Universal Selftrapping in Nonlinear Tight-binding Lattices

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We show that nonlinear tight-binding lattices of different geometries and dimensionalities, display an universal selftrapping behavior. First, we consider the single nonlinear impurity problem in various tight-binding lattices, and use the Green’s function formalism for an exact calculation of 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 $e^{1/2}$ at large exponent values. Then, we use the Discrete Nonlinear Schrödinger (DNLS) equation to examine the selftrapping dynamics of a single excitation, initially localized on the single nonlinear site, and compute the critical nonlinearity parameter for abrupt dynamical selftrapping. For a given nonlinearity exponent, this critical nonlinearity, 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 selftrapping 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, local modes in molecular systems, and power exchange among nonlinear coherent couplers in nonlinear optics. Its most striking feature is the possibility of “selftrapping”, 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

$$i \frac{d C_n}{dt} = \epsilon_n C_n + V \sum_m C_m - \chi_n |C_n|^\alpha C_n \quad (1)$$

where $C_n$ is the probability amplitude of finding the electron (or excitation) on site $n$ of a $d$-dimensional lattice, $\epsilon_n$ is the on-site energy, $V$ is the transfer matrix element, $\chi_n$ is the nonlinearity parameter at site $n$ and $\alpha$ is the nonlinearity exponent. The prime in the sum in (1) restricts the summation to nearest–neighbors only. In the conventional DNLS case, $\alpha = 2$ and $\chi_n$ is proportional to the square of the electron–phonon coupling at site $n$.

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 ($\epsilon_n = 0, \chi_n = \chi$) and the effects of point linear impurities on the stability of the 2-D DNLS solitons. We also point out the effects of nonlinear disorder ($\epsilon_n = 0, \chi_n$ random) and of linear disorder ($\chi_n = \chi, \epsilon_n$ random) on the selftrapping dynamics of initially localized and extended excitations in a chain. The results obtained in these studies suggest that, in general, the effect of nonlinearity is quite local for initially localized excitations, and that disorder leaves the narrow selftrapped excitations unaffected, although it does affect the propagation of the untrapped portion (“radiation”). In this Letter we show that, for an initially localized excitation, the dynamics of selftrapping 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, and much more weakly on other topological features of the lattice.

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 selftrap an initially completely–localized excitation: the critical nonlinearity strength for dynamical selftrapping 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 lattice that contains a single generalized nonlinear impurity at the origin $n = 0$. The Hamiltonian is $H = H_0 + H_1$, where $H_0 = V \sum_{n,m} |\langle n|m\rangle + \text{h.c.} |$ is the unperturbed tight–binding Hamiltonian with hopping constant $V$ and $H_1 = \chi |C_0|^\alpha |0\rangle\langle 0|$ corresponds to the nonlinear impurity perturbation. The $\{|n\}\rangle$ represent Wannier electronic states, and we have set $\epsilon_0 = 0$. For convenience we normalize all energies to a half bandwidth, $B$ and define: $z \equiv E/B$, $H \equiv H_0/B$ and $\gamma \equiv \chi/B$. The dimensionless lattice Green function $G = 1/(z - H)$ can be formally expanded as $G = G^{(0)} + G^{(0)} H_1 G^{(0)} + G^{(0)} H_1 G^{(0)} H_1 G^{(0)} + \ldots$, where $G^{(0)}$ is the unperturbed ($\gamma = 0$) Green function and $H_1 = \gamma |C_0|^\alpha |0\rangle\langle 0|$. The sum can be carried out exactly to yield

$$G_{mn} = G_{mm}^{(0)} + \frac{\gamma |C_0|^\alpha G_{m0}^{(0)} C_{0n}^{(0)}}{1 - \gamma |C_0|^\alpha G_{00}^{(0)}} \quad (2)$$
where $G_{mn} = \langle m | G | n \rangle$. The energy of the bound state(s), $z_b$ is obtained from the poles of $G_{mn}$, i.e., by solving $1 = \gamma |G^{(b)}_{0}|^2 G^{(0)}_{0}$. The bound state amplitudes $C_n^{(b)}$ are obtained from the residues of $G_{mn}(z)$ at $z = z_b$. In particular, $|C_0^{(b)}|^2 = \text{Res}\{G_{00}(z)\}_{z=z_b} = -G^{(0)}_{00}(z_b)/G^{(00)}_{00}(z_b)$. Inserting this into the bound state energy equation leads to

$$1 = \frac{\gamma G^{(0)}_{00} + 1}{-G^{(00)}_{00}(z_b)} |G^{(0)}_{00}(z_b)|^{1/2}. \quad (3)$$

We proceed to solve (3) numerically, using the exact, known expressions for $G^{(0)}_{00}$ for several lattices: one-dimensional (1-D), 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 $\alpha$ value there will be a minimum value of $\chi$ 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 1-D lattice where one needs in addition, $\alpha \geq 2$.\[22\]

![FIG. 1: The critical nonlinear parameter, $\gamma_c/z_b$, for Bound States. Thick lines correspond to Cubic, Square and 1D cases. Thin lines correspond to Bethe lattices with $K = 3, 5$ and 100 in ascending order near $\alpha = 0$. Dotted lines represent the Triangular cases: $\text{sgn}(\chi/V) > 0$ (upper line) and $\text{sgn}(\chi/V) < 0$](image)

