Universal features of self-trapping in nonlinear tight-binding lattices

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We use the discrete nonlinear Schrödinger (DNLS) equation to show that nonlinear tight-binding lattices of different geometries and dimensionalities display a universal self-trapping behavior. First, we consider the problem of a single nonlinear impurity embedded in various tight-binding lattices, and calculate the minimum nonlinearity strength to form a stationary bound state. For all lattices, we find that this critical nonlinearity parameter (scaled by the energy of the bound state), in terms of the nonlinearity exponent, falls inside a narrow band, which converges to $e^{1/2}$ asymptotically. Then, we examine the self-trapping dynamics of an excitation, initially localized on the impurity, and compute the critical nonlinearity parameter for abrupt dynamical self-trapping. For a given nonlinearity exponent, this critical parameter, properly scaled, is found to be nearly the same for all lattices. Same results are obtained when generalizing to completely nonlinear lattices, suggesting an underlying self-trapping universality behavior for all nonlinear (even disordered) tight-binding lattices described by DNLS.

The discrete nonlinear Schrödinger (DNLS) equation is a paradigmatic equation describing among others, dynamics of polarons in deformable media,[1] local modes in molecular systems[2] and power exchange among nonlinear coherent couplers in nonlinear optics.[3] Its most striking feature is the possibility of ''self-trapping'', that is, the clustering of vibrational energy or electronic probability or electromagnetic energy in a small region of space. In a condensed-matter context, the DNLS equation has the form

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

where $C_{\mathbf{n}}$ is the probability amplitude for finding the electron (or excitation) on site $\mathbf{n}$ of a d-dimensional lattice, $\epsilon_{\mathbf{n}}$ is the on-site energy, V is the transfer matrix element, $\chi_{\mathbf{n}}$ is the nonlinearity parameter at site $\mathbf{n}$ and α is the nonlinearity exponent. The prime in the sum in (1) restricts the summation to nearest-neighbors only.

Considerable work has been carried out in recent years to understand the stationary and dynamical properties of Eq. (1) in various cases. In particular, we point out the studies on the stability of the stationary solutions in one and two dimensions for the homogeneous case ($\epsilon_{\mathbf{n}}=0$, $\chi_{\mathbf{n}}=\chi$),[4,5] the effect of point linear impurities on the stability of the two-dimensional (2D) DNLS solitons,[6] the effects of nonlinear disorder ($\epsilon_{\mathbf{n}}=0$, $\chi_{\mathbf{n}}$ random)[7] and of linear disorder ($\chi_{\mathbf{n}}=\chi$, $\epsilon_{\mathbf{n}}$ random)[8] on the self-trapping dynamics of initially localized and extended excitations in a chain. The results of these studies suggest that in general, the effect of nonlinearity is quite *local* for initially localized excitations, and that disorder leaves the narrow self-trapped excitations unaffected, although it does affect the propagation of the untrapped portion (''radiation''). This suggests that the solution of the single nonlinear impurity problem might contain the essentials required to understand self-trapping in more general contexts. In that spirit, we have previously examined the problem of a single nonlinear impurity embedded in a linear chain and a linear square lattice.[9,10] In this work we extend these studies and show that, for an initially localized excitation, the dynamics of self-trapping in various different lattices of different dimensionalities, is universal and depends mainly on the nonlinearity strength at the initial site, the nonlinearity exponent and the coordination number.

Some symmetry considerations are useful at this point: The transformation $(\epsilon_{\mathbf{n}},V,\chi_{\mathbf{n}})\rightarrow(-\epsilon_{\mathbf{n}},-V,-\chi_{\mathbf{n}})$ turns Eq. (1) into an equation for the complex conjugate variable $C_{\mathbf{n}}^{*}$ and as a result, the site probability $|C_{\mathbf{n}}|^2$ remains invariant (provided the initial conditions are also transformed). Since we will be dealing with homogeneous lattices with a single impurity or completely nonlinear, we set $\epsilon_{\mathbf{n}}=0$ hereafter. Thus for a complete parameter study it is sufficient to take $\chi>0$ and consider the two possible signs of V. A further simplification is possible however, since Eq. (1) is also invariant under the change $(V,\chi,C_{\mathbf{n}})\rightarrow(-V,\chi,\Pi_i(-1)^{n_i}C_{\mathbf{n}})$, where $\mathbf{n}=(n_1,n_2,\ldots)$ for all the lattices considered in this work, with the exception of the triangular lattice. Thus, this case excepted, we can consider both $\chi_{\mathbf{n}}$ and V in Eq. (1) as positive.

