Nonlinear surface impurity in a semi-infinite lattice

M. I. Molina
Departamento de Física, Facultad de Ciencias, Universidad de Chile, Casilla 653, Santiago, Chile
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We examine the formation of bound states on a generalized nonlinear impurity located at or near the beginning (surface) of a linear, tight-binding semi-infinite lattice. Using the formalism of lattice Green functions, we obtain in closed form the number of bound states as well as their energies and probability profiles, for different nonlinearity parameter values and nonlinearity exponents, at different distances from the surface. It is shown that close to the surface, the amount of nonlinearity needed to create a bound state or to effect dynamical self-trapping, increases (decreases) depending on whether the exponent is smaller (larger) than, approximately, 2.

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The interplay of nonlinearity and discreteness has received considerable attention recently[1] because it plays a vital role in the emergence of a different kind of excitation in extended, nonlinear systems with discrete translational invariance, known as intrinsic localized modes (ILM). These ILMs are generic to physical systems of interest, such as arrays of nonlinear optical waveguides,[2] molecular crystals,[3] biopolymers,[4] arrays of Josephson junctions,[5] and even Bose-Einstein condensates in magneto-optical traps.[6]

Given the strictly local manner in which nonlinearity enters into the effective evolution equations in all these cases (see below), one is led to the idea that in the limit of strong nonlinearity, one could approximate a typical nonlinear system by a linear one containing a small cluster of nonlinear sites or even a single nonlinear impurity. The system, thus simplified, is amenable to exact mathematical treatment, and the influence of other potentially competing effects, such as dimensionality, boundary effects, noise, etc., can be more easily studied without losing the essential physics.

For a one-dimensional discrete system in the presence of a single nonlinear impurity, located at $n=d$, the dynamics is given by the well-known discrete nonlinear Schrödinger (DNLS) equation

$$i\frac{dC_n}{dt} = V(C_{n+1} + C_{n-1}) - \chi|C_n|^\beta C_n \delta_{n,d} \quad (\hbar \equiv 1), \qquad (1)$$

where C_n is the probability amplitude for finding the excitation on site n, V is the nearest-neighbor transfer matrix element, χ is the nonlinearity parameter, and β is the nonlinearity exponent. Usually, but not always, $\beta=2$, which, in a condensed-mater context, corresponds to an underlying harmonic oscillator degree of freedom "enslaved" to the excitation (electron) at the impurity site. When this vibrational impurity is anharmonic in nature, other β values are possible, in principle, with $\beta<2$ corresponding to a "hard" vibrational impurity while $\beta>2$ corresponds to a "soft" case.[7]

Bound states for single nonlinear impurities embedded in infinite lattices include chains,[8–10] Cayley trees,[11] triangular,[13] and cubic[12,13] lattices. Now, since the creation of a bound state, or the dynamical self traping at the impurity site implies the localization of energy on a scale of the order of the lattice spacing, one might surmise that, by placing the nonlinear impurity at or near the surface of a semi-infinite lattice, the nonlinearity strength needed to affect localization would decrease, facilitating in this way its creation and experimental observation. As a step in that direction, in this work we examine a simple model consisting of an electron (or excitation) propagating in a semi-infinite, linear chain, which contains a single nonlinear impurity at a distance d from the beginning ("surface") of a semi-infinite chain (Fig. 1), we examine the conditions for the existence of bound state(s) and the dynamical self-trapping properties, and we compare them to the results obtained for the infinite chain.[9]