Figure 1 shows the critical nonlinearity parameter $\gamma_c$, scaled by the energy of the bound state, in terms of $\alpha$, the nonlinearity exponent, for all the lattices examined. These curves are independent of $\text{sgn}(\chi/V)$, except for the triangular lattice, due to the asymmetry of its Green function with respect to the energy variable. In this case there are two curves depending on $\text{sgn}(\chi/V)$. All curves in Fig.1 fall inside a “band” which narrows as $\alpha$ increases, converging towards a constant value. To calculate it, we solve (3) exactly in two cases: the one-dimensional lattice\[12\] and the Bethe lattice in the limit of infinite connectivity (numerically indistinguishable from $K = 100$). In both cases we obtain:

$$\lim_{\alpha \to \infty} \left( \frac{\gamma_c}{z_b} \right) = e^{1/2} \sim 1.65. \quad (4)$$

We have traced the validity of (4) for the other lattices and the Bethe lattice in the one-dimensional lattice\[12\] and the Bethe lattice in the limit of infinite connectivity (numerically indistinguishable from $K = 100$). In both cases we obtain:

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Selftrapping Dynamics. We now examine the ability of a given lattice to dynamically selftrap an excitation, originally placed completely on the impurity site, by computing the minimum nonlinearity needed to give rise to abrupt selftrapping. The time evolution is given by Eq. (4) with $\gamma_0 = 0$ and $\chi_0 = \chi \delta_{n,0}$. 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\[8\]. To ascertain the presence or absence of a sharp selftrapping transition, we compute the long-time average probability at the impurity site, defined by

$$P_0 = \lim_{T \to \infty} \frac{(1/T) \int_0^T |C_0(t)|^2 dt}{|C_0(0)|} = 1. \quad (5)$$

Typically, $P_0$ vanishes for nonlinearity parameters below a critical value $\chi_c$ 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 $\left\langle u(t) \right\rangle = \sum_n n^2 |C_n|^2$. For nonlinearity values greater than $\chi_c$, $P_0$ remains finite and increases with $\chi$, converging towards unity at large $\chi$. The untrapped portion escapes to infinity, also in a ballistic manner, but with a much lower “speed” $\sqrt{\left\langle u(t)^2 \right\rangle}/Vt$. Thus, from the examination of $P_0$ we determine the critical nonlinearity parameter $\chi_c$ for dynamical selftrapping (usually for $P_0 \approx 1/2$).

For a particular lattice and a given exponent $\alpha$, we numerically determine the critical nonlinearity parameter $\chi_c$, scaled by $E_b$ (where $E_b$ is the unnormalized bound state energy corresponding to this $\chi_c$) for abrupt selftrapping. Figure 2 shows $\chi_c/E_b$ for all the lattices examined, and for several $\alpha$ values that give rise to sharp selftrapping (for $\alpha < 1$, the selftrapping 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. This is specially true in the all–important conventional DNLS case ($\alpha = 2$). It would seem that, in the $\alpha$ regime where abrupt selftrapping takes place ($\alpha \geq 1$), 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 $\chi/V$. For the triangular lattice we note that $\chi_c/E_b$ gets shifted a bit upon changing the sign of $\chi/V$. This probably trails back to the asymmetry of the unperturbed triangular lattice’s Green function $G^{(0)}_{00}$ under a sign change of its argument. All the rest of the lattices are symmetric in that respect. The increase of $\chi_c$ with $\alpha$ is to be expected since, in the continuum limit, increasing $\alpha$ is equivalent to increasing the dimensionality of the system; this in turns increases the effective coordination number making it harder to selftrap the excitation; hence, the need for larger nonlinearities. Also, the obtained values of $\chi_c$ in the dynamical case are all higher than for the bound state case, confirming the conjecture that the onset of the stationary bound state is a precursor for dynamical selftrapping. However, the lack of a superposition principle, makes it hard to establish formally the (observed) connection between the dynamical and the stationary DNLS problem. An alternative normalization for $\chi_c$ is to use the half bandwidth $B$ instead of $E_b$. In that case, all the curves in figure 2 lose a bit of flatness, but the tendency is otherwise unaltered.

We now recompute all of the above selftrapping dynamics calculations, this time using completely nonlinear lattices ($\epsilon_n = 0$, $\chi_n = \chi$) and same initial conditions ($C_n = \delta_{n,0}$).

Figure 3 shows the results obtained for the critical nonlinearities. The curves are virtually the same as the ones in Fig. 2. (The case $\alpha = 1$ does not display abrupt selftrapping like the rest, thus $\chi_c$ is not precisely defined here). This is due to the fact that, once the abrupt selftrapping is set, most of the probability is on the initial site, which gives, by conservation of probability, very small probability amplitudes for the rest of the lattice sites, making their nonlinear contribution negligible: they have become, in fact, linear for all selftrapping purposes and, in this way we are back to the single nonlinear impurity results. The greater the $\alpha$ value, the closer the system to the nonlinear impurity case. This is vividly illustrated by the limiting curves for large $\alpha$ in Figs. 2 and 3., which coincide.

This characterization of the selftrapping properties of nonlinear tight–binding lattices of different geometries and dimensionalities, in terms of a single parameter, namely the bound state energy for the one–impurity problem (or the half bandwidth $B$ for quick estimations), could be useful in several areas, given the paradigmatic character of DNLS.

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