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The Self Trapping Transition in the two dimensional system with nonlinear impurities

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Abstract : The Self–trapping transition(STT) of the quasiparticle in the two–dimensional square lattice is studied within the frame work of the discrete nonlinear Schrödinger equation. The STT shows a strong dependence on the escape probability of quasiparticle. Furthermore, near the STT the dynamics is mostly confined to a few neighbors. Reasons are discussed.

Keywords: Discrete Nonlinear SchrodingerEquation, Self–trapping transition.
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1 Introduction

The dynamics of quasiparticles such as electrons or excitons in solids are in general influenced by lattice vibrations. Different methods are used to study the effects of the lattice strongly interacting with the moving quasiparticle. One recent approach in this field formulates this problem within the framework of the discrete nonLinear Schrödinger equation(DNLSE) [1-4]. A widely used form of the DNLSE in d–dimensional Bravais lattices is

$$\frac{i dC_{\underline{n}}}{dt} = (\epsilon_{\underline{n}} + \chi_{\underline{n}} \mid C_{\underline{n}} \mid^2) C_{\underline{n}} + \sum_{\alpha} C_{\underline{n}+1_\alpha} \tag{1}$$

where $\underline{n}=(n_1, n_2, n_3, \ldots\ldots, n_d)^T$ and $1_\alpha = (0_1, 0_2, 0_3 \ldots\ldots\ldots \pm 1_\alpha \ldots\ldots 0_d)$. The summation over α in (1) considers only the nearest neighbors, although the hopping between any two sites can be included. All hopping matrix elements are taken to be same and the value has been set to unity without any loss of generality. $C_{\underline{n}}$ is the probability amplitude of the $\underline{n}$th site at a time t . $\epsilon_{\underline{n}}$ and $\chi_{\underline{n}}$ are respectively the site energy and the nonlinearity parameter associated with $\underline{n}$th site.

To obtain the linear dependence of the site–energy on the on–site probability two assumptions are invoked, namely, (i) the motion of the quasiparticle is coupled directly and linearly to the optical modes and (ii) the adiabatic approximation can be used for the lattice dynamics. Certain interesting cases of the above DNLSE have been solved analytically. The most important of them is, of course, the nonlinear dimer. It can be used as a model for hopping of protons to trapped oxygen–sites in metals like niobium. For the symmetric nonlinear dimer, a self–trapping transition(STT) has been obtained for $\chi = 4$ [5]. By the STT we imply that the quasiparticle over a sufficiently long time is preferentially found at one of the sites. The absorption of light energy by photosynthetic units has also been modeled by asymmetric nonlinear dimer [6].

The dynamics of quasiparticles in nonlinear lattices has also been studied. For example, a single nonlinear impurity in one to three dimensional Bravais lattices is found to produce a STT of the quasiparticle. The sharpness in the transition and the critical value of χ are also shown to increase with increasing the dimensionality(d) [7]. In another recent study one dimensional nonlinear clusters embedded in a perfect one dimensional lattice are considered. This system is found to exhibit a cluster–trapping transition and a STT. Propagating soliton–like waves are also found in between these transitions in large clusters [8]. In this paper we plan to study numerically the STT of quasiparticles in the two dimensional square lattice with various arrangements of nonlinear sites. Furthermore, the effect of the boundary condition is also examined.

2 Results and discussion

Fourth order Runge–Kutta method is used to compute the probability amplitude. We use 10^4 time steps with a time interval 0.01. The conservation of the probability is checked at every step to ensure the accuracy of the result. To discern the STT we primarily examine the time average probability of the initially excited site as a function of χ. The time dependence of the probability of the initial site is considered in some cases. Furthermore, the dependence on χ of the mean–square displacement(MSD) of the quasiparticle, and hence its velocity is studied. The MSD of a particle placed initially at a site $\underline{m}$ in a d–dimensional Bravais lattice is

$$<| \underline{n} - \underline{m} |^2> (t) = \sum_{n} | \underline{n} - \underline{m} |^2 | C_{\underline{n}\,\underline{m}}(t) |^2 \qquad (2)$$

and in a perfect linear lattices this quantity grows as t^2 with a speed of $\sqrt{2d}$. In nonlinear lattices, the MSD grows ballistically but $\frac{<|\underline{n}-\underline{m}|^2>}{t^2}$ depends on the nonlinearity parameter [9]. Our results are presented below.

CASE I: We consider a 7×7 square lattice with three types of boundary conditions, namely, (i) reflecting on both directions, (ii) semiperiodic (periodic in one of the directions) and (iii) fully periodic. A single nonlinear impurity is introduced in the middle of the lattice which is also the site for the initial excitation. For the reflecting and semiperiodic boundary conditions, we obtain the STT at $\chi_{cr} \sim 6.82$, where χ_{cr} denotes the critical value of χ. In the other case $\chi_{cr} \sim 6.87$. The transition in this system is characterized by a lot of fluctuation in the time averaged probability of the initially occupied site followed by a steep rise to the asymptotic value (cf Fig1.).

