Nonlinear impurity in a square lattice

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We use the Green's-function formalism for an exact, numerical calculation of the stationary states of an electron propagating in a square lattice in the presence of a single, Holstein-type, impurity of arbitrary nonlinearity exponent. We find that two bound states exist above a certain exponent-dependent critical nonlinearity strength. The localization length of the lower (higher) energy bound state increases (decreases) with nonlinearity strength. The dynamics of an electron, initially placed on the impurity site, reveals a sharp, self-trapping transition for any nonzero nonlinearity exponent: below a certain nonlinearity threshold, the electron escapes from the impurity site ballistically; above the threshold, there is partial trapping at the impurity site while the untrapped fraction escapes to infinity, also ballistically. The self-trapping features are sharper in time and space than for its one-dimensional analogue. [S0163-1829(99)07027-7]

The effects of nonlinear impurities on the electronic properties of solids is an old topic in solid-state physics, whose importance has not diminished throughout the years. As is well known,[1] in one and two dimensions, a linear impurity embedded in a lattice has always a bound state no matter how small the strength of the impurity. When the lattice contains a finite fraction of these (linear) impurities, distributed randomly, it gives rise to the interesting phenomenon of ''Anderson localization'' where all the eigenstates are localized, no matter how weak the disorder is. This, in turn, precludes any electronic transport.

Recently, attention has been given to the problem of *nonlinear* impurities. They appear in problems where strong electron-phonon interactions are considered. In that case, the lattice vibrations have the ability to adapt to the presence of the electron and give rise to polaronic effects. Under certain assumptions, the ''effective'' equation for the electronic amplitude turns into that of an electron moving inside a lattice that contains *nonlinear* impurities, i.e., where the local site energy at an impurity site depends on the electronic probability at that site. The electronic evolution equation, known as the discrete nonlinear Schrödinger (DNLS) equation has the form

$$i\frac{dC_{\mathbf{n}}}{dt}=V\sum_{n.n}C_{\mathbf{m}}-\chi_{\mathbf{n}}|C_{\mathbf{n}}|^{\alpha}C_{\mathbf{n}}, \tag{1}$$

where $\mathbf{n}$ is a site of a d-dimensional lattice, V is the transfer-matrix element, $\chi_{\mathbf{n}}$ is the nonlinearity parameter, and α is the nonlinearity exponent. The summation in Eq. (1) is restricted to nearest neighbors (nn) only. In the *conventional* DNLS case, $\alpha=2$ and χ is proportional to the square of the electron-phonon coupling at site $\mathbf{n}$ (Ref. 2). A previous study of Eq. (1) for the one-dimensional nonlinear random binary alloy,[3] revealed marked deviations from Anderson localization: it was found that the disorder is completely overcome by the presence of nonlinearity, leading to a partial trapping of an initially localized electron (for nonlinearity above a certain threshold) and a ballistic propagation of the untrapped fraction. The transmittance of plane waves through the medium displayed a *power-law decay* as a function of system size.

An interesting mathematical equivalence was found by Economou and coworkers[4] between the property that all states are localized in a disordered d-dimensional system (where $d\leqslant 2$) and the property that a potential well always traps a particle in d dimensions (also for $d\leqslant 2$). From this perspective, it is interesting to pursue the examination of various types of impurity problems since they might ultimately contain all the information needed to understand Anderson localization in several kind of disordered systems. For the case of a single nonlinear impurity, we have examined in previous works the one-dimensional case in detail. By using the Green's-function formalism in a self-consistent way, we obtained the stationary states analytically and obtained a phase diagram showing the number of bound states as a function of nonlinearity exponent and nonlinearity strength. We also examined the transmission of plane waves across the nonlinear impurity and the self-trapping dynamics of an electron (or excitation) initially located at the impurity site.[5–7]

In the present paper, we extend these previous studies to two dimensions and consider the stationary states and self-trapping dynamics of a nonlinear impurity embedded in a square lattice. A recent work considers the calculation of the bound states for this problem by using an approximate Green's-function approach.[8] We will pursue the bound state problem using the exact Green's functions and will solve the relevant equations numerically. Then, we will examine the self-trapping properties of the impurity by following the time evolution of an electron (or excitation) initially located on the nonlinear impurity.