Bound states. A tight correlation has been observed between the existence of bound states for a given nonlinear lattice and the ability of the lattice to self-trap an initially completely-localized excitation: the critical nonlinearity strength for dynamical self-trapping is always greater than the one needed to produce bound state(s). We begin by showing that the minimum nonlinearity needed to produce a bound state in different lattices, shows universal features. We consider the problem of determining the bound state for an electron in a d-dimensional homogeneous ($\epsilon_{\mathbf{n}}=0$) lattice that contains a single generalized nonlinear impurity at the origin $\mathbf{n}=\mathbf{0}$. We use a straightforward generalization of a Green's function formalism used previously by one of the authors (M.I.M.) in one-dimensional chains[9] and the square lattice.[10] With a scaled nonlinearity $\gamma=\chi/B$ and energy $z=E/B$, where B is the half bandwidth, the energy of the bound state(s) z_b is obtained from

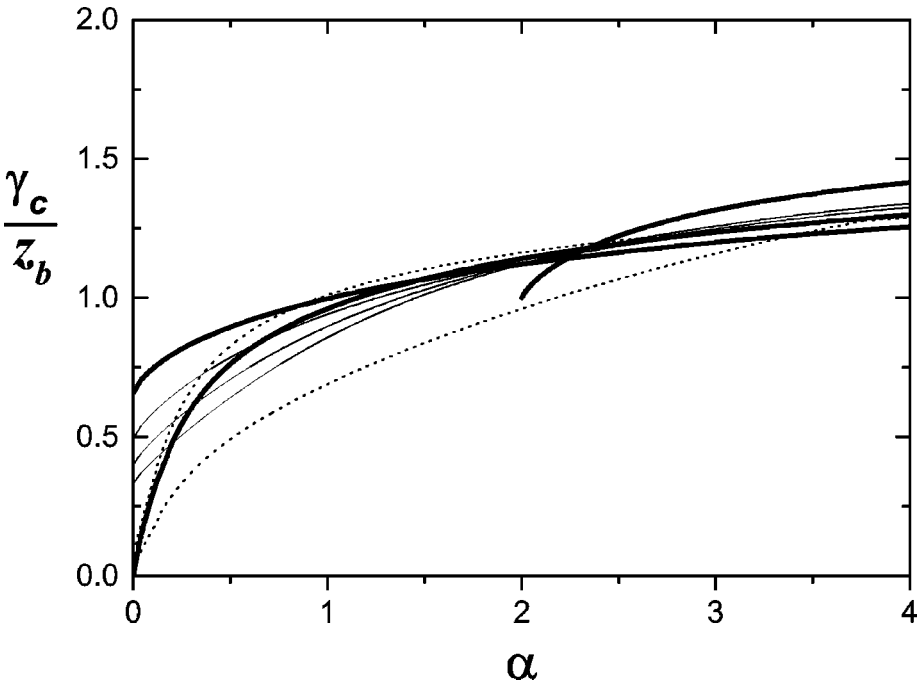

FIG. 1. Minimum nonlinearity γ_c/z_b to form a bound state in several lattices, containing a single nonlinear impurity. Thick lines correspond to 1D, square and simple cubic lattices. Thin lines correspond to Bethe lattices with $K=3$, 5 and 100 in ascendent order near $\alpha=0$. Dotted lines represent the triangular lattice cases: $\chi/V>0$ (upper line) and $\chi/V<0$ (lower line).

