Impurity modes and wave scattering in discrete chains with nonlinear defect states

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Abstract

We study the properties of localized impurity modes and the transmission of plane waves across a general nonlinear impurity embedded in an infinite one-dimensional linear chain. Using the formalism of the lattice Green function, we obtain nonlinear equations for the bound state energy and the transmission coefficient, for a wide class of nonlinear impurities. We specialize to a saturable nonlinear impurity, obtaining closed form expressions for the bound state energy and transmission coefficient.

1. Introduction

Impurities (or defects) are known to break the translational symmetry of physical systems leading to several novel features such as wave reflection, resonant scattering, and excitation of impurity modes [1]. When the wave interaction with the defect is attractive, it can lead to the energy trapping and localization in its vicinity, that occurs in the form of spatially *localized impurity modes*.

When nonlinearity becomes important, it may lead to self-trapping and energy localization even in a perfect (or homogeneous) system in the form of intrinsic localized modes [2]. When both nonlinearity and defects are present simultaneously, it is expected that competition between two different mechanisms of energy localization (i.e., one, due to the self-action of nonlinearity, and the other one, due to localization induced by defect) will lead to a complicated and somewhat nontrivial physical picture of localized states and their stability.

In this Letter, we consider one of the examples of such a competition, and analyze different types of localized impurity in the framework of the generalized discrete nonlinear model. In particular, being driven by the recent analysis of the weakly coupled arrays of optical waveguides in realistic physical systems [3], we apply our theory to the analysis of the effect of nonlinearity saturation on the existence, properties and stability of nonlinear localized impurity modes.

The local character of nonlinearity [see Eq. (1) below] suggests that in the case of attraction nonlinearity is important at the impurity site and the mode will be mainly localized at the defect decaying rapidly away from it. The local character of nonlinearity suggests that idea that in the limit of strong nonlinearity (and therefore, very localized excitation), one can 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 definiteness, we will work in a condensed-matter context, although the main results can be applied to other systems as well (e.g., nonlinear optics), for which the main equation (1) applies (see below). Thus, let us consider the propagation of an electron along a one-dimensional tight-binding chain and

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interacting strongly with a single vibrational degree of freedom at site $n = 0$. This oscillator is modelled either as a harmonic [4] or anharmonic [5] classical Einstein oscillator. In the limit when the oscillator vibration is completely correlated (or "enslaved") with the presence of the electron, it is possible to solve formally for the oscillator's displacement in terms of the electron's probability amplitude and thus arrive to an effective evolution equation for the electron, known as the discrete nonlinear Schrödinger (DNLS) equation:

$$i\left(\frac{dC_n}{dt}\right) = -V(C_{n+1} + C_{n-1}) + \chi\delta_{n,0} f\left(|C_n|^2\right)C_n, \qquad (1)$$

where $C_n(t)$ is the probability amplitude for finding the excitation on the nth site at time t, V is the coupling parameter and χ is the nonlinearity parameter. The specific form of $f(|C_n|^2)$ determines the nature of the nonlinear impurity in a physical problem. For instance, when $f(|C_n|^2) \sim |C_n|^\beta$, one could be dealing with a harmonic oscillator [4] ($\beta = 2$), or a "hard" anharmonic oscillator ($\beta < 2$) or a "soft" anharmonic oscillator ($\beta > 2$) [5]. In the case of the harmonic vibrational impurity, it must be pointed out that, a fully quantum treatment reveals some departures from the behavior predicted by Eq. (1) in some parameters regime [6].