Bound States. Let us consider the problem of determining the existence of bound states for an electron (or an excitation) moving on a square lattice that contains a single generalized nonlinear impurity at the origin $\mathbf{n}=\mathbf{0}$. The Hamiltonian is

$$\tilde{H}=\tilde{H}_0+\tilde{H}_1, \tag{2}$$

where

$$\tilde{H}_0 = V\sum_{n.n} (|\mathbf{n}\rangle\langle\mathbf{m}| + \text{h.c.}) \tag{3}$$

and

$$\tilde{H}_1 = \chi |C_{\mathbf{0}}|^{\alpha} |\mathbf{0}\rangle\langle\mathbf{0}|, \tag{4}$$

where the $\{|\mathbf{n}\rangle\}$ represent Wannier electronic states, V is the nearest-neighbor transfer-matrix element, and χ is the nonlinearity parameter. The $\{C_{\mathbf{n}}\}$ are the electronic probability amplitudes at site $\mathbf{n}$ and $\alpha > 0$ is the nonlinearity exponent. The sum in Eq. (3) is restricted to nearest neighbors only.

To get a preliminary feeling on our problem, let us consider a simple estimate of the existence of bound states around a single generalized nonlinear impurity of strength χ and exponent α embedded in a d-dimensional linear lattice, with lattice spacing a. If we assume an electronic bound state Ψ with localization length λ, then on normalization grounds we have $|\Psi|^2 \sim 1/\lambda^d$. Now, in order to have a bound state, the decrease in potential energy must overcome the increase in kinetic energy due to localization. The decrease of potential energy is, in magnitude

$$\Delta V = \int d^d r V(r) |\Psi(r)|^2 = \int d^d r \chi |\Psi(r)|^{\alpha} |\Psi(r)|^2 \sim \frac{\chi a^d}{\lambda^d [1 + (\alpha/2)]}. \tag{5}$$

While the increase in kinetic energy is

$$\Delta K \sim \frac{h^2}{2m\lambda^2}. \tag{6}$$

Potential energy dominates over kinetic energy if

$$\frac{h^2}{2m\chi a^d} \lambda^{d[1+(\alpha/2)]-2} < 1. \tag{7}$$

Now, if we let $\chi \to 0$, then we should have $\lambda \to \infty$. To be consistent with Eq. (7) we must have

$$d(2+\alpha) < 4. \tag{8}$$

For a two-dimensional lattice ($d=2$), Eq. (8) predicts that as soon as $\alpha > 0$, a minimum nonlinearity strength is needed to create a bound state. The borderline case $\alpha = 0$, i.e., the linear impurity, is well known and always displays a bound state.[1]

The above prediction will be confirmed indeed by the formal solution, based on lattice Green's Functions. For convenience, we normalize all energies to a half bandwidth, $4V$ and define: $z \equiv E/4V$, $H \equiv \tilde{H}/4V$, and $\gamma \equiv \chi/4V$. The dimensionless lattice Green's function $G = 1/(z - H)$ can be formally expanded as[1]

$$G = G^{(0)} + G^{(0)} H_1 G^{(0)} + G^{(0)} H_1 G^{(0)} H_1 G^{(0)} + \cdots, \tag{9}$$

where $G^{(0)}$ is the unperturbed ($\gamma = 0$) Green's function and $H_1 = \gamma |C_{\mathbf{0}}|^{\alpha} |\mathbf{0}\rangle\langle\mathbf{0}|$. The sum in Eq. (9) can be carried out exactly to yield

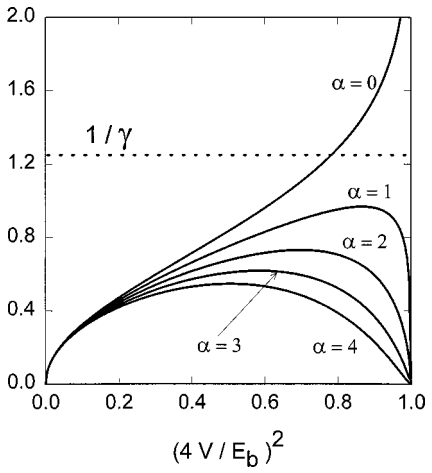

FIG. 1. Solid lines: Real part of the right-hand side of Eq. (13) $vz(4V/E_b)^2$, for different α values. Dashed line: $1/\gamma$. Intersection(s) of these two curves outside the band determine the energy(ies) of the bound state(s).

