

Self-trapping transition for nonlinear impurities embedded in a Cayley tree

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The self-trapping transition due to a single and a dimer nonlinear impurity embedded in a Cayley tree is studied. In particular, the effect of a perfectly nonlinear Cayley tree is considered. A sharp self-trapping transition is observed in each case. It is also observed that the transition is much sharper compared to the case of one-dimensional lattices. For each system, the critical values of χ for the self-trapping transitions are found to obey a power-law behavior as a function of the connectivity K of the Cayley tree.

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I. INTRODUCTION

The interaction of an electron or an exciton with the lattice vibrations is of fundamental importance in understanding the electric properties of solids. For example, the transport of quasiparticles such as electrons or excitons in solids is highly influenced by the electron-phonon interactions. The consequences have been investigated using different methods.¹ Recently, these systems have been studied based on the rigorous analytical treatments and numerical solutions of simple models such as nonlinear Schrödinger equations.^{2,3} One of them with varieties of applications in different areas of science is the one-dimensional discrete nonlinear Schrödinger equation, given as⁴⁻¹⁸

$$i \frac{dC_n}{dt} = V(C_{n+1} + C_{n-1}) + (\epsilon_n - \chi_n |C_n|^2) C_n, \quad (1)$$

where ϵ_n is the static site energy at site n and χ_n is the nonlinearity parameter associated with the n th grid point. Since $\sum_n |C_n|^2$ is set to be unity by choosing appropriate initial conditions, $|C_n|^2$ can be considered as a probability of finding a particle at the n th grid point. One way to derive this set of equations is to couple in the adiabatic approximation (in which the lattice oscillations are much faster than the exciton motion) the vibration of masses at lattice points of a lattice of N sites to the motion of a quasiparticle in the same lattice. The motion of a quasiparticle is described, however, in the frame work of a tight binding Hamiltonian (TBH). In other physical context, the set of equations are often called the discrete self-trapping equations (DST).

The analytical solutions of Eq. (1) are, in general, not known. However, for nonlinear quantum dimers which are two-site systems with the nonlinearity either on both the site-energies or in one of them can be solved analytically for any arbitrary initial condition. From the analytical solutions, a self-trapping transition is found in this model.⁶⁻¹⁰ The self-trapping transition for the symmetric dimer is found at $\chi/V = 4$.⁶ The trapping of hydrogen ions surrounding oxygen atoms in metal hydrides and the energy transport from the absorption center to the reaction center in photosynthetic unit have been modeled by the effective quantum nonlinear dimer.^{6-10,12,13,17} The nonlinear dimer analysis has also been applied to several experimental situations such as neutron scattering of hydrogen atoms trapped at the impurity sites in

metals,⁷ fluorescence depolarization,⁹ muon spin relaxation,¹⁰ nonlinear optical response of superlattices,¹⁹ etc. The self-trapping transition also occurs in the extended nonlinear systems.^{5,17} An interesting experimental example in this context is the observation that trapped hydrogen atoms in metals such as Nb move among the sites in the neighborhood of impurity atoms such as oxygen.²⁰ All these studies have been performed for finite number of nonlinear sites by assuming that the quasiparticle is localized within the nonlinear sites.

Later, the effect of nonlinear sites embedded in a host lattice on the dynamics of quasiparticles has been studied because of its importance in real systems. Dunlap *et al.*²¹ studied the self-trapping transition due to a single nonlinear impurity embedded in an infinite one-, two-, and three-dimensional host lattices. Self-trapping transitions were found at $\chi/V = 3.2, 6.72,$ and 9.24 for one-, two-, and three-dimensional simple host lattices, respectively. Furthermore, the effect of the presence of a nonlinear cluster on the self-trapping transition has also been considered in one-dimensional host lattices.²² The study has also been extended to the case where the inertial effect of the lattice oscillators has been taken into account and rich trapping-detrapping transitions depending on the masses of oscillators have been observed.²³ All these studies have been made in one-dimensional host lattices. However, one needs to know whether or not the self-trapping transition occurs in hosts of different geometrical structure. It would also be interesting to note the differences compared to the results for one-dimensional systems.