I. BOUND STATES

We consider Eq. (1) for a semi-infinite lattice ($n=0,1,\ldots$) and normalize all energies to the half bandwidth of the infinite chain case. The Hamiltonian is given by

$$H = \frac{1}{2}\sum_{n=0}^{\infty}(|n\rangle\langle n+1| + |n+1\rangle\langle n|) + \gamma|C_d|^\beta|d\rangle\langle d|, \qquad (2)$$

where $\{|n\rangle\}$ are Wannier states and $\gamma \equiv \chi/(2V)$. The dimensionless Green function $G=1/(z-H)$ can be formally expanded as[14] $G=G^{(0)}+G^{(0)}H_1G^{(0)}+G^{(0)}H_1G^{(0)}H_1G^{(0)}+\cdots$, where $G^{(0)}$ is the unperturbed ($\gamma=0$) Green function and $H_1=\gamma|C_d|^\beta|d\rangle\langle d|$. The series can be resumed to all orders to yield

$$G_{mn} = G^{(0)}_{mn} + \frac{\gamma|C_d|^\beta G^{(0)}_{md}G^{(0)}_{dn}}{1-\gamma|C_d|^\beta G^{(0)}_{dd}}, \qquad (3)$$

where $G_{mn} \equiv \langle m|G|n\rangle$. Now, we cannot use Eq. (3) directly because we do not know C_d, but we will determine it through an exact self-consistent procedure. The energy of the bound state(s) is obtained from the poles of G_{mn}, i.e., by solving

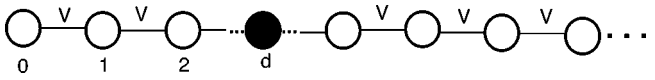

FIG. 1. A nonlinear impurity near the surface of a one-dimensional chain.

$1=\gamma|C_d|^\beta G_{dd}^{(0)}(z_b)$. On the other hand, the bound-state amplitudes C_n are obtained from the residues of G_{mn} at $z=z_b$. In particular, at the impurity site, $|C_d|^2=\mathrm{Res}\{G_{dd}(z)\}_{z=z_b}=-G_{dd}^{(0)^2}(z_b)/G_{dd}'^{(0)}(z_b)$. Inserting this back into the bound-state energy equation leads to

$$\frac{1}{\gamma}=\frac{G_{dd}^{(0)\beta+1}(z_b)}{[-G_{dd}'^{(0)}(z_b)]^{\beta/2}}. \tag{4}$$

The unperturbed Green function $G_{mn}^{(0)}$ for the semi-infinite lattice can be calculated by the method of mirror images. Since there is no lattice to the left of $n=0$, $G_{mn}^{(0)}$ should vanish identically at $n=-1$. Thus, $G_{mn}^{(0)}(z)=G_{mn}^{\infty}(z)-G_{m,-n-2}^{\infty}(z)$, where $G_{mn}^{\infty}(z)$ is the Green function for the infinite lattice $G_{mn}^{\infty}(z)=\mathrm{sgn}(z)(1/\sqrt{z^2-1})[z-\mathrm{sgn}(z)\sqrt{z^2-1}]^{|n-m|}$, where $\mathrm{sgn}(z)=+1(-1)$ for $z>0(<0)$. Therefore,

$$G_{mn}^{(0)}(z)=\mathrm{sgn}(z)\frac{1}{\sqrt{z^2-1}}[z-\mathrm{sgn}(z)\sqrt{z^2-1}]^{|n-m|}$$
$$-\mathrm{sgn}(z)\frac{1}{\sqrt{z^2-1}}[z-\mathrm{sgn}(z)\sqrt{z^2-1}]^{|n+2+m|}. \tag{5}$$

From Eq. (5) we note the parity property $G_{dd}^{(0)}(-z)=-G_{dd}^{(0)}(z)$, which implies $G_{dd}'^{(0)}(-z)=G_{dd}'^{(0)}(z)$. This means, according to Eq. (4) that the change $\gamma\to-\gamma$ reverses the sign of z_b. On the other hand, from Eq. (1), it is possible to deduce that the change $\gamma\to-\gamma$ is equivalent to the change $C_n\to(-1)^n C_n^*$. Since we are interested in a localized state, where C_n can be chosen as real, we conclude that a change in sign of the nonlinearity parameter reverses both the "staggered" character of the bound state and the sign of the localized state energy.