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

where $G_{\mathbf{mn}} = \langle \mathbf{m}|G|\mathbf{n}\rangle$. The energy of the bound state(s), z_b is obtained from the poles of $G_{\mathbf{mn}}$, i.e., by solving $1 = \gamma |C^{(b)}_{\mathbf{0}}|^{\alpha} G^{(0)}_{\mathbf{00}}$. The bound state amplitudes $C^{(b)}_{\mathbf{n}}$ are obtained from the residues of $G_{\mathbf{mn}}(z)$ at $z = z_b$. In particular,

$$|C^{(b)}_{\mathbf{0}}|^2 = \text{Res}\{G_{00}(z)\}_{z=z_b} = -\frac{G^{(0)2}_{\mathbf{00}}(z_b)}{G'^{(0)}_{\mathbf{00}}(z_b)}. \tag{11}$$

Inserting this in the bound state energy equation leads to

$$1 = \frac{\gamma G^{(0)\alpha+1}_{\mathbf{00}}(z_b)}{[-G'^{(0)}_{\mathbf{00}}(z_b)]^{\alpha/2}}. \tag{12}$$

Now, for the square lattice, $G^{(0)}_{\mathbf{00}}(z) = (2/\pi)\sqrt{m} K[m]$, where we have defined $m \equiv 1/z^2$ and $K[m]$ is the complete elliptic integral of the first kind $K[m] = \int_0^{\pi/2} [1 - m \sin^2(\phi)]^{-1/2} d\phi$. Inserting this into Eq. (12), and using $K'[m] = (1/2m)((1-m)^{-1} E[m] - K[m])$ where $E[m]$ is the complete elliptical integral of the second kind: $E[m] = \int_0^{\pi/2} [1 - m \sin^2(\phi)]^{1/2} d\phi$, we finally obtain the following nonlinear equation for the bound state energies

$$\frac{1}{\gamma} = \frac{\{(2/\pi)\sqrt{m} K[m]\}^{\alpha+1}}{\left\{(2/\pi)\left(\frac{m}{1-m}\right) E[m]\right\}^{\alpha/2}}. \tag{13}$$

Analysis of Eq. (13) reveals that, for $m \leqslant 1$ (i.e., outside the band), its right-hand side is real and positive. Figure 1 shows the shape of the right-hand side of Eq. (13) for several different α values. For a given $\alpha > 0$, there exists a critical nonlinearity threshold γ_c below which, there is no root (no bound state). At $\gamma = \gamma_c$ there is exactly one root (one bound state), while above threshold, $\gamma > \gamma_c$, there are two roots (two bound states). The value of γ_c increases with the nonlinear exponent, α. Figure 2 displays a phase diagram in nonlinearity strength—nonlinearity exponent space showing the critical curve above which two bound states exist, while

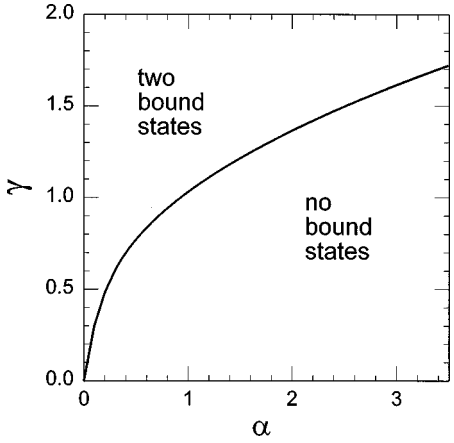

FIG. 2. Phase diagram showing the number of bound states as a function of the normalized nonlinearity parameter γ and the exponent α. The solid line is the critical line where only one bound state exists.

none (one) bound state exists below (on) the critical curve. For the conventional (DNLS) case where $\alpha=2$ the critical nonlinearity is $\gamma_c=1.366$, that is, $\chi_c/V=5.464$, substantially larger than for the one-dimensional case ($\chi_c/V=2$).[5] In Fig. 3, we show the normalized bound state energies as a function of normalized nonlinearity, for several values of the exponent, ranging from $\alpha=0$ (linear impurity) up to $\alpha=4$. By denoting the solution(s) of Eq. (13) by m_b, the bound state probability at the impurity site can be written as

$$|C_{\mathbf{0}}^{(b)}|^2=\left(\frac{2}{\pi}\right)\frac{(1-m_b)K[m_b]^2}{E[m_b]}. \tag{14}$$

