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Nonlinear impurities in a linear chain

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We use the Green's function formalism to evaluate analytically the stationary states for an electron moving in a one-dimensional chain in the presence of one and two adiabatic Holstein-type *nonlinear* impurities. For the case of one nonlinear monomer we find that, contrary to what occurs in the linear impurity problem, the strength of the impurity must be greater than half the bandwidth for a bound state to exist. In the case of a nonlinear dimer resonance phenomena are observed that lead to *complete* transmission through the dimer.

The nonlinear features of the motion of a strongly interacting particle in one-dimensional lattices were given considerable attention in recent years.[1] This problem, aside from the purely theoretical interest pertaining to the properties of self-trapping in ordered and disordered lattices has practical ramifications in biology,[1] condensed matter[2] as well as optics.[3] Most of the past studies were confined in studying systems where the discrete crystalline symmetry of the lattice is preserved. Two notable exceptions are the works in Ref. 4 where numerical studies were done for nonlinear discrete segments embedded in an infinite, linear discrete host. In the present Rapid Communication we cast the approach of Ref. 4 into a tight-binding type formalism and present an *analytical* treatment of the problem of one and two nonlinear impurities embedded in a linear host. Due to its generality, our method can also be extended to arbitrary nonlinear segments.[5] Our findings in the dimer case show that some of the results obtained in the context of the linear random dimer model[6] have a direct counterpart in the present nonlinear case.

Consider an electron moving in a one-dimensional periodic lattice in the presence of a number of substitutional *nonlinear* (adiabatic) Holstein-type impurities[7] located at lattice sites $r_1, r_2, \ldots, r_M$. These impurities have the same nonlinear features studied in the context of the discrete self-trapping equation.[8] We cast this problem into the tight-binding form where the "Hamiltonian" is

$$\tilde{H}=\tilde{H}_0+\tilde{H}_M , \tag{1}$$

where

$$\tilde{H}_0=V\sum_i(|i\rangle\langle i+1|+|i+1\rangle\langle i|) \tag{2}$$

and

$$\tilde{H}_M=\chi\sum_{i=1}^{M}|C_{r_i}|^2|r_i\rangle\langle r_i| \tag{3}$$

and the $\{|i\rangle\}$ represent Wannier electronic states, V is the hopping matrix element, χ is the nonlinearity parameter (proportional to the strength of the electron-phonon interaction at the impurity site), $|C_{r_i}|^2$ represents the probability of finding the excitation on site r_i and M is the total number of impurities. Note that the perturbation $\tilde{H}_M$ differs from the well-known problem of linear impurities in that it incorporates strong polaronic effects. For convenience, we introduce the following dimensionless quantities: $z\equiv E/2V$, $H\equiv\tilde{H}/2V$, and $\gamma\equiv\chi/2V$.

(a) *One nonlinear impurity.* The (dimensionless) lattice Green's function of our system $G\equiv 1/(z-H)$ can be formally expanded as[9]

$$G=G^{(0)}+G^{(0)}H_1G^{(0)}+G^{(0)}H_1G^{(0)}H_1G^{(0)}+\ldots , \tag{4}$$

where $G^{(0)}$ is the unperturbed ($\gamma=0$) Green's function, $H_1=\gamma|C_0|^2|0\rangle\langle 0|$ and where, without loss of generality, we have placed the impurity at the origin. by inserting H_1 into Eq. (4), we can formally resum the perturbative series to get, in the Wannier representation

$$G_{mn}=G_{mn}^{(0)}+\frac{\gamma|C_0|^2G_{m0}^{(0)}G_{0n}^{(0)}}{1-\gamma|C_0|^2G_{00}^{(0)}} . \tag{5}$$

We cannot use Eq. (5) yet, since we do not know $|C_0|^2$; we will however determine it subsequently in a self-consistent manner.