2. Bound states

We normalize all energies to a half bandwidth, $2V$ and look for stationary states: $C_n(t) = \exp(-iEt)C_n$, obtaining

$$EC_n = -\frac{1}{2}(C_{n+1} + C_{n-1}) + \gamma\delta_{n,0} f\left(|C_n|^2\right)C_n, \qquad (2)$$

where $\gamma \equiv \chi/2V$. The dimensionless Hamiltonian that gives rise to Eq. (2) is

$$H = H_0 + H_1, \qquad (3)$$

where

$$H_0 = -\frac{1}{2}\sum_n \left(|n\rangle\langle n+1| + |n+1\rangle\langle n|\right), \qquad (4)$$

$$H_1 = \gamma f\left(|C_0|^2\right)|0\rangle\langle 0|, \qquad (5)$$

where $\{|n\rangle\}$ are the Wannier states. The dimensionless Green function $G = 1/(z - H)$ can be formally expanded as [7] $G = G^{(0)} + G^{(0)}H_1G^{(0)} + G^{(0)}H_1G^{(0)}H_1G^{(0)} + \cdots$, where $G^{(0)}$ is the unperturbed (at $\gamma = 0$) Green function. The series can be resumed to all orders to yield

$$G_{mn} = G_{mn}^{(0)} + \frac{\mathcal{E}G_{m0}^{(0)}G_{0n}^{(0)}}{1 - \mathcal{E}G_{00}^{(0)}}, \qquad (6)$$

where $\mathcal{E} \equiv \gamma f(|C_0|^2)$, and $G_{mn} \equiv \langle m|G|n\rangle$. Now, we cannot use Eq. (6) directly since we do not know C_0, but we will determine it through an exact self-consistent procedure: the energy of the bound state(s) is obtained form the poles of G_{mn}, i.e., by solving $1 = \mathcal{E}G_{00}^{(0)} = \gamma f(|C_0|^2)G_{00}^{(0)}(z_b)$. On the other hand, the bound state amplitudes C_n are obtained form the residues of G_{mn} at $z = z_b$. In particular, at the impurity site, $|C_0|^2 = \mathrm{Res}\{G_{00}(z)\}_{z=z_b} = -{G_{00}^{(0)}}^2(z_b)/G_{00}'^{(0)}(z_b)$. Inserting this back into the bound state energy equation leads to

$$\frac{1}{\gamma} = f\left(-\frac{{G_{00}^{(0)}}^2(z_b)}{G_{00}'^{(0)}(z_b)}\right)G_{00}^{(0)}(z_b). \qquad (7)$$

Now we use the exact expression for the Green function for the one-dimensional infinite lattice,

$$G_{mn}^{(0)}(z) = \mathrm{sgn}(z)\frac{1}{\sqrt{z^2-1}}\left[z - \mathrm{sgn}(z)\sqrt{z^2-1}\right]^{|n-m|},$$

where $\mathrm{sgn}(z) = +1$ (-1) for $z > 0$ (< 0). After replacing into Eq. (7), we obtain the following nonlinear equation for z_b:

$$\frac{1}{\gamma} = f\left(-\frac{\sqrt{z_b^2-1}}{|z_b|}\right)\frac{\mathrm{sgn}(z_b)}{\sqrt{z_b^2-1}}. \qquad (8)$$

We notice from Eq. (8), that the change $\gamma \to -\gamma$ is equivalent to reversing the sign of the bound state energy: $z_b \to -z_b$. On the other hand, from Eq. (1), it can be proven that the change $\gamma \to -\gamma$ (i.e., $\chi \to -\chi$) is equivalent to the change $C_n \to (-1)^n C_n^*$. Since we are interested in a localized state inside an infinite lattice, where the C_n can be chosen as real, we conclude that a change in sign of the nonlinearity parameter reverses both the sign of the bound state energy and the "staggered" character of the bound state.

For each possible solution $z_b(|z_b| > 1)$ of Eq. (8), the associated bound state probability profile is obtained from the residues of $G_{mn}(z)$ at $z = z_b$ as:

$$|C_n|^2 = \frac{\sqrt{z_b^2-1}}{|z_b|}\left[z_b - \mathrm{sgn}(z_b)\sqrt{z_b^2-1}\right]^{2|n|}. \qquad (9)$$

This describes an exponentially decreasing spatial probability profile $\sim e^{-|n|/\lambda}$ with localization length

$$\lambda = -\frac{1}{2}\log\left|z_b - \mathrm{sgn}(z_b)\sqrt{z_b^2-1}\right|.$$

