Nonlinear impurity in a lattice: Dispersion effects

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We examine the bound state(s) associated with a single cubic nonlinear impurity, in a one-dimensional tight-binding lattice, where hopping to first- and second-nearest neighbors is allowed. The model is solved in a closed form via the use of the appropriate lattice Green function, and a phase diagram is obtained showing the number of bound states as a function of the nonlinearity strength and the ratio of second- to first-nearest-neighbor hopping parameters. Surprisingly, a finite amount of hopping to second-nearest neighbors helps the formation of a bound state at smaller (even vanishingly small) nonlinearity values. As a consequence, the self-trapping transition can also be tuned to occur at relatively small nonlinearity strength, by this increase in the lattice dispersion.

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The effects of impurities on the transport properties of materials continues to be an interesting subject. When the concentration of impurities inside a material is finite, we speak of a disordered system. In one-dimensional systems, this disorder gives rise to the well-known phenomenon of Anderson localization, where all states acquire a finite localization length. This precludes any amount of transport in the system. More recently, the problem of *nonlinear* impurities has received considerable attention. In a condensed matter context, they appear in strongly coupled electron-vibration systems, when the vibrational degrees of freedom have the ability to adapt quickly to the presence of the electron, giving rise to a polaronic behavior.[1] Nonlinear impurities also appear in other fields, such as nonlinear optics. For instance, an array of linear waveguides containing a single or several nonlinear, Kerr-like guides. The transversal dynamics describing the energy exchange among waveguides is formally identical to the dynamics of an excitation propagating in a linear tight-binding lattice in the presence of one or more nonlinear impurities.[2]

In systems where an electron (or excitation) is propagating while strongly interacting with vibrational degrees of freedom, an ''effective'' nonlinear evolution equation for the electron can be obtained, under the assumption that the vibrations adapt instantly to the presence of the electron.[1] This equation, known as the discrete nonlinear Schrödinger (DNLS) equation, has the form

$$i\left(\frac{dC_{\mathbf{n}}}{dt}\right)=V\sum_{\mathbf{n.n.}} C_{\mathbf{m}}-\chi_{\mathbf{n}}|C_{\mathbf{n}}|^2C_{\mathbf{n}} \quad (\hbar\equiv 1), \tag{1}$$

where $C_{\mathbf{n}}$ is the probability amplitude of finding the electron on lattice site $\mathbf{n}$ at time t, V is the nearest-neighbor hopping parameter, and $\chi_{\mathbf{n}}$ is the nonlinearity parameter at site $\mathbf{n}$ proportional to the square of the electron-vibration coupling. In the conventional DNLS equation, the sum in Eq. (1) is restricted to nearest neighbors (n.n.).

For the case of a single nonlinear impurity in a one-dimensional lattice ($\chi_n=\delta_{n,0}\chi$), we have obtained in a previous work[3] its bound state analytically, via lattice Green functions, and have shown that a bound state is possible provided $|\chi/2V|>1$. This result deviated markedly from the well-known linear impurity case where, a bound state exists for any impurity strength. The extension to an impurity of arbitrary nonlinear exponent α [i.e., $|C_{\mathbf{n}}|^{\alpha}$ instead of $|C_{\mathbf{n}}|^2$ in Eq. (1)], revealed[4,5] that for $\alpha<2$ there is always a bound state for any finite χ/V. At $\alpha=2$ (the standard DNLS case) there is one bound state for $|\chi/2V|>1$, while for $\alpha>2$ there is a critical curve in χ-α space, below which there is no bound state, while above it, there are two bound states. On the critical curve, there is a single bound state.