The Cayley tree is one possible example of host lattices with different geometrical structure. An important variable characterizing the geometry of the Cayley tree is the connectivity K , which is the number one smaller than the coordination number, i.e., $K = Z - 1$, Z being the coordination number. The Cayley tree reduces to a one-dimensional chain if $K = 1$. The structure of the Cayley tree will be described in the next section.

In this work, we study the self-trapping of an exciton in the Cayley tree with a single as well as a dimer impurity embedded in it. We also consider the fully nonlinear Cayley tree to observe the self-trapping effect.

II. FORMALISM

The structure of a Cayley tree with connectivity $K = 2$ is shown in Fig. 1. For $K = 1$, the system reduces to a one-

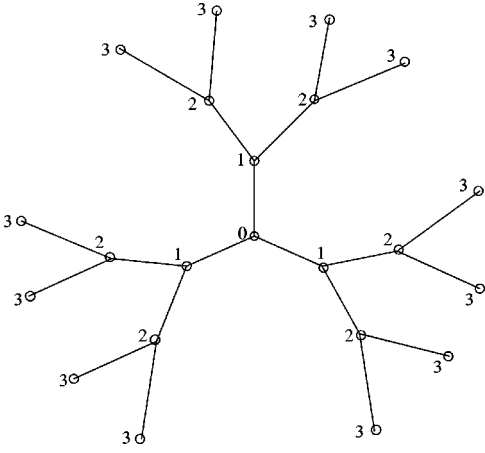


FIG. 1. The Cayley tree of the connectivity $K=2$. The impurity is embedded at the site marked by 0. The sites in the first shell are numbered as 1, the sites in the second shell as 2, and so on.

dimensional chain. In case of a single nonlinear impurity embedded in the Cayley tree, the neighboring sites surrounding the impurity site are symmetric. We thus consider the symmetric shells around the impurity site. The impurity site is designated as the zeroth site, and the n th shell is denoted by n , where n takes the values of $1, 2, 3, \dots$, as the sites are away from the zeroth site (see Fig. 1).

Thus, the n th shell contains ZK^{n-1} sites. All sites in the lattice have three nearest neighbors. While all the nearest-neighbor sites of the zeroth site fall in the first shell, two of the nearest-neighbor sites of any site in the n th shell fall in the $(n+1)$ th shell and the rest one falls in the $(n-1)$ th shell. We further notice that all sites in the same shell have an equal probability amplitude. Therefore, under the tight-binding formalism, the time evolution of a particle (initially placed at the impurity site) on the Cayley tree may be governed by the following equations:

$$i \frac{dC_0}{dt} = ZC_1 - \chi |C_0|^2 C_0,$$

$$i \frac{dC_n}{dt} = KC_{n+1} + C_{n-1}, \quad n \geq 1, \quad (2)$$

where C_0 is the probability amplitude at the zeroth site and C_n for $n \geq 1$ represents the probability amplitude at any site in the n th shell. The χ represents the nonlinear strength at the zeroth site of the Cayley tree. Without loss of generality, we take the nearest-neighbor hopping element to be unity. The normalization condition for the site amplitudes is given by

$$|C_0|^2 + \sum_{n=1}^{\infty} ZK^{n-1} |C_n|^2 = 1. \quad (3)$$

Therefore, to observe the self-trapping transition due to a single nonlinear impurity, Eq. (1) should be solved.