Bound state. The bound state energy z_b is given by the pole(s) of G_{mn}: $1=\gamma|C_0^{(b)}|^2G_{00}^{(0)}$. Since $G_{00}^{(0)}=1/\sqrt{z^2-1}$ (Ref. 9), we get for z_b

$$z_b=\pm\sqrt{1+\gamma^2|C_0^{(b)}|^4} . \tag{6}$$

The bound state amplitude coefficients $C_n^{(b)}$ can be obtained from the residues of $G_{mn}(z)$ at $z=z_b$ through the relation:[9]

$$C_n^{(b)}C_m^{(b)*}=\text{Res}\{G_{mn}(z)\}_{z=z_b} . \tag{7}$$

Now, since

$$G_{mn}^{(0)}(z)=\frac{1}{\sqrt{z^2-1}}\{z-\sqrt{z^2-1}\}^{|n-m|} \tag{8}$$

we get, with the help of Eqs. (5) and (7):

$$|C_n^{(b)}|^2 = \frac{|\gamma||C_0^{(b)}|^2}{\sqrt{1+\gamma^2|C_0^{(b)}|^4}} \times \{\sqrt{1+\gamma^2|C_0^{(b)}|^4} - |\gamma||C_0^{(b)}|^2\}^{2|n|} . \quad (9)$$

We now determine $|C_0^{(b)}|^2$ by the self-consistency requirement that Eq. (9) be obeyed at $n=0$. We get

$$|C_0^{(b)}|^2 = \sqrt{1-(1/\gamma)^2}\Theta(|\gamma|-1) \quad (10)$$

which implies, from Eq. (6): $z_b = \pm[1+\Theta(|\gamma|-1)(|\gamma|-1)]$. At $|\gamma|=1$, $z_b=\pm 1$ and so it is the state at the band edge which separates from the band to form the discrete level. By replacing Eq. (10) into Eq. (9) we have the final expression for the bound state profile:

$$|C_n^{(b)}|^2 = \sqrt{1-(1/\gamma)^2}(|\gamma| - \sqrt{\gamma^2-1})^{2|N|}\Theta(|\gamma|-1) . \quad (11)$$

In addition, it can be shown from Eq. (7) that we can choose all the amplitudes for the bound state to be *real and positive.* The bound state described by Eq. (11) exists only for $\gamma > 1$ in which case it decays exponentially away from the impurity site, with a localization length λ given by

$$\frac{\lambda}{a} = \frac{-1}{2\ln(|\gamma| - \sqrt{\gamma^2-1})} , \quad (12)$$

where a is the lattice spacing. For $|\gamma|<1$, no bound state exists and all the eigenstates are scattering states $[|C_n|^2 = O(1/N)]$. This is markedly different from the *linear* impurity case, where there is always a bound state no matter how small the impurity parameter is.[9] In our case, in order to have a bound state at all, the strength of the nonlinearity parameter must be at least equal to half the bandwidth: $|\gamma| = \chi/2V = 1$. Figure 1 shows the probability profile $|C_n^{(b)}|^2$ for the bound state versus the lattice site n, for several different values of the nonlinearity parameter γ. Figure 2 shows the probability of finding the excitation on the impurity site versus the nonlinearity parameter γ

Extended states. All states inside the band $-1<z<1$ are extended (scattering states) with $z=\cos(k)$. They are formally given by[9]

$$|\Psi_z\rangle = |k\rangle + G^{(0)+}(z)T^+(z)|k\rangle , \quad (13)$$

where $|k\rangle$ are the eigenstates of $G^{(0)}$ (plane waves). T is given by

$$T = H_1 + H_1 G^{(0)} H_1 + H_1 G^{(0)} H_1 G^{(0)} H_1 + \cdots . \quad (14)$$

After resumming, we get

$$T = \frac{\gamma|C_0|^2|0\rangle\langle 0|}{1-\gamma|C_0|^2 G_{00}^{(0)}} . \quad (15)$$

From Eqs. (13) and (15) we get for the scattering amplitude at site n

$$\langle n|\Psi_z\rangle = \langle n|k\rangle + \frac{\gamma|C_0|^2\langle n|G^{(0)+}(z)|0\rangle\langle 0|k\rangle}{1-\gamma|C_0|^2 G_{00}^{(0)}} . \quad (16)$$

