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Effects of a nonlinear impurity in a diatomic chain

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Abstract. The problem of the existence of bound states outside the continuum of the bands due to the presence of a nonlinear impurity is studied within a two-band tight-binding model in one dimension. The nonlinear impurity deviates from the ordinary sites by an on-site energy of the form $\chi(|\psi_0|^2)^{\beta/2}$, where $|\psi_0|^2$ is the probability of finding the particle at the impurity site, χ is referred to as the strength and β is the nonlinearity of the impurity. For $\beta > 2$, there exist threshold values for χ below which there is no bound state. For $0 < \beta \leqslant 2$, there is always one bound state above the upper band for $\chi > 0$; and two bound states, one with energy inside the band gap and another below the lower band, for $\chi < 0$. For $\beta < 0$, there is always a bound state above (below) the upper (lower) band for $\chi > 0$ ($\chi < 0$). For $|\beta| < 2/3$ ($\beta < 0$), there is always a state inside the gap; while for $|\beta| > 2/3$, there exists an upper bound for $|\chi|$ above which no bound states are found inside the gap.

1. Introduction

Recently, there has been much interest in studying phenomena in which nonlinearity and disorder are present simultaneously [1]. One class of studies looked into the spreading of a wave packet in a system with nonlinear impurities, and the transmission of an incident wave through a segment with nonlinear impurities [2, 3]. These nonlinear impurities have the property that their strength is proportional to the probability of finding the particle at the impurity site, i.e., the projection of the wavefunction onto the impurity site. Very different diffusion and transmission behaviours, e.g., self-trapping, have been found as a result of the presence of nonlinear impurities [4]. This problem, in general, is related to the more difficult problem of solving a nonlinear Schrödinger equation [3].

A related problem with very interesting results is that of the existence of bound states outside the band continuum in the presence of nonlinear impurities. The classic problem of the effects of a single linear impurity in an otherwise ordered solid has been treated in detail by Koster and Slater [5]. For a linear impurity within a one-band model, it was found that a bound state is formed in one dimension (1D) and two dimensions (2D) regardless of the strength of the impurity, and a threshold exists for the strength of the impurity for the existence of a bound state in three dimensions (3D) [5–7]. Recently, similar problems have been studied for a single nonlinear impurity in one-band tight-binding models [8–11]. It was found that nonlinearity leads to qualitatively different results. There may exist a threshold below which there is no bound state and above which there are two bound states.

In the present work, we study in detail the problems of the existence of bound states in a *two-band* model in 1D. In particular, a diatomic linear chain model is used. In contrast

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to the case for one-band models, which have no band gap, we can consider the impurity levels within the band gap. The presence of states in the band gap depends on where the impurity is located, i.e., at which site of a diatomic chain, and on the sign of the strength of the impurity. The interplay between the strength and the nonlinearity provides a very rich behaviour regarding the existence of bound states.

As in the diffusion and transmission problems, in which such phenomena as self-trapping are studied. the nonlinearity may be due to many-body effects in solids, e.g., the polarization due to localized electron. Nonlinearity may also be introduced by doping of materials with foreign species with nonlinear properties. The dependence of the strength of an impurity on the probability of finding the particle at the impurity site can also be regarded as an approximation for treating, to a certain degree, on-site repulsion effects. The present problem can be readily generalized to that of electromagnetic wave propagation in inhomogeneous nonlinear media; the corresponding ordered systems in this case are usually referred to as photonic band-gap materials.

The plan of the paper is as follows. In section 2, the formalism of the problem is presented and results for a linear impurity in a two-band model are briefly reviewed. In section 3, we present results for a nonlinear impurity, with particular attention being paid to the effects of the sign of the strength of the impurity and that of the nonlinearity. In section 4, we summarize the results and discuss possible generalizations of the present problem.