Let us now focus on the family of functions

$$f\left(|C_n|^2\right) = \left(a + b|C_n|^2\right)^d, \qquad (10)$$

with $a, b > 0$, which contains several physically relevant cases. For instance, for $a = 0$, $b = 1 = d$, we obtain $f(|C_n|^2) = |C_n|^2$, the standard cubic nonlinear impurity [8]. For $a = 0$, $b = 1$, $d = \beta/2$, we obtain $f(|C_n|^2) = |C_n|^\beta$, the generalized nonlinear impurity, described in Ref. [9]. For $a = 1 = b$, $d = -1$, one obtains the saturable impurity case, i.e., $f(|C_n|^2) = 1/(1 + |C_n|^2)$ [3]. After replacing Eq. (10) into (8), the bound state equation becomes

$$\frac{1}{\gamma} = \left(a + b\frac{\sqrt{z_b^2-1}}{|z_b|}\right)^d \frac{\mathrm{sgn}(z_b)}{\sqrt{z_b^2-1}}. \qquad (11)$$

We distinguish two main cases:

(i) $a = 0$. In this case, we have

$$\frac{1}{\gamma} = \frac{b^d}{|z_b|^d}\left(z_b^2 - 1\right)^{(d-1)/2}\mathrm{sgn}(z_b). \qquad (12)$$

The RHS of the equation above shows different behaviors, according to whether d is smaller or greater than one. If $d < 1$, the RHS always diverges at $|z| = 1$ (the band edge) and decreases monotonically with increasing z, implying a unique solution for a bound state, for any γ value. The cases discussed in Refs. [8,9] fall in this category. At $d = 1$, there is a unique solution, $z_b = b\gamma$, provided $\gamma \geqslant 1/b$. When $d > 1$, the right-hand side of Eq. (12) starts from zero, at $z = 1$, then raises and reaches a maximum and decreases afterwards towards zero as $O(1/|z|)$ when $z \to \infty$. Thus, there is a minimum value for the nonlinearity parameter γ_c, above which there are two bound states, and below which there are no bound states. At precisely $\gamma = \gamma_c$, there is a single bound state. From analysis of Eq. (12), one obtains a closed-form expression for this nonlinearity threshold:

$$\gamma_c = \frac{\sqrt{d-1}}{b^d}\left(\frac{d}{d-1}\right)^{d/2} \quad (d > 1). \tag{13}$$

Now, as nonlinearity is increased, one of the two states approaches the continuum band ($z = 1$) while the other gets away from it. Since an increase in γ is equivalent to a decrease in site coupling, one would expect that the corresponding bound state should decrease its localization length, which is tantamount to drifting away from the continuum band. Therefore, we conclude that the state which, upon increasing nonlinearity, approaches the band must be *unstable*, while the one that gets away from it must be *stable*.

(ii) $a > 0$. We notice that, at $z = 1^+$ and also at $z \gg 1$, the right-hand side of Eq. (11) is dominated by the inverse square root of the second term, which would seem to imply a unique bound state solution, for all possible values of a, b and d. However, a closer look reveals the possibility of additional intermediate solutions. Algebraic analysis of the RHS of Eq. (11) shows two important sub-regimes: for $d < 1$, there is only one bound state solution, for any γ value, while for $d > 1$, we can have up to three bound states, depending on the value of the ratio (b/a). For $(b/a) < (b/a)_{\text{crit}}$, there is a unique solution, while for $(b/a) > (b/a)_{\text{crit}}$, we can have up to three bound states, for some nonlinearity parameter range. Following the same arguments shown in (i), we can show that only two of these states is stable while the third one is unstable. The critical parameter $(b/a)_{\text{crit}}$ is given in closed form by

$$\left(\frac{b}{a}\right)_{\text{crit}} = \frac{3}{2}\frac{\sqrt{3d}}{(d-1)^{3/2}}, \tag{14}$$

and the bound state energy associated with this intermediate state is $z_b = \sqrt{3d/(1+2d)} < d$. It lies between 1^+ at $d = 1^+$ and $\sqrt{3/2} = 1.22$, at large d values.