For the perfectly nonlinear Cayley tree, the time evolution for the site amplitudes on the Cayley tree of a particle (initially placed at the zeroth site) may be governed by

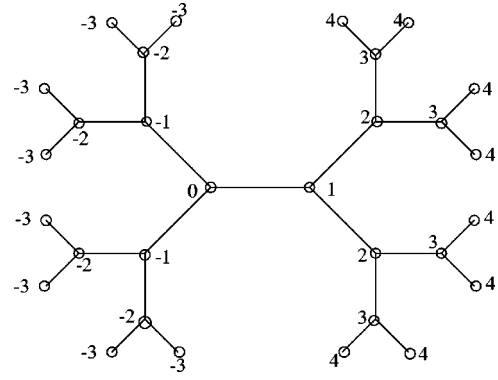


FIG. 2. The Cayley tree with the connectivity $K=2$. The dimeric impurity is embedded at the sites marked by 0 and 1.

$$i \frac{dC_0}{dt} = ZC_1 - \chi |C_0|^2 C_0,$$

$$i \frac{dC_n}{dt} = KC_{n+1} + C_{n-1} - \chi |C_n|^2 C_n, \quad n \geq 1 \quad (4)$$

because the system may be treated in a similar way as it is treated for the single impurity case.

If there is a dimeric impurity in the system, the symmetry about one of the impurity sites does not hold anymore. The system, however, remains symmetric about the bond connecting the two impurity sites. In this case, the Cayley tree with dimeric impurity may be transformed to a one-dimensional system which might be studied more conveniently. The transformation has been reported in the earlier work²⁴; however, for completeness, we briefly describe it in what follows.

We pick a bond and assign the numbers 0 and 1 on its two ends. The neighboring sites of site 1 are numbered with an increasing order and those of the site 0 are numbered with a decreasing order, as shown in Fig. 2. Thus, all points with the same number are assumed to be in the same generation and, accordingly, the number of points in the n th generation is K^{n-1} if $n \geq 1$ and $K^{|n|}$ if $n \leq 0$. We note that all sites in a given generation have the same probability amplitude.

We now consider the motion of a particle on a Cayley tree of the connectivity K with a dimeric impurity embedded at sites 0 and 1. In the tight-binding formalism with nearest-neighbor hopping only, equations governing the motion of a particle are

$$i \frac{dC_n}{dt} = KC_{n+1} + C_{n-1}, \quad n > 1,$$

$$i \frac{dC_n}{dt} = KC_{-|n|-1} + C_{-|n|+1}, \quad n < 0,$$

$$i \frac{dC_1}{dt} = KC_2 + C_0 + \epsilon_1 C_1,$$

$$i \frac{dC_0}{dt} = KC_{-1} + C_1 + \epsilon_0 C_0, \quad (5)$$

where C_n denotes the probability amplitude at any point in the n th generation. We assume that the matrix element of the nearest-neighbor hopping is unity, and that all points in a given generation arising due to a specific organization have the same site energy. The normalization condition for the site amplitudes gives

$$\sum_{n=-\infty}^0 K^{|n|} |C_n|^2 + \frac{1}{K} \sum_{n=1}^{\infty} K^n |C_n|^2 = 1. \quad (6)$$

We now make the following transformations: (i) $\tau = \sqrt{K}t$, (ii) $\epsilon_0 = \tilde{\epsilon}_0/\sqrt{K}$ and $\epsilon_1 = \tilde{\epsilon}_1/\sqrt{K}$, (iii) $C_n = K^{-(n-1)/2} \tilde{C}_n$ for $n \geq 1$ and $C_{-|n|} = K^{-|n|/2} \tilde{C}_n$ for $n \leq 0$. Substituting these in Eq. (5) we obtain

$$i \frac{d\tilde{C}_n}{d\tau} = \tilde{C}_{n+1} + \tilde{C}_{n-1}, \quad \text{for } n > 1 \text{ and } n < 0,$$

$$i \frac{d\tilde{C}_1}{d\tau} = \tilde{C}_2 + \frac{1}{\sqrt{K}} \tilde{C}_0 + \tilde{\epsilon}_1 \tilde{C}_1,$$

$$i \frac{d\tilde{C}_0}{d\tau} = \tilde{C}_{-1} + \frac{1}{\sqrt{K}} \tilde{C}_1 + \tilde{\epsilon}_0 \tilde{C}_0. \quad (7)$$