After inserting Eq. (5) into (4), the general structure for the number of bound states emerges. For any finite distance d from the surface and any positive value of the exponent β, there is a critical amount of nonlinearity γ below which there is no bound state and above which there are two bound states. For β exponents smaller than 2 and as d is increased, one of the bound states tends to merge with the band edge, so that in the limit of a very deep impurity, there is only a single localized bound state. For $\beta>2$, however, as d is increased, both bound states remain localized. In the special case of a linear impurity ($\beta=0$), there is a single bound state provided $\gamma>1/(d+1)$. Thus, in the limit $d\to\infty$ these results are consistent with the case of a completely infinite lattice:[9] a single bound state for $\beta<2$, and for $\beta>2$, a critical curve in nonlinearity strength and nonlinearity exponent space, separating a region with no bound states from a region with two bound states. At the surface ($d=0$), the critical curve is given by

$$\gamma_c=\frac{(1+\beta)^{(1+\beta)/2}}{2\beta^{\beta/2}}. \tag{6}$$

In particular, for the DNLS case, $\gamma_c=3^{3/2}/4\approx1.3$, larger than the value for the infinite chain ($\gamma_c=1$). Figure 2 shows phase diagrams in γ-β space showing the number of bound states at different distances d between the impurity and the "surface" of the system.

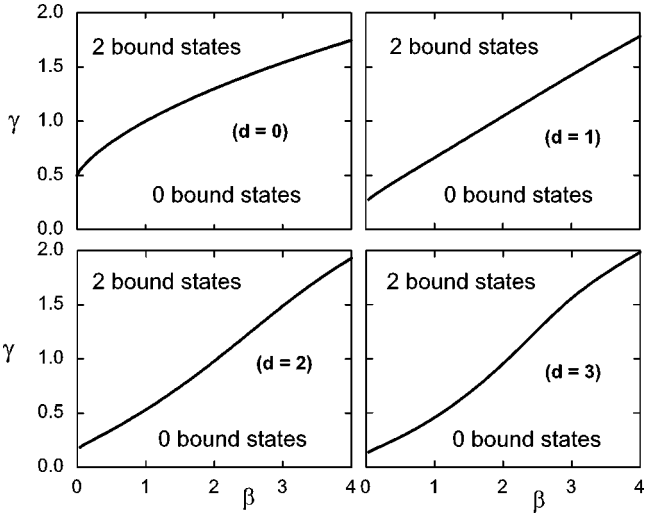

FIG. 2. Phase diagram in γ-β space showing the number of bound states for different distances impurity surface (in units of the lattice constant).

As to the stability of these bound states, it is easy to see from a graphical analysis of the structure of Eq. (4) that, as nonlinearity γ is increased, one of the bound states becomes more and more localized while the other becomes more and more delocalized. Since, in the limit of high nonlinearity, the effective coupling among sites is negligible, one would expect the bound state to become more and more localized. Therefore, the state with the smaller localization length is stable, the other unstable. This qualitative argument is confirmed by the more rigorous procedure of examining the Hamiltonian flow of the system around the two fixed points (bound states).

Figure 3 shows the critical nonlinearity for the onset of a bound state, as a function of the distance from the impurity to the lattice "surface" ($n=0$), for different nonlinearity exponents. Significant differences from the infinite lattice case are apparent. As the impurity is placed closer and closer to the surface, the critical nonlinearity to create a bound state increases or decreases, depending on whether the nonlinear exponent is below or above ~2. In particular, for the all-important standard DNLS case $\beta=2$, the presence of a surface increases the nonlinearity needed to create a bound state, which is contrary to popular belief that a surface would help localize the electron.

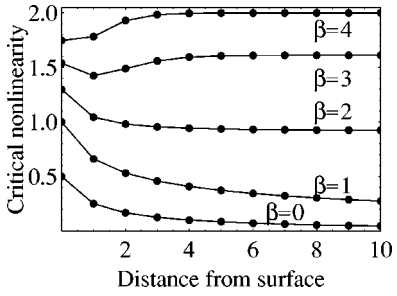

FIG. 3. Scaled critical nonlinearity for onset of a bound state as a function of the distance from the nonlinear impurity to the "surface" of the chain.