The electronic probability at the impurity site for the bound state(s), as a function of nonlinearity, is shown in Fig. 4, for several exponent values. For a given nonzero exponent, as nonlinearity is increased beyond threshold value, one of the bound states ''shrinks'' quickly around the impurity site, while the other ''spreads'' increasing its localization length. This can be seen from the fact that in any dimension d, the bound state localization length λ for $|E_b|-ZV\ll ZV$, obeys:[4] $\lambda^{-1}\approx\sqrt{(|E_b|/V)-Z}$, where Z is the coordination number. In

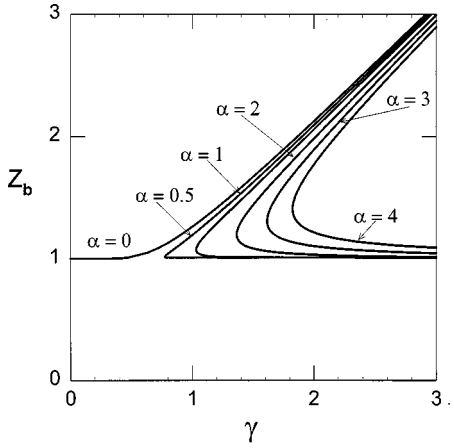

FIG. 3. Normalized bound state energy z_b as a function of the normalized nonlinearity parameter γ, for different values of the exponent α.

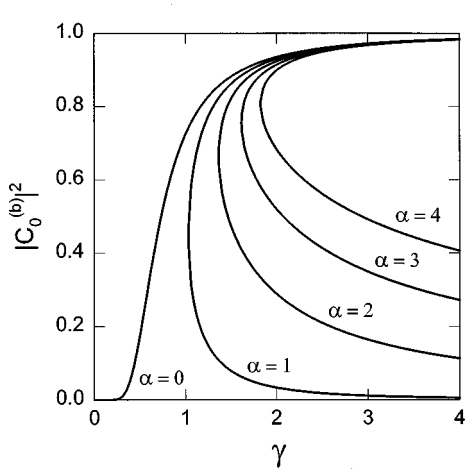

FIG. 4. Occupation probability of the nonlinear impurity site in the bound state(s) as a function of the normalized nonlinearity parameter γ for different exponents α.

our case this implies $\lambda^{-1}\approx\sqrt{|z_b|-1}$. A similar feature was also observed in the one-dimensional case.[6] We note, in passing, that Figs. 2 and 3 are very similar to the ones obtained if one uses a Hubbard-type Green's function.[8]

Self-trapping Dynamics. We place the electron at the impurity site at $t=0$ and observe its time evolution [Eq. (1)] for relatively long times. The numerical scheme is that of a fourth-order Runge-Kutta, where the accuracy is monitored through total probability conservation. To avoid undesired boundary effects, a self-expanding lattice is used.[3] To ascertain the presence or absence of a self-trapping transition, we compute the long-time average probability at the impurity site, defined by

$$P_{\mathbf{0}}=\lim_{T\to\infty}(1/T)\int_0^T|C_{\mathbf{0}}(t)|^2dt,\quad |C_{\mathbf{0}}(0)|=1. \tag{15}$$

To quantify the electronic propagation, we also examine the mean-square displacement

$$\langle\mathbf{n}^2\rangle=\sum_{\mathbf{n}}\mathbf{n}^2|C_{\mathbf{n}}(t)|^2, \tag{16}$$

where the normalization $\Sigma_{\mathbf{n}}|C_{\mathbf{n}}(t)|^2=1$ has been used. The increase in the coordination number with respect to the one-dimensional chain, makes the propagation time scale shorter: In the absence of any impurity, $\langle\mathbf{n}^2\rangle=4(Vt)^2$ whereas for one dimension, $\langle\mathbf{n}^2\rangle=2(Vt)^2$. The extra dimensionality also has the effect of making any nontrapped wave-packet decay faster in space (as $O(1/N)^2$). The square symmetry of this one-impurity problem reduces the computational demands considerably with respect to a case with say, many impurities randomly distributed.