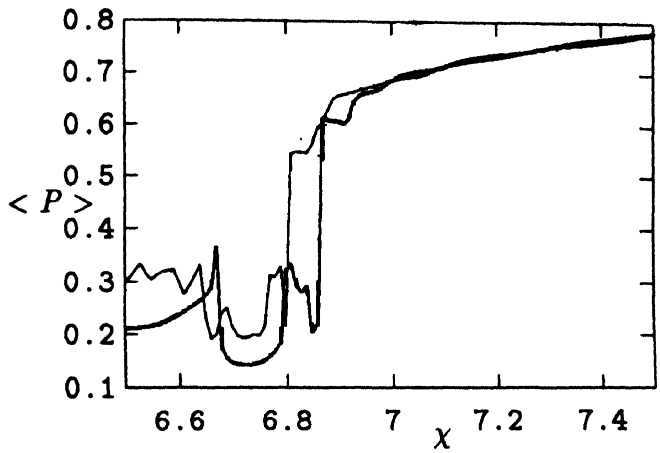

Fig1. The plot of time averaged probability of the initially occupied site as a function of nonlinear parameter χ. The lattice is a 7×7 square containing one nonlinear impurity in the middle and initial excitation has been put in the middle site of the lattice. The light solid curve corresponds to reflecting boundary condition($\chi_{cr} \sim 6.82$), Dotted curve cirresponds to semiperiodic boundary condition($\chi_{cr} \sim 6.82$) and the heavy solid curve corresponds to the full periodic boundary condition($\chi_{cr} \sim 6.87$).

However for a 100×100 square lattice we find a very sharp transition at $\chi_{cr} \sim 6.81$ irrespective of the boundary conditions. A similar type of transition at $\chi_{cr} \sim 6.82$(cf. Fig2.) is obtained from the self-expanding lattice while previously reported result for this case ~ 6.72 [7].

The reported value of $\chi_{cr}(3.22)$ for the one dimensional self-expanding lattice is also obtained by gradually reducing the hopping to zero in one of the directions. The STT is also obtained at the reported value from a finite square lattice(say, 100x100) using the same procedure. We further find that $\chi_{cr}(W) \simeq 3.22 + 3.6W$, and $0 \leq W \leq 1$ defines the ratio of the hopping integrals in two directions. Similarly, we get a straight line with different intercept and slope for the same lattice with same χ at all sites. However, the time averaged probability at the trap-site reaches slowly to the asymptotic value.

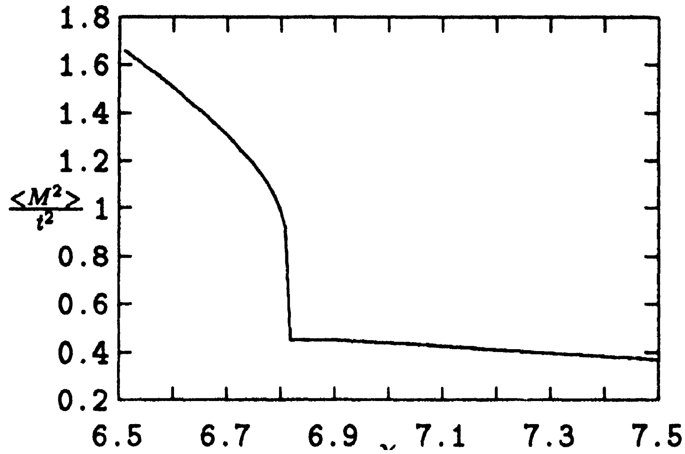

Fig2. The plot of velocity of the particle as a function of χ in a self-expanding square lattice. The lattice contains nonlinearity(χ) at the middle and the initial excitation is applied there. At the critical value of nonlinearity parameter($\chi \sim 6.82$) velocity jumps from a high value to a low value , there by indicating the transition.

CASE II: When a finite size linear cluster of nonlinear impurities is placed in the middle of a 100x100 lattice and one of the end sites is initially occupied, we obtain $\chi_{cr} \sim 6.91$. In the one dimensional lattice with the same initial condition χ_{cr} is ~ 4.2. However, no cluster trapping transition [8] is observed in this case in sharp contrast to its behavior in the one dimensional lattice. On the other hand, for a perfectly nonlinear trimer(all sites have same χ) χ_{cr} rises to ~ 6.98, if the particle is placed initially at the middle of the trimer. No well defined STT is observed with this initial condition if the trimer is embedded in the one dimensional lattice.