2. Formalism

Consider two types of site arranged alternately on a linear chain. The even- (odd-) numbered sites are occupied by type-A (type-B) atoms with on-site energy $+\epsilon$ $(-\epsilon)$. For simplicity, we consider interactions only between nearest neighbours. The Hamiltonian of the ordered chain can be written as

$$H_0 = \epsilon \sum_n (|2n\rangle\langle 2n| - |2n+1\rangle\langle 2n+1|) + V \sum_n (|2n\rangle\langle 2n+1| + |2n\rangle\langle 2n-1| + \text{HC}) \qquad (1)$$

where V is the hopping integral between neighbouring Wannier orbitals $|n\rangle$. The spacing between neighbouring atoms is assumed to be a and hence the lattice constant is $2a$. The Bloch sums associated with the type-A and type-B sites can be constructed as

$$|\phi_A(k)\rangle = \frac{1}{\sqrt{N}} \sum_n \mathrm{e}^{\mathrm{i}k2na} |2n\rangle \qquad |\phi_B(k)\rangle = \frac{1}{\sqrt{N}} \sum_n \mathrm{e}^{\mathrm{i}k(2n+1)a} |2n+1\rangle \qquad (2)$$

where N is the number of unit cells. The Schrödinger equation $H_0|\psi_k\rangle = E(k)|\psi_k\rangle$ can be solved by writing $|\psi_k\rangle$ as a linear combination of the Bloch sums:

$$|\psi_k\rangle = \alpha_A|\phi_A(k)\rangle + \alpha_B|\phi_B(k)\rangle. \qquad (3)$$

Substituting into the Schrödinger equation gives a 2×2 matrix with each k in the first Brillouin zone. The corresponding eigenvalues give the band structure

$$E(k) = \pm\sqrt{\epsilon^2 + (2V\cos ka)^2}. \qquad (4)$$

The band gap is given by 2ϵ and the band width of each band is $\sqrt{\epsilon^2 + 4V^2} - \epsilon$. Note that if we set $\epsilon = 0$, the model reduces to a one-band model with lattice constant a and band width $4V$. Another case worth studying, which also leads to a two-band situation, is the use of a chain of one type of site with two orbitals per site.

The Green's function corresponding to H_0 can be found exactly. In particular, the matrix elements connecting Wannier orbitals on type-A sites are given by

$$G^{(0)}_{2n,2m}(z) \equiv \langle 2n|G^{(0)}|2m\rangle = -\left(\frac{z+\epsilon}{2\pi \mathrm{i} V^2}\right)\oint \mathrm{d}w \; \frac{w^{|n-m|}}{w^2 - 2wx + 1} \tag{5}$$

where z is an energy parameter and the integral is over a unit circle and

$$x = \frac{1}{2V^2}(z^2 - \epsilon^2 - 2V^2). \tag{6}$$

Since we are primarily interested in the existence of bound states outside the band continuum due to the presence of an impurity, we focus on the Green's function with z above (below) the top (bottom) of the upper (lower) band and inside the band gap. The on-site matrix element at, say, the origin can be evaluated by carrying out a contour integration:

$$G^{(0)}_{00}(z) = \begin{cases} \dfrac{z+\epsilon}{2V^2\sqrt{x^2-1}} & \text{for } |z| > \sqrt{\epsilon^2 + 4V^2} \\ -\dfrac{z+\epsilon}{2V^2\sqrt{x^2-1}} & \text{for } |z| < \epsilon. \end{cases} \tag{7}$$

Note that $G^{(0)}_{00}(z)$ is positive for z above the top of the upper band and is negative for z within the band gap and below the bottom of the lower band.

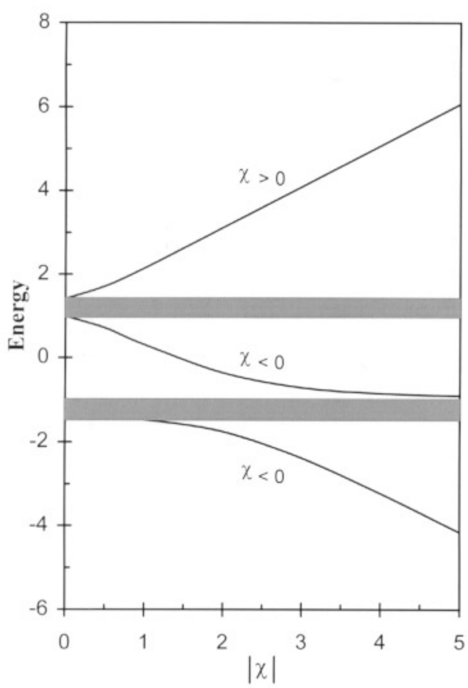

Figure 1. The dependence of the bound-state energies as a function of the linear impurity ($\beta = 0$) strength. For $\chi > 0$, there is always a bound state above the top of the upper band. For $\chi < 0$, there are always two bound states with one inside the gap and the other below the bottom of the lower band. The shaded regions are the band continua. The on-site energy is chosen to be $\epsilon = 1$ and the hopping integral $V = 0.5$.