The transmission coefficient t is the probability density at the *impurity* site, i.e., $t=|C_0|^2$. From Eq. (16), we have

$$t = \frac{1}{|1-\gamma t G_{00}^{(0)}|^2} . \quad (17)$$

By replacing $G_{00}^{(0)} = -i\sqrt{1-z^2}$ we get a cubic equation for t:

$$\gamma^2 t^3 + \sin(k)^2 t - \sin(k)^2 = 0 , \quad (18)$$

whose positive and real solution is

$$t = (1/\gamma)\left[\frac{9\gamma\sin(k)^2 + \sqrt{3}\sqrt{27\gamma^2\sin(k)^4 + 4\sin(k)^6}}{18}\right]^{1/3} - (1/\gamma)\frac{(2/3)^{1/3}\sin(k)^2}{[9\gamma\sin(k)^2 + \sqrt{3}\sqrt{27\gamma^2\sin(k)^4+4\sin(k)^6}]^{1/3}} . \quad (19)$$

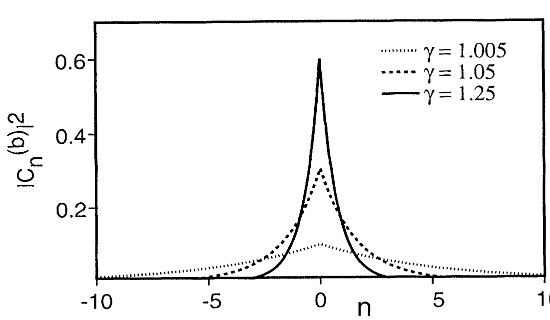

FIG. 1. One nonlinear impurity. Probability profile for the bound state for different values of the nonlinearity parameter $\gamma \equiv \chi/2V$.

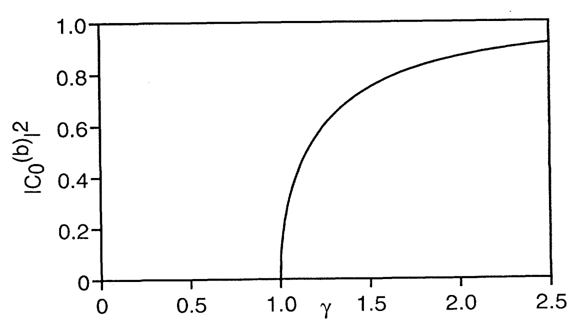

FIG. 2. One nonlinear impurity. Probability for finding the electron at the nonlinear impurity site, as a function of the nonlinearity parameter $\gamma \equiv \chi/2V$.

Figure 3 shows the transmission t versus $\cos(k)$ for $\gamma=1$; we also plot the transmission for the *linear* problem with $H_1=\epsilon|0\rangle\langle 0|$, for $\epsilon=1$.[9] We note that the nonlinear transmission is always larger than its linear counterpart but does not exhibit any additional features.

Finally, an examination of the density of states (DOS) shows that for $\gamma<1$ the DOS is not affected by the presence of the impurity (even though the transmittance decreases monotonically with increasing γ), while for $\gamma>1$, a discrete level is formed at the expense of the continuous spectrum, as expected.[5,9]

(b) *Two nonlinear impurities.* We specialize to the case of two nearest-neighboring impurities that form a dimer located at sites 0 and 1; the impurity "Hamiltonian" is $H_p=\gamma|C_0|^2|0\rangle\langle 0|+\gamma|C_1|^2|1\rangle\langle 1|$. This can be considered as the problem of one impurity in a chain, "perturbed" by an additional impurity. If $G^{(1)},G^{(2)}$ denote the Green's function for the one, two nonlinear impurity problem, respectively, using Eq. (5) we get for $G^{(2)}$

$$G_{mn}^{(2)}=G_{mn}^{(1)}+\frac{\gamma|C_1|^2G_{m1}^{(1)}G_{1n}^{(1)}}{1-\gamma|C_1|^2G_{11}^{(1)}} \tag{20}$$

with $G^{(1)}$ completely known from the previous calculations.