When this nonlinear impurity is embedded in a square lattice,[6] the χ-α bound state phase diagram shows a single curve separating two regimes. Below the curve, there are no bound states; on the curve there is a single bound state, while above the curve there are two bound states. One of these become more localized upon increment of the nonlinearity parameter while the other becomes more delocalized. Bound states for single nonlinear impurities have also been computed for other systems, including a Cayley tree,[7] a triangular lattice,[9] and a cubic lattice.[8,9]

In all the studies above, only dispersion to first nearest-neighbors has been considered. For systems with long-range dispersion, a continuumlike approximation that employs a nonlocal nonlinear Schrödinger equation has been proposed.[10] For the case of a discrete system with a hopping parameter of the form $V_{nm}=V/|n-m|^s$, another study[11] followed a variational approach, based on a plausible ansatz for the localized state. Among other things, they found that there is a critical s_{cr} such that all dispersive interactions decreasing faster than $r^{-s_{cr}}$ lead to similar qualitative behavior as the DNLS with only nearest neighbor transfer. In this work we solve in closed form via Green functions, the case of a single DNLS impurity in a tight-binding lattice, including hopping to first- and second-nearest neighbors. This configuration and similar others with a nonlinear topology appear naturally in quasi onedimensional systems, such as ''zigzag'' or coiled structures. In this last case, it is possible to engineer the main interactions to be between first neighbors and between mth neighbors, where m is the ''period'' of the helix. Now, since the phenomenon of selftrapping is the result of a struggle between the tendency to spread (dispersion) and the tendency to localize (nonlinearity), one might surmise that any increase in dispersion will have the simple effect of increasing the nonlinearity needed to selftrap. However, as we will see, this is not necessarily the case and a small incre-

ment in dispersion can actually favor the formation of a bound state at smaller nonlinearity strength.

I. ONE-DIMENSIONAL LATTICE WITH DISPERSION

Let us consider the problem of determining the existence of bound states and dynamic selftrapping characteristics for an electron (or an excitation) moving on a one-dimensional dispersive lattice with hopping up to second- nearest neighbors, which contains a single DNLS impurity at the origin $n=0$. DNLS equation (1) reduces to

$$i\left(\frac{dC_n}{dt}\right)=V_1(C_{n+1}+C_{n-1})+V_2(C_{n+2}+C_{n-2}) -\chi|C_0|^2C_0\delta_{n,0}. \tag{2}$$

For stationary states, one puts $C_n(t)=\exp(-iEt)\,\phi_n$, obtaining

$$E\,\phi_n=V_1(\phi_{n+1}+\phi_{n-1})+V_2(\phi_{n+2}+\phi_{n-2}) -\chi|\phi_0|^2\phi_0\delta_{n0}. \tag{3}$$

The Hamiltonian that gives rise to Eq. (2) is

$$H=H_0+H_1, \tag{4}$$

where

$$H_0=V_1\sum_n\,(|n\rangle\langle n+1|+|n+1\rangle\langle n|) +V_2\sum_n\,(|n\rangle\langle n+2|+|n+2\rangle\langle n|) \tag{5}$$

and

$$H_1=-\chi|\phi_0|^2|0\rangle\langle 0|. \tag{6}$$

$\{|n\rangle\}$ represent Wannier electronic states and $V_1(V_2)$ is the nearest- (next-to-nearest-) neighbor transfer matrix element. In the absence of impurity, the energy band is given by

$$E(k)=2\,V_1\cos(k)+2\,V_2\cos(2k). \tag{7}$$

A simple analysis shows that, for positive $\delta\equiv V_2/V_1$, the upper and lower band edges obey

$$z_{max}(\delta)\equiv E_{max}/V_1=2(1+\delta), \tag{8}$$

$$z_{min}(\delta)\equiv E_{min}/V_1=\begin{cases}-2(1-\delta), & \delta<1/4\\ -(1/4\delta)-2\delta, & \delta>1/4.\end{cases} \tag{9}$$

As a result, while the upper edge always increase linearly with V_2, the lower edge shows the presence of a "waist": At first it decreases (in magnitude), reaching a minimum value of $2[1-(1/\sqrt{8})]V_1\approx 1.29V_1$ at $V_2=(1/\sqrt{8})V_1$. Afterwards, the lower edge increases in magnitude with V_2. At large V_2, this increase will be almost linear. These features will of importance in Sec. I A, where we determine the position of the impurity bound state(s).