Consider a nonlinear impurity at a type-A site. Without loss of generality, we assume that the impurity is placed at the origin. The impurity is assumed to lead to a perturbation term in the Hamiltonian of the form

$$H_1 = \chi(|\psi_0|^2)^{\beta/2}|0\rangle\langle 0| \tag{8}$$

where $|\psi_0|^2 = |\langle 0|\psi_k\rangle|^2$ is the probability of finding the particle at the impurity site, χ is referred to as the strength of the impurity and β the nonlinearity. Since $|\psi_0|^2 < 1$, by the normalization of the wavefunction, the factor $(|\psi_0|^2)^{\beta/2}$ acts as a reduction factor to χ for $\beta > 0$ and as an enhancement factor for $\beta < 0$. With this form of H_1, the site at the origin has an on-site energy $\epsilon + \chi(|\psi_0|^2)^{\beta/2}$, i.e., a nonlinear term added to the original on-site energy. Note that χ can either be positive or negative.

The matrix elements of the perturbed Green's function G corresponding to the total Hamiltonian $H = H_0 + H_1$ can be expressed exactly as

$$G_{mn} = G_{mn}^{(0)} + G_{m0}^{(0)} T_{00} G_{0n}^{(0)} \tag{9}$$

where the t-matrix T_{00} is

$$T_{00} = \frac{\chi(|\psi_0|^2)^{\beta/2}}{1 - \chi(|\psi_0|^2)^{\beta/2} G_{00}^{(0)}} \tag{10}$$

with $G_{00}^{(0)}$ given by equation (7) and $G_{mn} \equiv \langle m|G|n\rangle$. It is our aim to investigate the interplay between ϵ and β as regards the existence of bound states outside the continuum of the band.

The poles of the perturbed Green's function G give the energies of the bound states. Since $G_{mn}^{(0)}$ has poles (branch cut) only within the bands, it is sufficient to solve for the energies z_b corresponding to the poles of T_{00}, i.e.,

$$1 - \chi(|\psi_0|^2)^{\beta/2} G_{00}^{(0)}(z_b) = 0. \tag{11}$$

However, the factor $|\psi_0|^2$ depends also on z_b, as it is known only after G is solved. Using a standard relation between G and $|\psi_0|^2$, and equation (9) for G, $|\psi_0|^2$ can be written in terms of the unperturbed Green's function as [6]

$$|\psi_0|^2 = -\frac{[G_{00}^{(0)}(z_b)]^2}{[G_{00}^{(0)\prime}(z)]_{z=z_b}} \tag{12}$$

where the denominator is the derivative of $G_{00}^{(0)}(z)$ with respect to z evaluated at $z = z_b$. Equations (11) and (12) form a set of equations to be solved simultaneously for the bound-state energies.

For comparison with results for a nonlinear impurity, it is useful to discuss briefly the case of a linear impurity (i.e., $\beta = 0$). In this case, it is then sufficient to solve equation (11) alone with $G_{00}^{(0)}$ given by equation (7). Figure 1 shows the energies of the bound states as functions of the impurity strength χ. For $\chi > 0$, there is always one bound state with energy above the top of the upper band. For $\chi < 0$, there are always two bound states, one inside the gap and another below the bottom of the lower band. This behaviour is closely related to our choice of $+\epsilon$ on-site energy at type-A sites. If the linear impurity is placed at a type-B site, say site 1, then the role of $G_{00}^{(0)}$ in equation (11) is taken by $G_{11}^{(0)}$. In this case, we have one bound state below the bottom of the lower band for $\chi < 0$, and two bound staes for $\chi > 0$.