Bound states. Since for $\gamma<1$ $|C_0|^2=O(1/N)$ and $|C_1|^2=O(1/N)$ where N being the number of lattice sites, there cannot be a bound state. This can easily be seen by the fact that for $N\to\infty$, $G^{(2)}\to G^{(1)}\to G^{(0)}$. Therefore, for $|\gamma|<1$ there can be no bound state in a linear chain doped with a finite number of identical nonlinear impurities of the type considered here. The above observation can be also generalized to any finite number of *nonidentical nonlinear impurities,* provided $|\gamma_i|<1\forall i=1,\ldots,M$. For $\gamma>1$, on the other hand, we use Eqs. (5) and (11) and get

$$G_{mn}^{(1)}=(1/\sqrt{z^2-1})\left[1+\frac{\sqrt{\gamma^2-1}}{\sqrt{z^2-1}-\sqrt{\gamma^2-1}}\times[z-\sqrt{z^2-1}]^{2|n|}\right]. \tag{21}$$

As previously the bound state energies of our two-impurity problem are given by the poles of $G_{mn}^{(2)}$, i.e.,

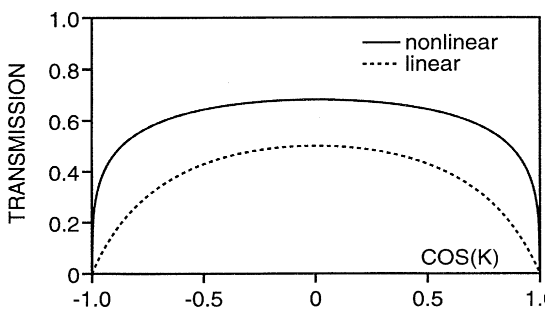

FIG. 3. One nonlinear impurity. Transmission coefficient t vs $\cos(k)$ (solid line) at $\gamma\equiv\chi/2V=1$. The dashed line represents the transmission coefficient for the linear impurity with $\epsilon=1$.

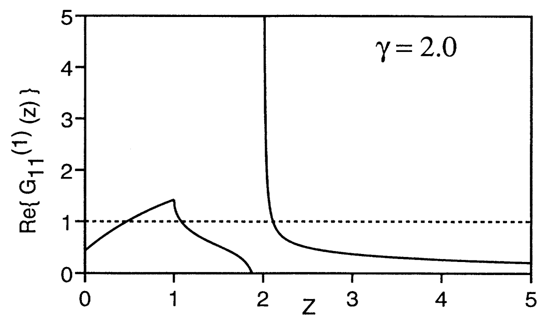

FIG. 4. Two nonlinear impurities. Solid line: Real part of $G_{11}^{(1)}(z)$ vs $z\equiv E/2V$, for the case $\gamma=2.0$. Dashed line: $1/\gamma|C_1|^2$, taken equal to 1 for definiteness. Intersection(s) of these two curves outside the band determine the energy(ies) of the bound state(s).

$$\gamma|C_1|^2G_{11}^{(1)}=1\ . \tag{22}$$

It is not possible to solve Eq. (22) for z in terms of $|C_1|^2$ in closed form. However, some general features can be deduced by examining a plot of the real part of $G_{11}^{(1)}(z)$

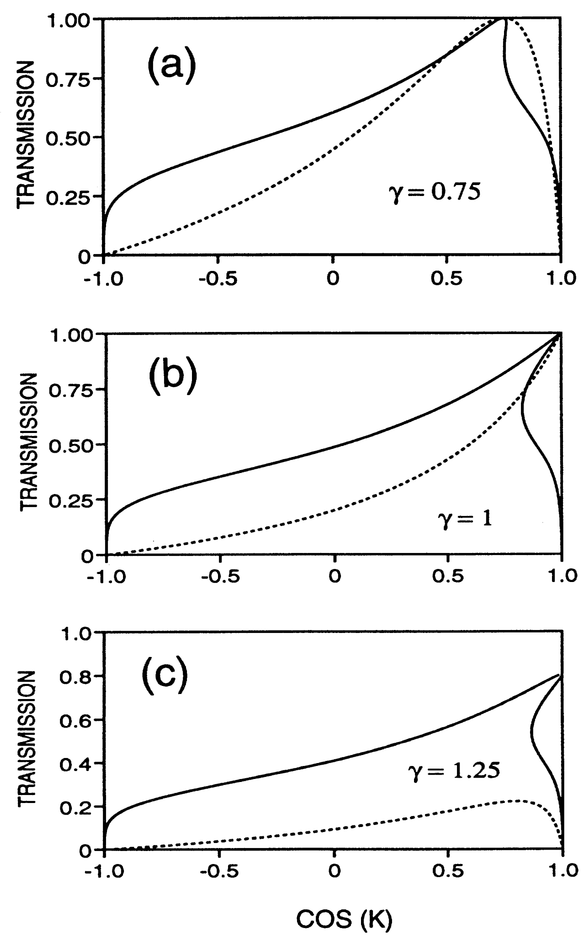

FIG. 5. Two nonlinear impurities. Transmission t vs $\cos(k)$ for (a) $\gamma=0.75$, (b) $\gamma=1$, and (c) $\gamma=1.25$ (solid lines). In each case the dashed line represents the transmission for the corresponding problem with two linear impurities.