A. Bound states

We use lattice Green functions as described in Refs. 3 and 12, where the perturbative series for the Green function is resumed to all orders, to obtain

$$G_{mn}(z)=G^{(0)}_{mn}(z)-\frac{\gamma|\phi_0|^2G^{(0)}_{m0}(z)G^{(0)}_{0n}(z)}{1+\gamma|\phi_0|^2G^{(0)}_{00}(z)}, \tag{10}$$

where $G_{mn}=\langle m|G|n\rangle$, $\gamma=\chi/V_1$, and

$$G^{(0)}_{mn}(z)=\frac{1}{2\pi}\int_{-\pi}^{\pi}d\phi\,\frac{\exp[i\phi(m-n)]}{[z-\cos(\phi)-\delta\cos(2\phi)]} \tag{11}$$

is the Green function in the absence of nonlinearity ($\gamma=0$). By using residues, we evaluate it in a closed form,

$$\mathrm{Re}[G^{(0)}_{00}(z)]=\begin{cases}2\sqrt{2}\delta[(\gamma_1\delta+\gamma_2)\sqrt{1-\delta(4\delta-2z+\gamma_1)}+(\gamma_1\delta-\gamma_2)\sqrt{1+\delta(-4\delta+2z+\gamma_1)}]^{-1}, & z>z_{max}(\delta)\\ -2\sqrt{2}\delta[(\gamma_1\delta+\gamma_2)\sqrt{1-\delta(4\delta-2z+\gamma_1)}-(\gamma_1\delta-\gamma_2)\sqrt{1+\delta(-4\delta+2z+\gamma_1)}]^{-1}, & z<z_{min}(\delta)\\ 0 & \text{otherwise,}\end{cases} \tag{12}$$

where $\gamma_1(z)\equiv\sqrt{8+(1/\delta^2)+(4z/\delta)}$ and $\gamma_2(z)\equiv 1-4\delta^2+2\delta z$, and

$$\mathrm{Im}[G^{(0)}_{00}(z)]=\frac{\Theta[(1/4)-\delta]\{\Theta[z-2(\delta-1)]-\Theta[z-2(1+\delta)]\}}{2\sqrt{1-d_1(z)^2}|1+4\delta\,d_1(z)|}+\frac{\Theta[\delta-(1/4)]\{\Theta(z+[1/(4\delta)]+2\delta)-\Theta[z-2(1+\delta)]\}}{2\sqrt{1-d_1(z)^2}|1+4\delta\,d_1(z)|} +\frac{\Theta[\delta-(1/4)]\{\Theta(z+[1/(4\delta)]+2\delta))-\Theta[z-2(\delta-1)]\}}{2\sqrt{1-d_2(z)^2}|1+4\delta\,d_2(z)|}, \tag{13}$$

where $d_1(z)\equiv(1/4\ \delta)(-1+\sqrt{1+8\ \delta[\delta+(z/2)]})$ and $d_2(z)\equiv(1/4\ \delta)(-1-\sqrt{1+8\ \delta[\delta+(z/2)]})$.

The (dimensionless) energy of the bound state, z_b is obtained from the poles of $G_{mn}(z)$, while the bound state amplitudes $\phi^{(b)}_n$ are obtained from the residues of $G_{mn}(z)$ at $z=z_b$. This leads to a nonlinear equation for z_b:

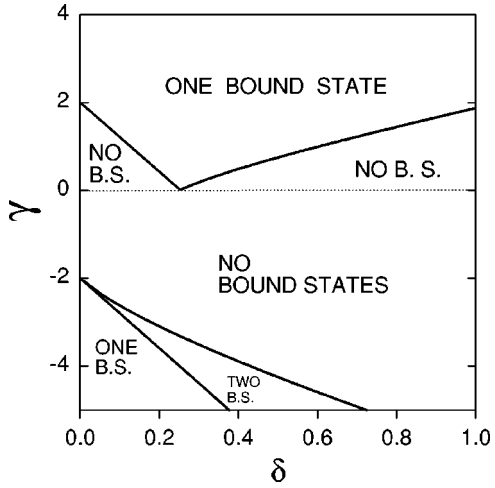

FIG. 1. Bound state phase diagram in nonlinearity-dispersion space ($\gamma \equiv \chi/V_1, \delta \equiv V_2/V_1$).