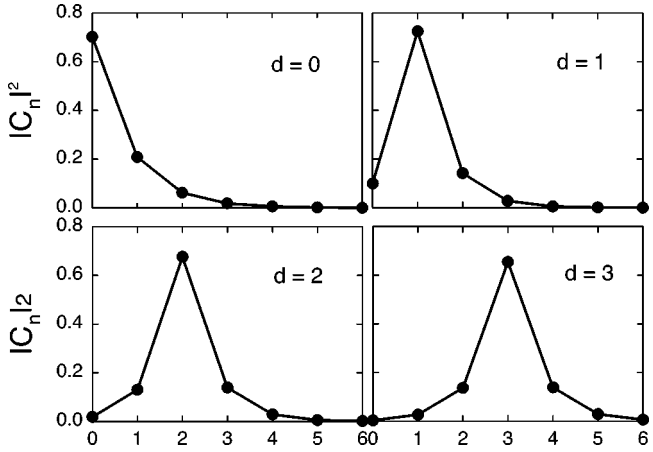

FIG. 4. Probability profile for the stable bound state at different impurity positions ($\beta=2$, $\gamma=1.305$).

For a given value of exponent β and any inclusion distance d, the bound state probability profile $|C_n|^2$ is given in closed form by $|C_n|^2=A[Q^{|n-d|}-Q^{|n+d+2|}]$, where $Q\equiv z_b-\sqrt{z_b^2-1}$, $A\equiv(z_b-Q)/\{z_b+[z_b+2(1+d)\sqrt{z_b^2-1}]Q^{2(1+d)}\}$ and z_b is the solution of Eq. (4). Simple analysis of this profile shows that $|C_n|^2$ has always a single hump at $n=d$. This profile is shown in Fig. 4 for the standard DNLS ($\beta=2$) and a nonlinearity strength γ just above critical, at four different impurity locations under the surface. Its general features are shared by other β exponents. Below the surface, the probability profile converges quickly to the infinite lattice case as d increases past 4.

II. DYNAMICAL SELF TRAPPING

We numerically compute the long-time average probability at the impurity site $P_d=\lim_{T\to\infty}(1/T)\int_0^T dt|C_d|^2$ for several distances d from the surface ($n=0$). As the initial condition, we use a completely localized excitation on the impurity site $C_n(0)=\delta_{nd}$. Figure 5 shows the critical nonlinearity for self trapping ($P_d>0$) as a function of the distance between the nonlinear impurity and the chain surface, for different nonlinearity exponent values. In general, the behavior is qualitatively similar to the one observed for the onset of a bound

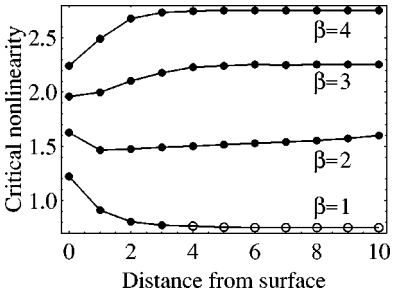

FIG. 5. Right: Scaled critical nonlinearity for dynamical self trapping as a function of the distance from the impurity to the chain surface, for several nonlinearity exponents. The empty circles shown for $\beta=1$ and $d=4$ through $d=10$ indicate approximate values since the self-trapping is not abrupt.

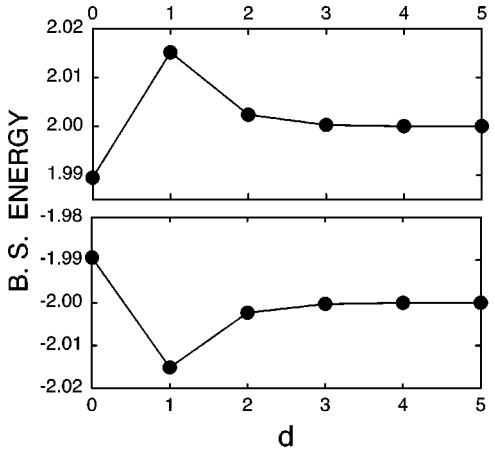

FIG. 6. Nonlinear impurity bound-state energy as a function of distance impurity surface for $\beta=2$ and $\gamma=2$ (upper) and $\gamma=-2$ (lower).

