [11,12] and shows abrupt dynamical self-trapping for a given value of the nonlinearity parameter. We observe the same phenomenon for nonlinearity exponents larger than 2 occurring at progressively larger nonlinearity parameters. It is worth pointing out, however, that for $d<2$ there seems to be a continuous change in the survival probability as a function of the nonlinearity parameter. This is compatible with the findings of the stationary-state analysis for the same exponent regime that are presented in Fig. 3.

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