(Fig. 4). For values of γ close to 1, we expect $|C_1|^2$ to be small and then, the line $1/\gamma|C_1|^2$ is located in the upper part of the plane in Fig. 4 and therefore there is only one intersection outside the band (i.e., there is a unique bound state). This intersection occurs at a z value slightly higher than the one in the one-impurity case, viz. the presence of the second impurity merely shifts the bound state energy. As the value of γ increases, $|C_1|^2$ increases as well and the line $1/\gamma|C_1|^2$ will shift to the lower part of Fig. 4. There will be a value of γ for which there will be a second intersection with $\text{Re}\{G_{11}^{(1)}(z)\}$ just outside the band ($z=1^+$) and thus a second bound state appears. The value of such critical γ_c will satisfy the condition $G_{11}^{(1)}(z\rightarrow 1)=1/\gamma_c|C_1|^2$, or [using Eq. (21)]:

$$2-\frac{1}{\sqrt{\gamma_c^2-1}}=\frac{1}{\gamma_c|C_1|^2} \ . \tag{23}$$

Since $|C_1|^2$ is unknown, a precise value of γ_c can only be obtained via a numerical calculation. A simple estimate may be obtained by assuming that $|C_1|^2$ has behavior similar to $|C_0|^2$ in the one-impurity problem. In the latter case we obtain $\gamma_c \sim \sqrt{13}/2 \sim 1.80$. Other simple estimates place γ_c slightly below or above this value. The important feature here is the existence of this second threshold value of nonlinearity beyond which two bound states can exist. This behavior is reminiscent of localization on a Bethe lattice (with connectivity 4) doped with two *linear* nearest-neighbor impurities.[9]

Transmission coefficient. The simplest way to obtain the transmission coefficient through the nonlinear dimer is by studying the scattering properties of plane waves sent towards it. The eigenvalue equation becomes in this case:

$$zC_n=(1/2)(C_{n+1}+C_{n-1}) +\delta_{n0}\gamma|C_0|^2C_0+\delta_{n1}\gamma|C_1|^2C_1 \ . \tag{24}$$

We set

$$C_n=\begin{cases} e^{ikn}+Re^{-ikn}\ , & n\le 0\ ,\\ Te^{ikn}\ , & n\ge 1 \end{cases} \tag{25}$$

with R, T representing the reflected and transmitted part of the wave, respectively. Inserting Eq. (25) into Eq. (24) we get after some tedious algebra the following nonlinear equation for the transmission coefficient $t\equiv|T|^2$:

$$t=\frac{4\sin^2(k)}{(b-a)^2+ab\,[ab-2(a+b)\cos(k)+4\cos^2(k)]+4\sin^2(k)}\ , \tag{26}$$

where $a=2\gamma t$ and $b=2\gamma t|1-2\gamma\exp(ik)|^2$. It can be seen from Eq. (26) that for $|\gamma|<1$ the wave vector with value $k_c=\arccos(\gamma)$ always leads to complete transmission, i.e., $t=1$. This type of resonant phenomenon is not dissimilar to the one observed in the context of plane wave scattering through a completely *linear* dimer leading to enhanced transport properties even in the presence of spatial randomness.[6] This makes doping with nonlinear impurities an attractive candidate method for fabricating quasi-one-dimensional materials with desired transport properties. In Fig. 5 we plot the transmission t as a function of $\cos(k)$ for different values of γ (solid line) and compare it with the linear case (dashed line). In the nonlinear case, t is significantly larger than that of the linear case, especially for values of $\gamma>1$. At about $\gamma\sim 0.75$, t begins to develop a window of bistability, whose width decreases as the nonlinearity parameter is increased. This bistability seems to be related to the multistability observed in periodically modulated one-dimensional nonlinear structures.[4]

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