$$\frac{1}{\gamma} = \frac{G_{00}^{(0)3}(z_b)}{G_{00}^{\prime(0)}(z_b)}. \tag{14}$$

For a complete parameter space examination of all possible eigenvalues, we only need to consider a fixed sign for the dispersion parameter δ (say, positive) and the two possible signs of γ. A graphical examination of Eq. (14) (not shown) reveals that, when $\gamma > 0$ and as δ increases from zero, the right hand side of Eq. (14) moves toward the origin and increases its height, until δ reaches 1/4, where the height diverges. Further increase in δ decreases the height of the curves, but they continue to approach the origin until $\delta = 1/\sqrt{8}$. Afterwards, the curves move away from the origin while their heights continue to decrease. For the case of $\gamma < 0$, the situation is quite different: For a given δ value, there is a minimum $|\gamma_a|$ at which there is a bound state. Further increase in $|\gamma|$ creates two bound states, one of which will ultimately disappear at a further finite $|\gamma_b|$ value, leaving only a single bound state. These results are nicely summarized in Fig. 1, which shows a phase diagram in nonlinearity-dispersion space showing the number of bound state(s). For positive nonlinearity, the critical curve separating the region with no bound states from the region with one bound state, decreases with increasing δ, and reaches zero at $\delta = 1/4$. Afterwards, it increases monotonically with further dispersion. Thus, there is a finite dispersion interval, $0 < \delta < 1/4$ where, contrary to what might be expected, an increase in dispersion actually *reduces* the nonlinearity needed to create a bound state. This can also be seen in Fig. 2(a), which shows the bound state energy as a function of (positive) nonlinearity, for several values of dispersion δ. This reduction in nonlinearity needed to sustain a bound state is, of course due to the reduction in the width of the negative portion of the band with a small positive dispersion, and thus, it has a *linear* origin.[15] In the negative nonlinearity sector, in Fig. 1 we have two critical curves separating regions with no bound states, two bound states, and one bound state. Here an increase in dispersion causes a corresponding increase in the minimum nonlinearity needed for the creation of a bound

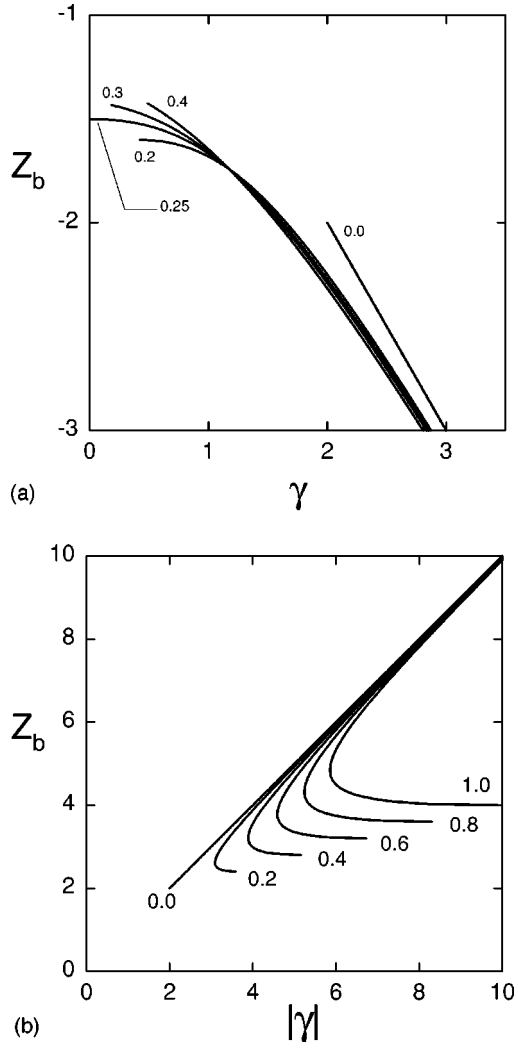

FIG. 2. Bound state energy as a function of positive (a) and negative(b) nonlinearity, for several dispersion values.