3. Results

3.1. $\beta > 0$

For $\chi > 0$, bound states appear above the top of the upper band. Using equation (7) for $G_{00}^{(0)}$ and equations (11) and (12), z_b satisfies the equation

$$\frac{1}{\chi} = (z_b + \epsilon)\left[z_b^2 - \epsilon^2 - \frac{4\epsilon V^2}{z_b + \epsilon}\right]^{-\beta/2} [(z_b^2 - \epsilon^2)(z_b^2 - \epsilon^2 - 4V^2)]^{(\beta-2)/4}. \tag{13}$$

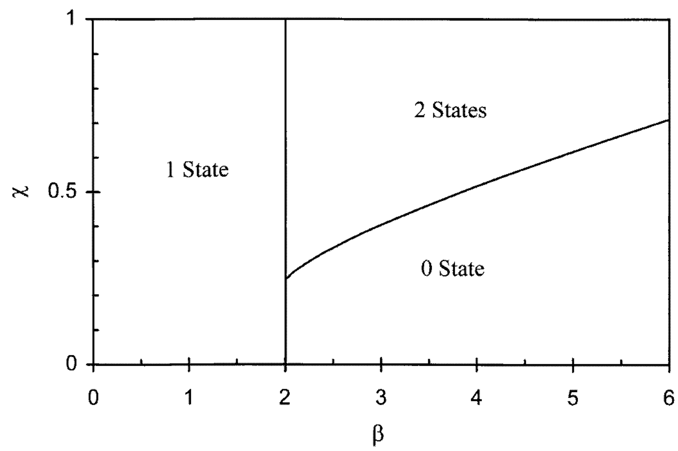

Figure 2. The behaviour of the bound states on the χ–β plane with $\chi > 0$ and $\beta > 0$. When $\beta < 2$, there is always one bound state above the top of the upper band. When $\beta > 2$, there exists a threshold value of χ below which there are no bound states. Above the threshold, there are two bound states above the top of the upper band. The parameters are the same as in figure 1.

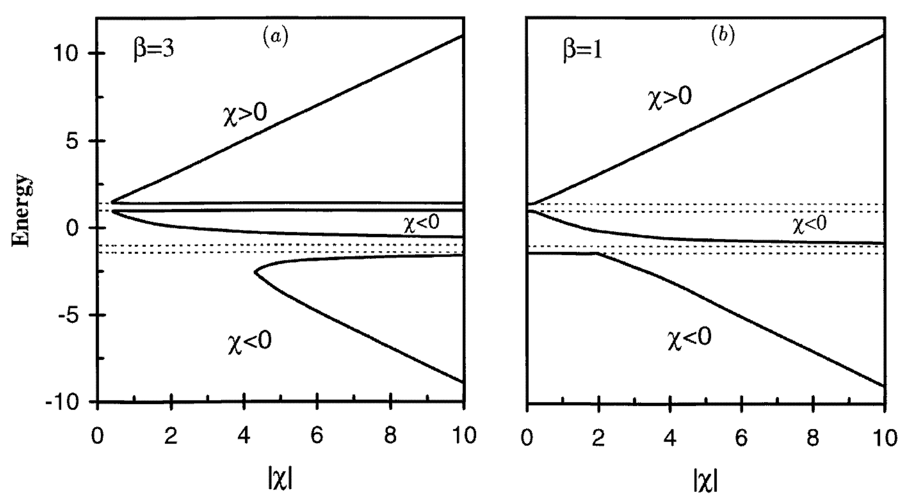

Figure 3. The dependence of the energies of the bound states on the strength $|\chi|$ in the cases of (a) $\beta = 3$ and (b) $\beta = 1$. The upper portions of the figures correspond to $\chi > 0$. For (a) $\beta > 2$, two bound states can be found above the top of the upper band when χ is above the threshold. For (b) $\beta < 2$, there is always one bound state regardless of the value of χ. The lower portions of the figures correspond to $\chi < 0$. For (a) $\beta > 2$, a maximum of four bound states, two of which are inside the gap and the other two of which are below the bottom of the lower band, can be found if $|\chi|$ is large enough. For (b) $\beta < 2$, there are always two bound states, with one inside the gap and one below the bottom of the lower band. The parameters are the same as in figure 1.