Figure 5 shows P_0 versus the normalized nonlinearity parameter γ for several different nonlinearity exponents α. As soon as $\alpha>0$, we observe a self-trapping transition around a specific γ whose value (and the sharpness of the transition) increases with α. In particular, for the conventional DNLS case ($\alpha=2$), the transition occurs at approximately $\gamma\approx1.69$. This value is substantially higher than for the one-

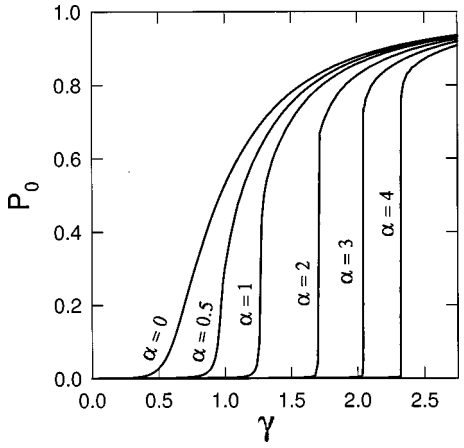

FIG. 5. Time-averaged probability at the nonlinear impurity site as a function of the normalized nonlinearity strength γ for different exponents α.

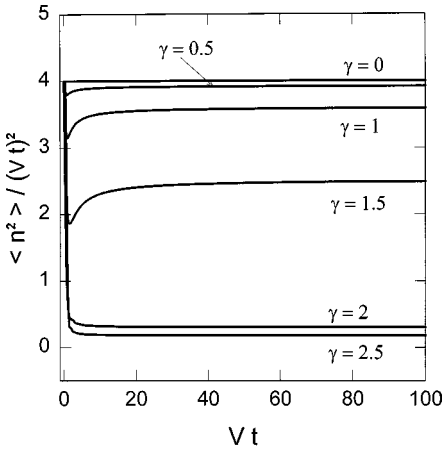

FIG. 7. Electronic mean square displacement as a function of time Vt for completely localized initial conditions and $\alpha=2$, and for several nonlinearity parameter values.

dimensional case ($\gamma\approx0.8$) and was first estimated using a different approach, by Dunlap, Kenkre, and Reineker.[9]

Figure 6 shows electronic probability snapshots for the conventional ($\alpha=2$) DNLS case for three different times and for two different nonlinearity parameter values. One corresponds to the linear impurity case ($\gamma=0$); the other to a nonlinear strength slightly larger than the critical one. In the first case, the probability profile spreads quickly away from the impurity site; in the second case, there is partial selftrapping at the impurity, while the untrapped fraction escapes away ballistically. This propagation feature is most prominent in Fig. 7, where we plot the electronic mean-square displacement as a function of time, for the conventional DNLS case and for several different nonlinearity parameter values. After a very short transient, the propagation approaches a ballistic behavior in all cases. The ''speed'' of the propagation gets substantially smaller past the nonlinearity threshold for selftrapping: the onset of trapping reduces the total probability wave that can escape to infinity. The trapped electronic fraction at the impurity site displays persistent oscillations (not shown), with amplitude (frequency) that decreases (increases) with nonlinearity strength. We associate this oscillations with the breather mode proved by Aubry and MacKay to exist in the large γ limit.[10]

Discussion. We have examined the problem of the bound states for a rather general nonlinear impurity embedded in a (linear) square lattice, by means of a straightforward generalization of the Green's-functions formalism. We found that a nonlinearity threshold exists beyond which, two bound states are possible. One of them increases its localization length upon increasing nonlinearity; the other decreases it. A quantum-mechanical argument shows that, for the nonlinear impurity, the marginal dimension for the existence of a bound state decreases with respect to the case of a *linear* impurity; in particular, for the conventional ($\alpha=2$) DNLS