From Eq. (7), the normalization condition reduces to $\sum_{n=-\infty}^{\infty} |\tilde{C}_n|^2 = 1$. Therefore, the motion of a particle on a Cayley tree is mapped to that on a one-dimensional chain. However, in this chain, the nearest-neighbor hopping matrix element between the zeroth and the first site is reduced from unity to $1/\sqrt{K}$. It can be shown that the Green's function $G_{0,0}(E)$ calculated from Eq. (7) would yield $\tilde{G}_{0,0}(\tilde{E} = E\sqrt{K})$ for a Cayley tree of the connectivity K . Here, in the dimeric impurity problem, the impurities are defined as $\tilde{\epsilon}_0 = \tilde{\chi}|C_0|^2$ and $\tilde{\epsilon}_1 = \tilde{\chi}|C_1|^2$ with $\tilde{\chi} = \chi\sqrt{K}$.

Equations (2), (4), and (7) cannot be solved analytically and, therefore, the numerical method, namely, the fourth order Runge Kutta method is employed. Since there is a conserved quantity in each case, the normalization condition is checked at every step of our numerical calculation. The time interval $\delta t = 0.001$ is used during the calculation. There are two ways to observe the self-trapping transition. One way is to look at the behavior of $|C_n|^2$ as a function of t for various values of the nonlinear strength, and another is to look at the time averaged probability of the particle at site n as a function of the nonlinear strength. The time averaged probability of the exciton at site n is defined as

$$\langle P_n \rangle = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T |C_n|^2 dt. \quad (8)$$

Therefore, we will look at the quantity $|C_n|^2$ or $\langle P_n \rangle$ or both of them for various situations to examine the occurrence of the self-trapping transition.

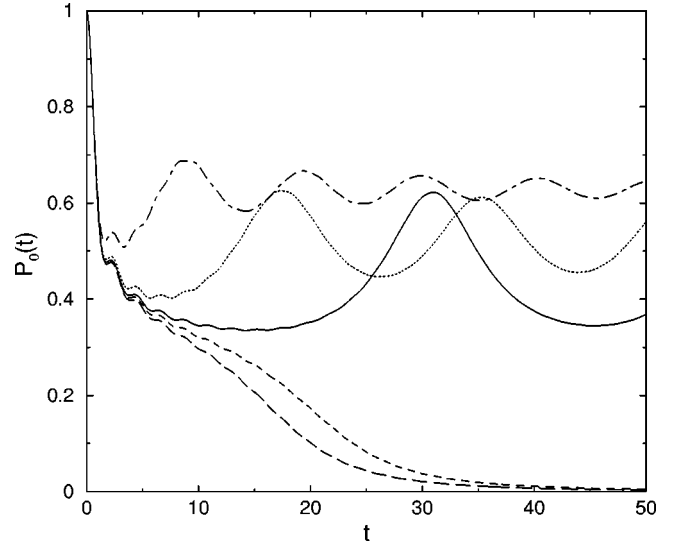


FIG. 3. The probability of the particle to be at the impurity site [$P_0(t)$] as a function of time for various values of the nonlinear parameter is shown. The long dashed curve, dashed curve, solid curve, dotted curve, and the dotted-dashed curve correspond, respectively, to $\chi = 4.75, 4.76, 4.77, 4.8,$ and 5.0 .

III. RESULTS AND DISCUSSIONS

First of all, we discuss the results for the Cayley tree with a single nonlinear impurity. The initial condition is set at the impurity site (zeroth site in Fig. 1).

The probability of finding a particle at the impurity site (initially populated site) is obtained by solving Eq. (2), and the results are plotted in Fig. 3 as a function of time. Different curves correspond to the different values of the nonlinear parameter χ . The long dashed, dashed, solid, dotted, and dotted-dashed curves correspond to the nonlinear strength of $\chi = 4.75, 4.76, 4.77, 4.8,$ and 5.0 , respectively. The connectivity for the Cayley tree considered here is $K = 2$.