CASE III: If the middle site as well as its nearest neighbor sites are nonlinear with same value of χ in a 100×100 square lattice with the initial excitation at the middle site, we obtain $\chi_{cr} \sim 7.12$. By extending the similar type nonlinearity to its next nearest neighbors, we obtain $\chi_{cr} \sim 7.18$ for the same initial condition. For the fully nonlinear lattice with all sites having same χ we obtain $\chi_{cr} \sim 7.17$ for both the semiperiodic and fully periodic boundary condition. Again the excitation is placed at the middle site initially. The self-expanding lattice with the same initial condition yields $\chi_{cr} \sim 7.18$ (cf. Fig3.). This shows that the motion of the quasiparticle in the neighborhood of the STT is mostly confined to the near neighbors of the initial site. We ascribe this to the restriction in our model that the quasiparticle can directly tunnel only to the nearest neighbors.

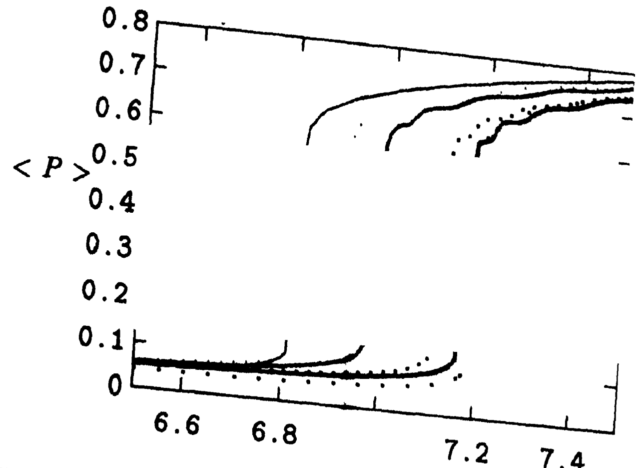

Fig3. The time averaged probability of the initial site versus χ is shown for a 100×100 square lattice. Left most solid curve corresponds to the system with one nonlinear impurity at the middle site($\chi_{cr}\sim6.82$). Light dotted curve corresponds to the system with a nonlinear dimer placed in the lattice with one site of the dimer at the middle of the lattice($\chi_{cr}\sim6.91$). Middle solid curve corresponds to the system with a nonlinear trimer embedded in the lattice, where the middle site of the trimer coincides with the middle of the lattice($\chi_{cr}\sim6.98$). Middle dotted curve refers to the system with same χ at the middle site as well as its nearest neighbor sites of the lattice($\chi_{cr}\sim7.12$). The solid curve in the extreme right corresponds to the system with same χ at the middle, nearest neighbors and next nearest neighbor sites of the lattice($\chi_{cr}\sim7.17$). The dotted curve in the extreme right corresponds to the system where all sites are nonlinear with same χ($\chi_{cr}\sim7.18$).

To explain our main results we first note that the tunneling between two sites, albeit decreases with the increase in the ratio of their site energy difference ($\Delta\epsilon$) to the hopping strength (V), goes truely to zero iff this ratio $|\frac{\Delta\epsilon}{V}|$ goes to infinity. Since, the coordination number(Z) of the Bravais lattice increases with its dimensionality, the escape probability of the quasiparticle from the initial site through the tunneling to the nearest neighbors increases. This reduces the onsite probability, reducing in consequecne the site–energy of the nonlinear impurity in our model. So, the effective $|\frac{\Delta\epsilon}{V}|$ reduces. On the other hand, $|\frac{\Delta\epsilon}{V}|$ must attain the same critical value for the STT to occur. Hence, the value of χ_{cr} increases with the increase in the dimensionality. We further note that the effective tunneling between two nonlinear sites is more than between a nonlinear site and a perfect site. So, the escape probability from the initial site will increase due to any increase in the nonlinear nearest neighbors. By the above argument we should then expect that the χ_{cr} will increase with the increase in the nonlinear nearest neighbors. For a linear cluster of nonlinear impurities with the initial excitation at the end site, the initial site has one nonlinear nearest neighbor. This increases to two and four respectively in a nonlinear trimer and in the square lattice with the nearest neighbor nonlinearity with the initial excitation at the middle site. So, the expected trend is observed.

The absence of a cluster-trapping transition in a finite size linear clusters of nonlinear impurities in a square lattice is also due to the enhancement of the escape probability. If we just keep the nearest neighbors and treat all the perfect sites as a single site, the effective hopping to this site increases by $\sqrt{(Z-1)}$. This then implies that the escape probability through the perfect sites will increase atleast by this factor. This will affect the site-energy difference. So, the χ_{cr} for this transition will shift towards the χ_{cr} for the STT.

3 Conclusion

Near the STT of the quasiparticle a few neighboring sites determine its dynamics. So, an accurate estimation of χ_{cr} can be obtained from relatively small samples. χ_{cr} is also strongly influenced by the probability of escape of the quasiparticle from the trap-site. A quantitative estimation of this aspect is, however, desirable. This work is in progress.

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