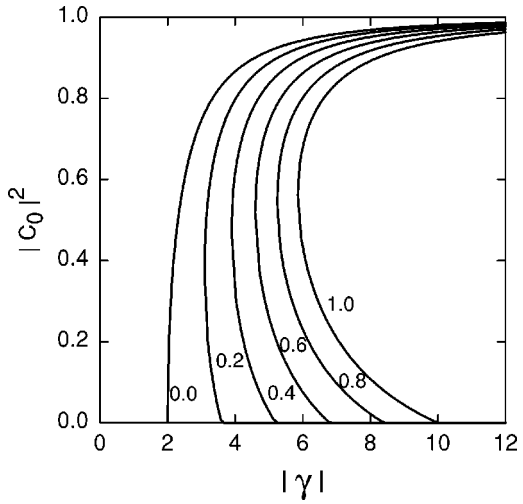

FIG. 3. Probability at the impurity site as a function of nonlinearity, in the negative nonlinearity sector, for several dispersion values.

state(s). This is correlated with the fact that the width of the positive portion of the band always increases linearly with δ. Figure 2(b) shows the bound state energy as a function of nonlinearity, for negative γ. Here, for a given value of δ, there exists a critical nonlinearity value γ_a for which there is a bound state, with energy outside the band. Further increase in nonlinearity creates two bound states, one of which increases its energy monotonically with nonlinearity while the other state decreases its energy toward the band, reaching it at a finite nonlinearity value γ_b. As Fig. 3 shows, in the regime with two bound states, as the magnitude of the nonlinearity is increased, one of the states becomes more localized on the impurity site, while the other becomes more delocalized, ultimately disappearing into the continuum at a finite nonlinearity value.

B. Transmission across the impurity

Again, following the formalism of Green functions,[3,12] we obtain the equation for the transmission coefficient t of plane waves across the nonlinear impurity,

$$t=\frac{1}{|1+\gamma\, t\, G_{00}^{(0)}|^2}=\frac{1}{1+\gamma^2\, t^2\, \mathrm{Im}[G_{00}^{0)}(z)]^2}, \qquad (15)$$

which leads to the cubic equation: $\gamma^2 t^3 \mathrm{Im}[G_{00}^{0)}(z)]^2+t-1=0$. This is invariant under $\gamma\rightarrow-\gamma$, implying that the transmission does not depend on the sign of the nonlinearity parameter. The physical solution for t is

$$t=\frac{-2\,6^{1/3}+(18\,\gamma\mathrm{Im}[G_{00}^{(0)}(z)]+2\sqrt{3}\sqrt{4+27\,\gamma^2\mathrm{Im}[G_{00}^{(0)}(z)]^2})^{2/3}}{2\;3^{2/3}\,\gamma\,\mathrm{Im}[G_{00}^{(0)}(z)](9\,\gamma\mathrm{Im}[G_{00}^{(0)}(z)]+\sqrt{3}\sqrt{4+27\,\gamma^2\mathrm{Im}[G_{00}^{(0)}(z)]^2})^{1/3}}, \qquad (16)$$

with $\mathrm{Im}[G_{00}^{(0)}(z)]$ given by Eq. (12). Figure 4 shows several transmission curves as functions of the plane waves dimensionless energy z, for several different dispersion ratios δ. The most remarkable new feature is the appearance of an abrupt ''dip'' on the transmission near the lower edge of the band at $\delta\sim0.4$. As δ increases further, the ''dip'' moves to the right and eventually (not shown) approaches the upper band edge and merges with it. This ''dip'' is related to the creation of a secondary ''branch'' in $\mathrm{Im}[G_{00}^{(0)}(z)]$.