state (Fig. 3). In both cases, for a fixed distance, an increase of the nonlinear exponent β results in an increase of the nonlinearity threshold for self-trapping. The same behavior was observed previously for an impurity in a completely infinite chain.[9] This phenomenon is not hard to explain. Since $|C_n|<1$, we see from Eq. (1) that as $\beta>0$ is increased, $|C_d|^\beta$ will necessarily decrease, which implies that a larger γ will be needed to keep the value of the *effective* impurity strength $\gamma|C_d|^\beta$. Thus, at a fixed impurity-surface distance, a higher β implies a higher γ_c. Another interesting behavior we observe from Figs. 5 and 3 is that for a fixed nonlinearity exponent, the critical nonlinearity depends roughly on whether the exponent is below or above ~ 2. For $\beta<2$, an increase in the impurity-surface distance d results on a decrease of γ_c, while for $\beta>2$, an increase in d increases γ_c. The explanation of this phenomenon seems to rest on the delicate balance between kinetic and potential energies. If we assume an electronic bound state Ψ with localization length λ, then on normalization grounds we have $|\Psi|^2\sim 1/\lambda$. The kinetic energy content is $\Delta K\sim h^2/2m\lambda^2$, while the average potential energy is, in magnitude, equal to $\Delta V=\int dx\ V(x)|\Psi(x)|^2=\int dx\ \gamma|\Psi(x)|^\beta|\Psi(x)|^2\sim \gamma a/\lambda^{[1+(\beta/2)]}$, where a is of the order of the lattice spacing. Thus,

$$\Delta V/\Delta K\sim \gamma\lambda^{1-(\beta/2)}. \tag{7}$$

On the other hand, as the impurity is brought closer to the surface, the wave function becomes more "compressed" (Fig. 4), i.e., λ decreases as d approaches zero. This implies, from Eq. (7), that for $\beta>2$, a decrease in λ increases ΔV with respect to ΔK, which means that less nonlinearity is needed to maintain a localized state. On the contrary, if $\beta<2$, a decrease in λ decreases ΔV with respect to ΔK and now, more nonlinearity is needed to maintain the localized state.

III. COMPLETELY NONLINEAR LATTICE

In the large nonlinearity limit where $\gamma\gg\gamma_{cr}$, the single nonlinear impurity results should approximate those corre-

sponding to a whole nonlinear lattice. For the particular case examined in this work, the "extended" problem consists of the formation of an intrinsic localized mode (ILM) in a semi-infinite nonlinear latice. Due to the presence of a surface, the discrete translational invariance is broken and a natural question arises: where will the localized state be formed? Our single nonlinear impurity analog can provide an answer. For each impurity position d, the bound-state energy can be computed as a function of d. The position corresponding to its minimum value will correspond to the position of the ILM. Also, the impurity energy and spatial probability profile should approximate the ones corresponding to the ILM. Figure 6 shows the impurity energies as a function of distance from the lattice surface, for the DNLS case, $\beta=2$ and $\gamma=\pm 2$. We see that for a positive value of the nonlinearity parameter γ, the preferred position is the very surface ($d=0$), while for a negative γ, the preferred position is one layer below the surface ($d=1$). These predictions are indeed confirmed by direct numerical computations, where the Hamiltonian corresponding to a semi-infinite nonlinear lattice $H=(1/2)\Sigma_{n=0}^{\infty}(|n\rangle\langle n+1|+|n+1\rangle\langle n|)+\gamma\Sigma_{n=0}^{\infty}|C_n|^{\beta}|n\rangle\langle n|$ is diagonalized by an iterative procedure. For the particular example in Fig. 6, the error obtained for the ILM energy is about 1%.

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