$$1=\frac{\gamma G_{\mathbf{00}}^{(0)^{\alpha+1}}(z_b)}{[-G_{\mathbf{00}}^{\prime(0)}(z_b)]^{\alpha/2}}, \tag{2}$$

where $G_{\mathbf{00}}^{(0)}=\langle \mathbf{0}|G^{(0)}|\mathbf{0}\rangle$ is a matrix element of the Green's function for the crystalline lattice (without impurity). We proceed to solve (2) numerically, using the exact, known expressions for $G_{\mathbf{00}}^{(0)}$ for several lattices:[11,12] one-dimensional (1D), square, triangular, simple cubic and Bethe lattices with connectivities 3, 5 and 100. This allows us to compare lattices with different dimensionality, coordination number Z, length of shortest loops, etc. In general, for a given α value there will be a minimum value of χ below (above) which, there is (are) no (two) bound state(s). Just at the critical nonlinearity value, we obtain exactly one bound state. The exception is the 1D lattice where for $\alpha\leqslant 2$ one has always one bound state regardless of χ.

Figure 1 shows the critical nonlinearity parameter γ_c, scaled by the energy of the bound state, in terms of α, the nonlinearity exponent, for all the lattices examined. There are two curves for the triangular lattice, depending on sgn(χ/V), due to the asymmetry of its Green function with respect to the energy variable. All curves fall inside a ''band'' which narrows as α increases, converging towards a constant value. To calculate it, we solve (2) exactly in two cases: the one-dimensional lattice[9] and the Bethe lattice in the limit of infinite connectivity (Hubbard model; practically indistinguishable from $K=100$). In both cases we obtain:

$$\lim_{\alpha\to\infty}\left(\frac{\gamma_c}{z_b}\right)=e^{1/2}\sim 1.65. \tag{3}$$

We have traced the validity of (3) for the other lattices up to high α values (10^3 for the square and cubic lattices; 10^5 for the rest) with no discernible deviation.

Self-trapping Dynamics. We now examine the ability of a given lattice to dynamically self-trap an excitation, originally placed completely on the impurity site, by computing the minimum nonlinearity needed to give rise to abrupt self-trapping. The time evolution is given by Eq. (1) with $\epsilon_{\mathbf{n}}=0$ and $\chi_{\mathbf{n}}=\chi\delta_{\mathbf{n},\mathbf{0}}$. Following an earlier treatment,[10] we compute the long-time average probability at the impurity site, defined by

$$P_{\mathbf{0}}=\lim_{T\to\infty}(1/T)\int_{\mathbf{0}}^{T}|C_{\mathbf{0}}(t)|^2dt, \quad |C_{\mathbf{0}}(0)|=1. \tag{4}$$

Typically, $P_{\mathbf{0}}$ vanishes for nonlinearity parameters below a critical value χ_c and the particle escapes from the impurity site in a ballistic manner. This is determined from an examination of the excitation's mean square displacement $\langle u(t)\rangle=\Sigma_{\mathbf{n}}\mathbf{n}^2|C_{\mathbf{n}}|^2$. For nonlinearity values greater than χ_c, $P_{\mathbf{0}}$ remains finite and increases with χ, converging towards unity at large χ. The untrapped portion escapes to infinity, also in a ballistic manner, but with a much lower ''speed'' $\sqrt{\langle u(t)\rangle}/Vt$. Thus, the examination of P_0 provide us with the critical nonlinearity parameter χ_c for dynamical self-trapping.

For a particular lattice and a given exponent α, we numerically determine χ_c, scaled by $E_{\min}^{(b)}$, the minimum unnormalized bound-state energy. Figure 2 shows $\chi_c^{(dyn)}/E_{\min}^{(b)}$ for all the lattices examined, and for several α values that give rise to sharp self-trapping (for $\alpha<1$, the self-trapping is not sharp). We see that, for the wide range of geometries and dimensionalities involved, this critical (dynamical) nonlinearity is nearly independent of the lattice and increases monotonically with the nonlinearity exponent. The left panel in Table I shows the ratio between this 'dynamical' critical parameter $\chi_c^{(dyn)}$ and the previously computed critical value needed to form a bound state, $\chi_c^{(b)}$, for several different exponents α. A quick and 'dirty' estimate for $\chi_c^{(dyn)}$ can be obtained as follows: From the analytical expression for $\chi_c^{(dyn)}$ in 1D and Hubbard model for the stationary impurity problem we can see that asymptotically, $\chi_c^{(dyn)}\sim B\sqrt{\alpha}$, where B is the half bandwidth. Table I central panel, shows that the quick estimation of $\chi_c^{(dyn)}$ as $B\sqrt{\alpha}$, is not bad at all,