It is observed from Fig. 3 that, for $\chi = 4.75$ and 4.76 (the long-dashed and dashed curves), the probability of finding the particle at the impurity site decreases rapidly and then approaches to zero as time increases. This implies that the particle goes away from the impurity site, i.e., the particle becomes fully delocalized. However, the situation is drastically different for $\chi = 4.77$ (solid curve). The probability of finding the particle at the initially populated site decreases down to about 0.35, then increases up to 0.61, and oscillates afterward between 0.35 to 0.61. Thus, the average probability of finding the particle at the initially populated site is approximately 0.48. For higher value of χ , the probability of finding the particle at the initially populated site increases as is obvious from the dotted and dotted-dashed curves in Fig. 3. Therefore, we observe that there is a distinct critical value of χ near (or below) 4.77, below which the particle escapes from the initially populated site and becomes fully delocalized, while above which the particle is most likely trapped at the initially populated site.

The time averaged probability is also plotted in Fig. 4 as a function of the nonlinear parameter χ . The sharp transition of the $\langle P_0 \rangle$ (the time averaged probability at the impurity

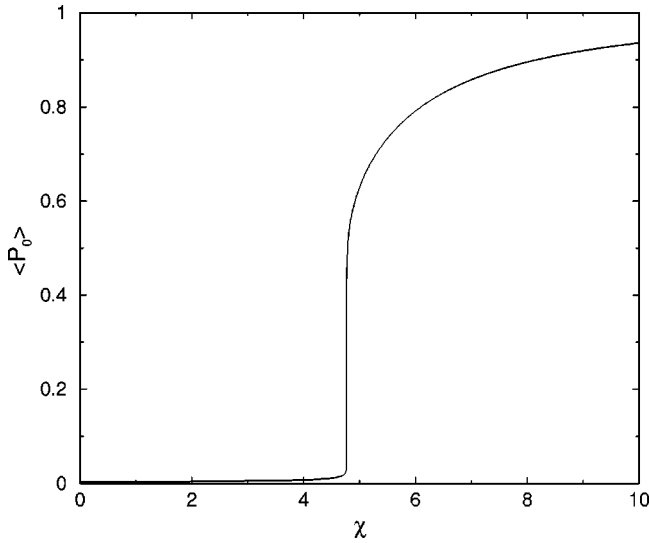


FIG. 4. The time averaged probability of finding the particle at the impurity site 0 (i.e., $\langle P_0 \rangle$) of the Cayley tree of $K=2$ plotted against χ . Sharp transition at $\chi=4.77$ is found.

site) at $\chi \approx 4.77$ is also clear from the Fig. 4.

The self-trapping transition for the $K=1$ case, i.e., for a single nonlinear impurity embedded in a one-dimensional lattice has been studied in detail by Dunlap *et al.*,²¹ and the transition is found at $\chi=3.205$. However, we notice that the self-trapping transition for a single impurity embedded in the Cayley tree with $K=2$ is sharper and clearer when compared with the case for the one-dimensional chain.

In order to observe the dependence of the critical value of χ as a function of the connectivity K of the Cayley tree, we plotted in Fig. 5 χ_{cr} for various values of $K \geq 2$ on a double logarithmic scale. The data points lie surprisingly well on the straight line, implying that the critical value obeys the power law

$$\chi_{\text{cr}} = \alpha K^\beta, \quad (9)$$

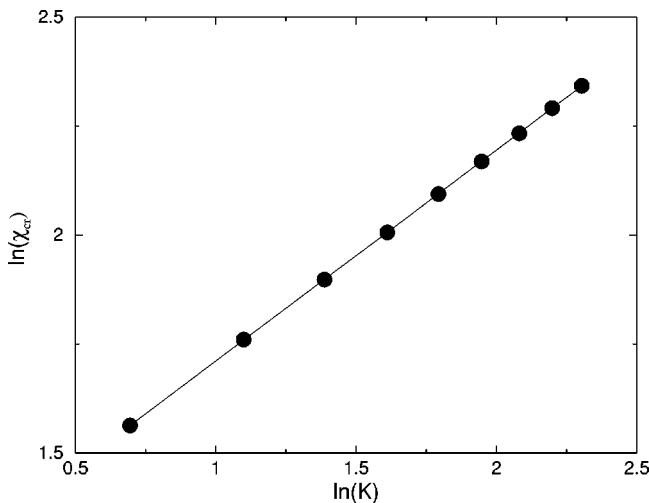


FIG. 5. The critical values of χ for self-trapping transition in a Cayley tree with a single nonlinear impurity is plotted as a function of the connectivity of the Cayley tree.