C. Dynamic self-trapping

We place the electron at the impurity site at $t=0$ and observe its time evolution, according to Eq. (2). The observable of interest here is the long-time average probability of finding the electron on the initial site after a relatively long time T:

$$P_0=\lim_{T\rightarrow\infty}(1/T)\int_0^T|C_{\mathbf{0}}(t)|^2dt, \quad |C_{\mathbf{0}}(0)|=1. \qquad (17)$$

Following earlier works,[4] we use a fourth-order Runge-Kutta numerical scheme, whose accuracy is monitored through total probability conservation: $1=\Sigma_n|C_n(t)|^2$. Figure 5 shows P_0 as a function of (positive) nonlinearity parameter γ, for several different dispersion δ values. As anticipated from the bound state results, an increase of dispersion reduces the critical nonlinearity for the onset of self-trapping. The minimum threshold occurs around $\delta\approx0.3$. In the immediate vicinity of this value, the self-trapping transition also seems to

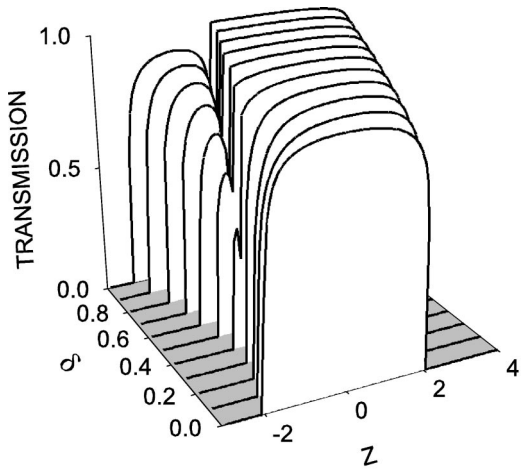

FIG. 4. Transmission coefficient of plane waves across the nonlinear impurity as a function of the plane wave dimensionless energy, for several dispersion values.

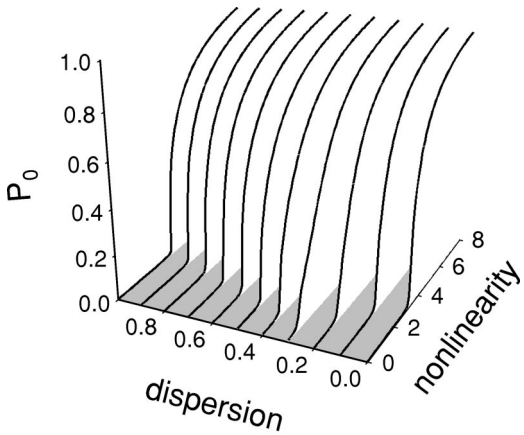

FIG. 5. Long-time average probability of finding the electron on the impurity site, as a function of nonlinearity, for several different dispersion values ($T=203V_1$).

lose some sharpness. A subsequent increase in δ increases the critical nonlinearity γ_c again and restores sharpness to the P_0 curve. At $\delta \approx 1$, the P_0 curve almost coincides with the $\delta = 0$ case. Thereafter, γ_c increases in an almost linear fashion with δ. For the case of a negative nonlinearity parameter (not shown), the critical nonlinearity always increases monotonically with dispersion. This case also corresponds to $\gamma > 0, \delta < 0$.

II. DISCUSSION

We have analytically examined the conditions for the formation of a bound state at a nonlinear impurity site, in a one-dimensional linear lattice with hopping to first and second nearest-neighbors. The formalism employed lattice Green functions, which have been evaluated in closed form for our system. We found a range in which this increment in dispersion can actually favor the formation of a bound state at smaller nonlinearity strength. As a consequence, the onset of dynamical self-trapping at the impurity site can also be shifted to lower nonlinearity thresholds. Given the paradigmatic character of the DNLS equation, these results could be applied to completely nonlinear optical or solid nanostructures, with nonlinear topology. For instance, a ''zigzag'' array of waveguides in nonlinear optics,[13] where one has coupling to first- and second- nearest neighbors, or a triangular/helicoidal stack of atoms, where the main couplings are to first- and third-nearest neighbors, etc. In these and other cases, the bound state profile found here could serve as a good initial condition for the launching of a discrete excitation (soliton) along a completely nonlinear system.[14] The transport properties of these nonlinear systems and the steering of their mobile excitations is currently an active field of research.

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