It is immediately clear that $\beta < 2$ and $\beta > 2$ represent two qualitatively different situations. For $\beta < 2$, the right-hand side (RHS) of equation (13), as a function of z_b, diverges as z_b approaches the band edge (i.e., as $z_b \to \sqrt{\epsilon^2 + 4V^2}$) and monotonically decreases to zero as $z_b \to \infty$. Hence for given χ and β less than two, there is always one solution for z_b. For $\beta > 2$, however, the RHS of equation (13) vanishes both at the band edge and as $z_b \to \infty$. Hence for given β, there exists a threshold χ_{min} below which there is no bound state. For $\chi > \chi_{min}$, there are two bound states. Figure 2 shows the corresponding regions of different behaviour on the χ–β plane for the case where $\chi > 0$. These results are similar to those in one-band models [9]. The upper portion of figure 3 shows the dependence of the energies of the two bound states on the strength χ ($\chi > 0$) for $\beta = 1$ and $\beta = 3$. For $\beta > 2$, the energy of one of the bound states decreases towards the top band edge of the upper band and that of the other increases as χ increases.

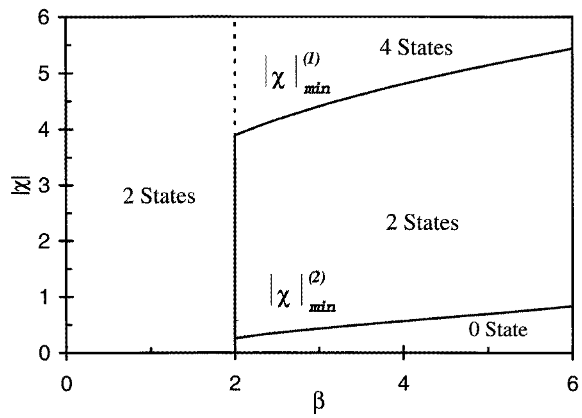

Figure 4. The dependence of $|\chi|^{(1)}_{min}$ and $|\chi|^{(2)}_{min}$ on β with $\beta > 0$ and $\chi < 0$. For $\beta > 2$, there exists a threshold $|\chi|^{(2)}_{min}$ above which there are two bound states. As $|\chi|$ increases further until $|\chi| > |\chi|^{(1)}_{min}$, four bound states are found, with two inside the gap and the other two below the bottom of the lower band. For $\beta < 2$, two states are found with one inside the gap and the other below the bottom of the lower band. On the dashed line, there are three bound states.

For $\chi < 0$, bound states, if they exist, appear inside the gap and below the bottom of the lower band. For z_b below the bottom of the lower band, it again satisfies equation (13). This leads to similar behaviour regarding the existence of a threshold, $|\chi|^{(1)}_{min}$, for the presence of bound states for $\beta > 2$. For the bound state inside the band gap, z_b satisfies the equation

$$\frac{1}{|\chi|} = (z_b + \epsilon)\left[\epsilon^2 - z_b^2 + \frac{4\epsilon V^2}{z_b + \epsilon}\right]^{-\beta/2} [(\epsilon^2 - z_b^2)(\epsilon^2 - z_b^2 + 4V^2)]^{(\beta-2)/4}. \tag{14}$$

Again, for $\beta > 2$, there exists a threshold, $|\chi|^{(2)}_{min}$, above which there are two bound states. Figure 3 also shows the dependence of the bound-state energies on χ for $\chi < 0$. We note that for some values of $|\chi|$ there are four bound states, two in the gap and two below the bottom of the lower band. The bound states in the gap lie closer to the upper band. As $|\chi|$ increases, one of them shifts towards the lower band edge of the upper band and the other shifts towards the upper band edge of the lower band. Figure 4 gives the dependence of $|\chi|^{(1)}_{min}$ and $|\chi|^{(2)}_{min}$ on β and shows the regions of different behaviour on the $|\chi|$–β plane.

3.2. $\beta < 0$

In a two-band model for an arbitrary value of $|\beta|$ ($\beta < 0$), there is always one bound state above (below) the top (bottom) of the upper (lower) band for positive (negative) values of