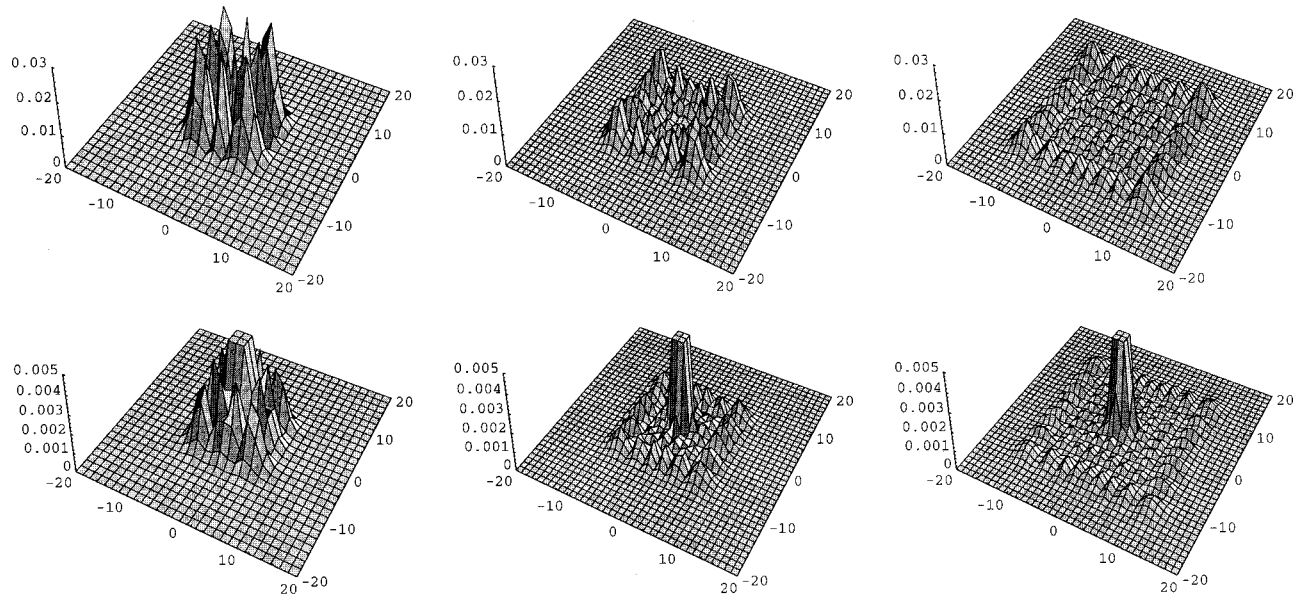

FIG. 6. Electronic probability density snapshots for an electron initially located on a single site (''site zero'') of a square lattice. Upper row: $\gamma=0$ (linear impurity). From left to right $Vt=2, 4$, and 6. Lower row: Same as before but for $\gamma=1.75$. The center peak, which has been truncated for visualization, extends up to a height of approximately 0.7.

impurity it is equal to one, whereas for the linear case the marginal dimension is equal to two. It would seem that the nonlinear character of the impurity has somehow produced a sort of ''dimensional reduction.'' If one were to apply the potential well analogy of Economou *et al*., it could be predicted that a two-dimensional nonlinear random binary alloy would not have all of its eigenstates localized. This is reinforced by the observation that one needs a minimum amount of nonlinearity to dynamically selftrap an initially localized electron around a nonlinear impurity. However, the usefulness of this is severely limited when it comes to predict the consequences for transport, given that, in the nonlinear system the eigenstates constitute just particular solutions and cannot be superposed to construct the time-dependent wave function.

The dynamics of an electron, initially localized on the impurity site, revealed the existence of an exponent-dependent self-trapping transition at a certain nonlinearity strength. The situation is qualitatively similar to the one-dimensional case, although the transition is, in general sharper and requires higher nonlinearity strength. This dynamical self-trapping transition has a higher threshold than that for the appearance of a bound(s) state(s), suggesting that the onset of a bound state is in a sense, a precursor for the onset of dynamical self-trapping. Unlike the case of a *linear* impurity though,[1] the exact connection between stationary and dynamical quantities is unknown due to the lack of the superposition principle, as noted above. After a short transient, the mean-square displacement assumes a ballistic form, with a ''speed'' that decreases significatively beyond the threshold for self-trapping. We expect these features to persist in the case of a two-dimensional nonlinear random binary alloy, where due to the increased dimensionality and on normalization grounds, one would expect nonlinear effects to be strictly local. The propagation of an initially localized excitation would be affected only by the local environment close to the initial site, with the rest of the impurities playing no role. They might affect though, the propagation of an extended excitation as they do in the one dimensional case.[3]

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