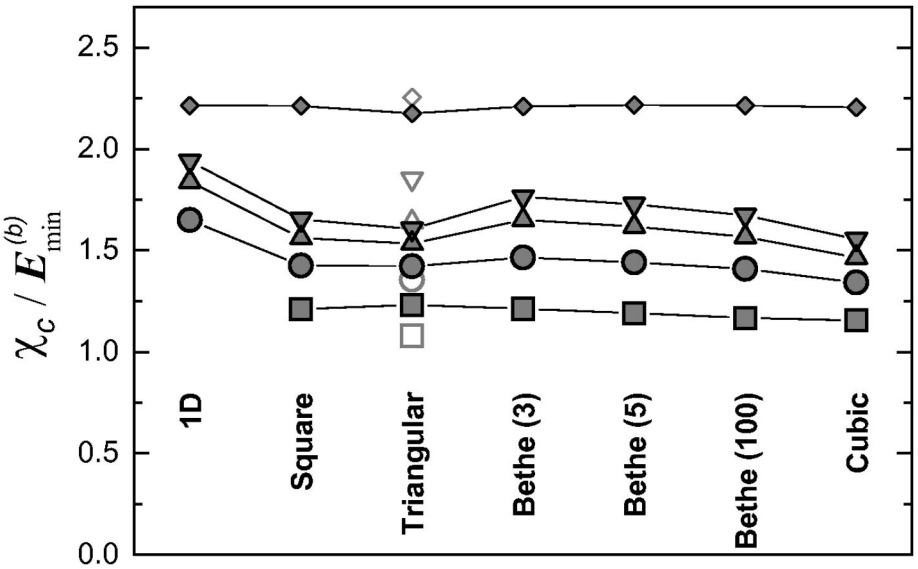

FIG. 2. Dynamical critical nonlinearity parameter χ_c scaled by the minimum bound-state energy $E_{\min}^{(b)}$ for one nonlinear impurity in various lattices. The values for the nonlinearity exponents are $\alpha=1$, 2, 3, 4 and 1000 from bottom to top. The hollow symbols for the triangular lattice case correspond to the case $\chi/V<0$.

and can be used as a good lower bound in all cases. It would seem that in the α regime where abrupt self-trapping takes place ($\alpha \geqslant 1$), the only relevant parameters are the nonlinearity at the impurity site and the coordination number of the lattice. The rest of the topological features is of secondary importance. In all cases, with the exception of the triangular lattice, the critical nonlinearity is independent of the sign of χ.

The increase of $\chi_c^{(dyn)}$ with α is to be expected since in the continuum limit, increasing α is equivalent to increasing the dimensionality of the system,[4,13,14] this in turn increases the effective coordination number making it harder to self-trap the excitation. Hence, the need for larger nonlinearities. Also, we notice that for all lattices, the values of $\chi_c^{(dyn)}$ are all higher than $\chi_c^{(b)}$ (see Table I), confirming the conjecture that the onset of the stationary bound state is a precursor for dynamical self-trapping. However, the lack of a superposition principle, makes it hard to establish formally the (observed) connection between the dynamical and stationary DNLS problem.

We now recompute all of the above calculations, this time using completely nonlinear lattices ($\epsilon_{\mathbf{n}}=0$, $\chi_{\mathbf{n}}=\chi$) and same initial conditions ($C_{\mathbf{n}}=\delta_{\mathbf{n},\mathbf{0}}$). The right panel in Table I shows the critical nonlinearity strength ratio between the completely nonlinear lattice and the linear lattice with a single nonlinear impurity. The critical values are virtually the same in both cases, except when the self-trapping is not abrupt and therefore χ_c is not so precisely defined. This similarity is due to the fact that, once the abrupt self-trapping is set, most of the probability is on the initial site, which gives, by conservation of the norm, very small probability amplitudes for the rest of the lattice sites, making their nonlinear contribution negligible: they have become, in fact, linear for all self-trapping purposes and, in this way we are back to the single nonlinear impurity results. The same argument would also be valid for a disordered lattice. The greater the α value, the closer the system is to the nonlinear impurity case. This is vividly illustrated by the limiting values in the right panel of Table I for large α, where the critical nonlinear parameter is the same for both cases. A similar situation could be found