2.1. Saturable impurity

We specialize now to the saturable impurity case, characterized by $a = 1 = b$, $d = -1$. According to the discussion above, in this case there is only one possible bound state for any impurity strength. The equation for z_b takes the form

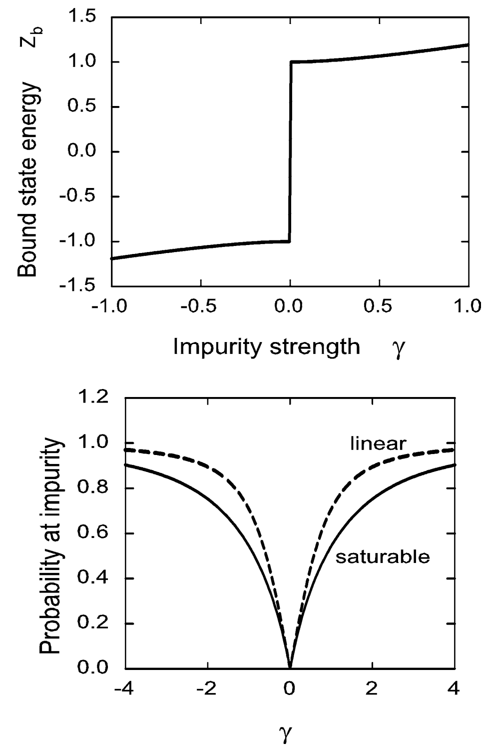

Fig. 1. Saturable impurity case. Top: normalized bound state energy of saturable impurity as a function of the normalized impurity strength. Bottom: probability at impurity site as a function of the normalized impurity strength. The curve corresponding to the linear impurity case is also shown, for comparison.

$$\frac{1}{\gamma} = \frac{z_b}{|z_b|\sqrt{z_b^2 - 1} + (z_b^2 - 1)}. \tag{15}$$

Eq. (15) is a cubic algebraic equation, with real solution,

$$z_b(\gamma) = -\frac{1-\gamma^2}{6\gamma} + \frac{1+10\gamma^2+\gamma^4}{6\gamma G^{1/3}} + \frac{G^{1/3}}{6\gamma},$$
$$\text{with } G = -1 + 39\gamma^2 + 15\gamma^4 + \gamma^6 + 6\sqrt{3}|\gamma|\sqrt{-1 + 11\gamma^2 + \gamma^4}. \tag{16}$$

Fig. 1 shows the bound state energy as a function of γ, as well as the probability at the impurity site, $|C_0(\gamma)|^2 = \sqrt{z_b^2(\gamma) - 1}/|z_b(\gamma)|$. Clearly, the growth of probability with impurity strength is sub-linear. This suggests that our saturable impurity is somewhat equivalent to an effective linear impurity. This is easy to see, since at small nonlinearity, $|C_0|^2 \ll 1$, implying an effective impurity Hamiltonian term of the form $\gamma|0\rangle\langle 0|$; while at large nonlinearity value, $|C_0|^2 \sim 1$, implying an impurity term of the form $(\gamma/2)|0\rangle\langle 0|$. Thus, at small and large nonlinearity, the impurity behaves as a linear impurity.

On Fig. 2 we display several bound states profiles for different impurity parameter values, going from small to large values.

3. Transmission across the impurity

We now consider the problem of computing the transmission of linear plane waves sent towards a single general nonlinear impurity of the form $f(|C_0|^2)\delta_{n0}$. We set $C_n(t) =$

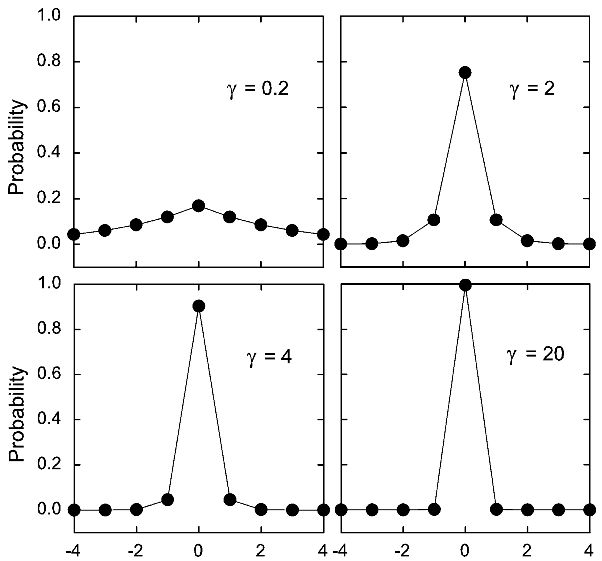

Fig. 2. Saturable impurity: bound state probability profiles for different values of the impurity strength.