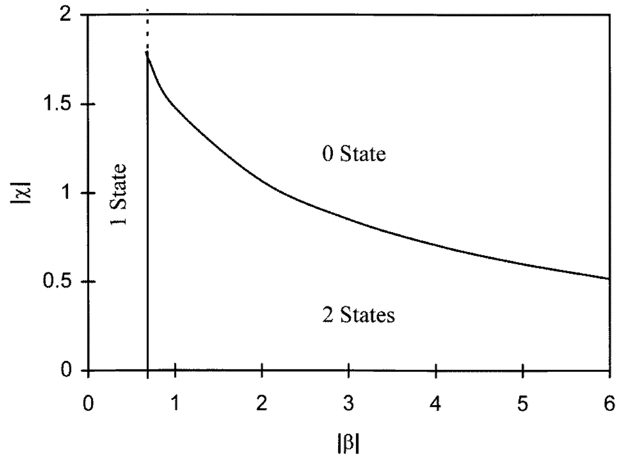

Figure 5. The behaviour of the existence of bound states within the gap on the $|\chi|$–$|\beta|$ plane for $\beta < 0$ and $\chi < 0$. For $|\beta| < 2/3$, there is always one bound state within the gap. However, for $|\beta| > 2/3$, there is an upper bound for the impurity strength, $|\chi|_{max}$, above which there is no bound state within the gap. However, if $|\chi|$ is below the threshold, two bound states can be found within the gap. On the dashed line, there is no bound state.

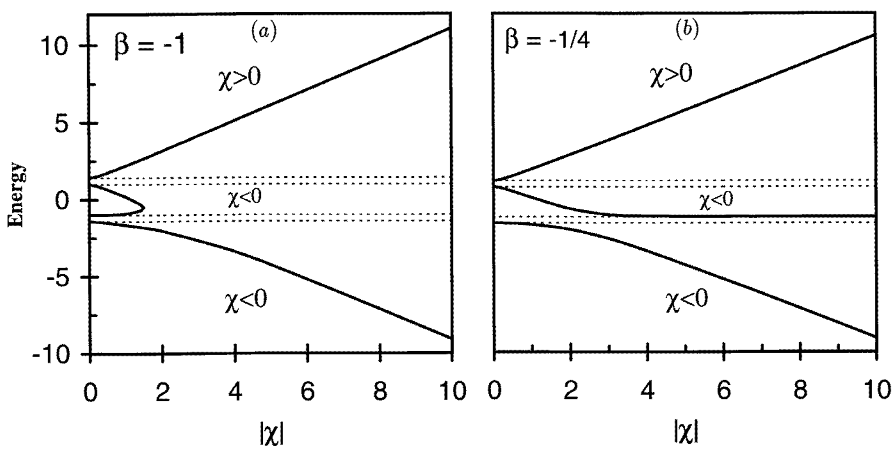

Figure 6. The dependence of the bound-state energies on $|\chi|$ ($\chi < 0$) with $\beta < 0$. (a) For $|\beta| > 2/3$, there exists an upper bound $|\chi|_{max}$ above which no bound states can be found within the gap. However, when $|\chi| < |\chi|_{max}$, two bound states can be found. (b) The situation is different for (b) $|\beta| < 2/3$, where one bound state can always be found within the gap.

χ. This behaviour is similar to that of a *linear* impurity and of a one-band model with negative nonlinearity. However, the states within the band gap which appear when $\chi < 0$ behave differently. The energy of the bound state within the gap satisfies equation (14). Figure 5 shows the regions corresponding to different behaviour regarding the existence of bound states within the gap on the $|\chi|$–$|\beta|$ plane. For $|\beta| < 2/3$, there is always one bound state within the gap regardless of the magnitude of the strength $|\chi|$. However, for $|\beta| > 2/3$, there exists an upper bound for the strength $|\chi|_{max}$, which depends on $|\beta|$, above which there is no bound state within the gap. For $|\beta| > 2/3$ and $|\chi| < |\chi|_{max}$, there are two bound states. The bound-state energies are shown in figure 6 for two different values of $|\beta|$.

Such a result becomes clear when we consider the behaviour of the RHS of equation (14) as a function of z_b. As z_b approaches the bottom of the upper band, i.e., $z_b \to +\epsilon$, the RHS of equation (14) diverges for arbitrary value of $|\beta|$. As z_b approaches the top of the lower band, the RHS of equation (14) behaves as $(z_b + \epsilon)^{(2-3|\beta|)/4}$, which goes to zero for $|\beta| < 2/3$ and diverges for $|\beta| > 2/3$. Hence for $|\beta| > 2/3$, the RHS of equation (14) diverges at both edges forming the gap and thus imposes a $|\chi|_{max}$ above which there is no bound state.