TABLE I. Left panel: Ratio between the critical nonlinearity parameter for dynamical self-trapping $\chi_c^{(dyn)}$ and the minimum nonlinearity value to form a bound state $\chi_c^{(b)}$. Central panel: Ratio between $\chi_c^{(dyn)}$ and the rough estimate $B\sqrt{\alpha}$. (For the triangular lattice we use $B=3$ for $\chi/V>0$; otherwise, $B=6$.) Right panel: Ratio between $\chi_c^{(dyn)}$ for the completely nonlinear lattice and the linear lattice with a single nonlinear impurity. Each column correspond to a different value for the nonlinearity exponent, $\alpha=1$, 2, 3, 4 and 1000. Values in brackets denote cases where the self-trapping is not abrupt and are therefore, approximate.

	$\chi_c^{(dyn)}/\chi_c^{(b)}$					$\chi_c^{(dyn)}/B\sqrt{\alpha}$				$\chi_c(\mathrm{NL})/\chi_c(\mathrm{imp})$				
Lattice	1	2	3	4	1000	1	2	3	4	1	2	3	4	1000
1D	-	1.65	1.40	1.37	1.34	(1.25)	1.17	1.30	1.37	(1.52)	(1.3)	1.08	1.02	1.00
Square	1.26	1.25	1.26	1.27	1.34	1.30	1.21	1.18	1.16	(0.98)	1.05	1.01	1.00	1.00
Simple cubic	1.16	1.20	1.22	1.24	1.34	1.24	1.09	1.03	1.00	(1.15)	1.02	1.00	1.00	1.00
Triang.														
$\chi/V>0$	1.32	1.39	1.41	1.42	1.35	1.12	1.06	1.12	1.18	(1.07)	1.04	1.00	1.00	1.00
$\chi/V<0$	1.22	1.22	1.24	1.25	1.34	1.34	1.22	1.17	1.14	(1.25)	1.04	1.01	1.00	1.00
Bethe														
$K=3$	1.41	1.31	1.31	1.32	1.34	1.26	1.19	1.21	1.22	(1.26)	1.06	1.01	1.00	1.00
$K=5$	1.33	1.28	1.30	1.3	1.35	1.25	1.17	1.18	1.18	(1.16)	1.03	1.01	1.00	1.00
$K=100$	1.24	1.25	1.27	1.28	1.34	1.24	1.15	1.13	1.12	(0.99)	1.00	1.00	1.00	1.00

in ''related'' models like Holstein's quantum molecular-crystal model, where the interaction is also on-site and proportional to the probability amplitude on this site. In this case the condition for small polaron formation (self-trapping line), effective mass, electron-phonon correlations and other polaron properties could display universal features like the ones found here for DNLS.[15] For instance, the electron-phonon coupling needed to get a small polaron is practically the same for a very short chain (two sites) and for longer chains (32 sites).[16] The localized solutions we have found resemble the intrinsic localized modes or ''breathers'' that are known to exist in systems of coupled anharmonic oscillators[17] and seem to exhibit the same kind of ''universal'' or dimension-independent features.[18] These phenomena could have a common origin, in light of Aubry's anti-integrable limit concept.[19] The fact that we are able to obtain them through the use of an impurity formalism, suggests that a suitable generalization of the Green's function concept applied to nonlinear systems is indeed relevant. When nonlinear or linear disorder is added into the picture, one could speculate that its effects are likely to be of significance only for the untrapped portion of the excitation. Results in that direction have already been observed for one-dimensional chains (see work by one of the authors in Ref. 8).

In summary, we have shown that it is possible to characterize the self-trapping properties of DNLS lattices of different geometries and dimensionalities, in terms of a single parameter, namely the minimum bound-state energy for the one-impurity problem (or the product $B\sqrt{\alpha}$ for quick estimations). Roughly speaking, it is possible to keep an excitation localized (self-trapped) when the nonlinearity parameter χ is larger than this bound-state energy. This characterization is satisfactory for the nonlinear impurity problem and for completely nonlinear systems and could also be valid for the case of disordered nonlinear lattices.

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