$\phi_n \exp(-iEt)$ and take ϕ_n of the form

$$\phi_n = \begin{cases} I\exp(ikn) + R\exp(-ikn), & \text{if } n \leqslant -1, \\ T\exp(ikn), & \text{if } n \geqslant 0, \end{cases} \tag{17}$$

with I, R and T being the amplitude of the injected, reflected and transmitted parts of the wave, respectively. After inserting this into Eq. (2) and after some algebra, we obtain a nonlinear equation for $|T|^2$,

$$|T|^2 = \frac{|I|^2}{1 + (\gamma/\sin(k))^2 f^2(|T|^2)}. \tag{18}$$

From Eq. (18) we immediately notice several general features: $|T|^2$ is even in γ and k; there are no resonances: $|T|^2 < |I|^2$; an increase in impurity strength γ always decreases $|T|^2$. Most interestingly, there is no bistability for any *monotonic* $f(x)$: this can most easily seen by rewriting Eq. (18) as

$$|I|^2 = |T|^2\left(1 + \left(\frac{\gamma}{\sin(k)}\right)^2 f^2(|T|^2)\right). \tag{19}$$

For a given input intensity $|I|^2$, the right-hand side of Eq. (19) is always monotonic in $|T|^2$, for $f(x)$ monotonic.

3.1. Saturable impurity

In this case $f(x) = 1/(1+x)$, and Eq. (18) can be cast as a cubic equation for the transmission coefficient $t \equiv |T|^2/|I|^2$,

$$1 = t\left(1 + \frac{(\gamma/\sin(k))^2}{(1+|I|^2 t)^2}\right), \tag{20}$$

and a real solution for t can be written down, although is not particularly illuminating. In Fig. 3 we show two transmission plots: one for a fixed impurity parameter γ and variable injected intensity $|I|$ and the other, for a fixed incoming intensity $|I|$ and variable impurity strength γ. As expected, an increase in injected intensity increases the transmission while an increase in the impurity parameter γ decreases it. In the limit $I \to 0$, we recover the well-known case of a linear impurity of strength γ: $t \to \sin(k)^2/(\gamma^2 + \sin(k)^2)$.

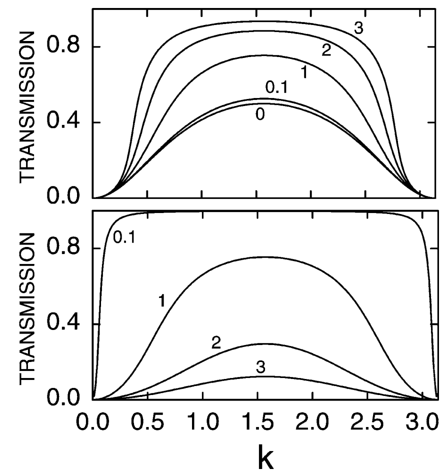

Fig. 3. Plane wave transmission coefficient versus wave vector. Top: fixed $\gamma = 1$ and varying input intensity $|I|$. Bottom: fixed input intensity $|I| = 1$ and varying γ.

In conclusion, we have studied the properties of localized impurity modes and the plane wave scattering in the framework of the generalized discrete nonlinear model. Using the formalism of lattice Green function, we have obtained nonlinear equations for the bound state energy and the transmission coefficient, for a wide class of nonlinear impurities. The results obtained are generic for a wide class of physical systems where the main Eq. (1) is applicable. As an example, we have studied in detail the case of saturable nonlinearity that corresponds to the recently analyzed arrays of weakly coupled optical waveguides. We found that only a single bound state is possible for any value of the impurity parameter. The transmission of plane waves across the saturable impurity shows no bistability.

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