3.3. Nonlinear impurity on type-B sites

We have considered in detail the effects of a nonlinear impurity on type-A sites. A similar treatment can be applied to an impurity located on type-B sites. Since the results are similar, we only discuss the major difference. In this case, we replace $G_{00}^{(0)}$ in equation (11) by $G_{11}^{(0)}(z)$, which is the on-site matrix element of the unperturbed Green's function at site 1 and is given by

$$G_{11}^{(0)} = \begin{cases} \dfrac{z-\epsilon}{2V^2\sqrt{x^2-1}} & \text{for} |z| > \sqrt{\epsilon^2+4V^2}E \\ -\dfrac{z-\epsilon}{2V^2\sqrt{x^2-1}} & \text{for } |z| < \epsilon \end{cases} \tag{15}$$

where x is defined by equation (6). The difference when placing an impurity on a type-B site is that for $\chi < 0$, bound states appear only with energies *below* the bottom of the lower band; while for $\chi > 0$, bound states appear in the band gap and above the top of the upper band. Other than this, the existence of the bound states for different values of β and χ is qualitatively similar to the behaviour discussed above.

4. Discussion

In summary, we have studied in detail the problem of the existence of bound states in a two-band tight-binding model in 1D. For $\beta > 2$, there exist threshold values for the strength of the impurity for the presence of bound states outside the continuum of the bands. For $0 < \beta < 2$, there are always bound states regardless of the strength of the impurity. For negative β and $|\beta| > 2/3$, there exists an upper bound, $|\chi|_{max}$, on the strength above which there is no bound state with energies inside the band gap.

Our work focused on the dependence of the bound-state energies on the strength χ and nonlinearity β of the impurity. It is equally interesting to look at the wavefunction associated with these bound states. Basically, they are localized around the impurity sites but the width of the wavefunction depends sensitively on χ and β and becomes quite widely spread when the bound-state energies approach one of the band edges. When extended to include many impurities, the interesting question becomes that of localization in a random chain with nonlinear impurities which has recently attracted much attention [2].

We conclude with a discussion on possible generalizations of the present work. A system of current interest is that of photonic band-gap (PBG) materials, which are basically periodic dielectric materials [12–14]. The dispersion relation for electromagnetic wave propagation in these PBG materials exhibits bands of allowed modes and forbidden frequency ranges with no propagating modes, analogous to bands and band gaps in electronic systems. These dispersion relations can be fitted to standard tight-binding form in order to establish an empirical tight-binding treatment for photonic bands [15]. Theoretically, this tight-binding description of photonic bands can be viewed as a result of overlaps of neighbouring localized Wannier orbitals associated with the sites on a lattice [16, 17]. These Wannier functions can be formed by linearly combining Bloch functions. If a single band or a pair of bands is of particular interest, then a one-band or two-band tight-binding model suffices to capture the basic essential features. Our formalism in treating impurities, linear and nonlinear, can then be applied to these PBG materials [16, 17]. In this case, a nonlinear impurity may represent the substitution at one site for the periodic dielectric material of another material with nonlinear optical properties. Experimentally, impurity levels have been observed within the photonic band gaps in intentionally doped PBG materials [18]. Our results indicate that one can control the position of the impurity levels by tuning the strength of the impurity. These doped PBG materials have potential applications in the design of novel optoelectronic devices such as lasers, resonators, and frequency filters. Impurity levels are sometimes useful in the operation of some of these devices. For example, doped PBG materials can be used to provide high-Q electromagnetic cavities. It should be pointed out that a complete treatment of the PBG problem should take into account the vectorial nature of EM fields. Qualitatively, a scalar wave approximation may be used to estimate the effects of nonlinear impurities. Note that even within the scalar wave approximation, the form of the wave equation is different from that of the Schrödinger equation, and hence slightly different results from those reported here will be obtained [19].

Our problem can naturally be extended to higher spatial dimensions. However, in higher dimensions we do not expect different behaviour for $\beta < 2$ and $\beta > 2$ as this merely comes from the special form of the Green's function in 1D which, in turn, is a result of the tight-binding energy band and the k-space integration in obtaining the Green's function. The formalism presented here for the single-impurity problem can be extended to treat an infinite number of impurities, which is equivalent to an alloy problem. The standard methods [20] such as the average t-matrix approximation and the coherent-potential approximation can be used to deal with this alloy problem, with the former being good in the limit of dilute concentration of nonlinear impurities.

Acknowledgments

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