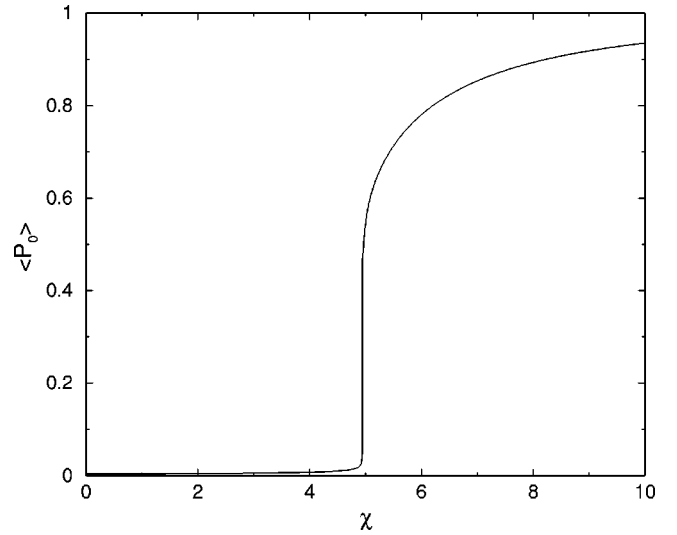


FIG. 6. The time averaged probability of finding the particle at the zeroth impurity site on a Cayley tree of $K=2$ with a dimeric nonlinear impurity plotted as a function of the nonlinearity parameter χ . Sharp transition is observed at $\chi=4.95$

with $\alpha \approx 3.41$ and $\beta \approx 0.484$. It should be noted that the critical value $\chi_{\text{cr}} \approx 3.41$ for $K=1$ is prominently different from the critical value for a one-dimensional system. This implies that the power law is valid only for $K \geq 2$. We therefore conclude that the geometry of the host lattice results in different critical values of χ for different values of $K \geq 2$, obeying the power-law behavior in Eq. (9).

We now consider the dimeric impurity embedded in the Cayley tree with connectivity $K=2$. The particle is initially populated at one of the impurity sites. The probability of finding the particle at the initially populated site is calculated by solving the Eq. (7) for various values of χ , and the time averaged result is plotted in Fig. 6. The sharp transition is found at $\chi_{\text{cr}}=4.95$. One interesting observation found from Fig. 6 is that there is no precursor (peak) in the $\langle P_0 \rangle$ before the permanent self-trapping transition occurs at $\chi \approx 4.95$, unlike the case in the one-dimensional system with two impurities (Fig. 5 in Ref. 23) for which a peak is observed at $\chi \approx 3.2$ just before the permanent transition occurs at $\chi \approx 4.22$. Thus, the particle in the Cayley tree is always influenced by both the impurities present in the host whereas the particle does not feel the presence of the second impurity in the one-dimensional system below $\chi \approx 3.2$. From Eq. (7) we note that the Cayley tree of connectivity K with dimeric impurity reduces to a one-dimensional chain with the hopping element between the impurity sites reduced from unity to $V_{\text{eff}} = 1/\sqrt{K}$. For the Cayley tree $K \geq 2$, the hopping element between the impurity sites in the transformed one-dimensional system becomes less than or equal to $1/\sqrt{2}$. Since the peak before the permanent transition disappears in the case of Cayley tree, we suspect that there must be a critical value for the hopping element (say, $V_{\text{eff}}^{\text{cr}}$) between the dimeric impurity sites of a one-dimensional chain while keeping the other hopping elements unity such that the peak disappears for $V_{\text{eff}} \leq V_{\text{eff}}^{\text{cr}}$. In order to verify this, we perform the numerical calculation of the time averaged probability

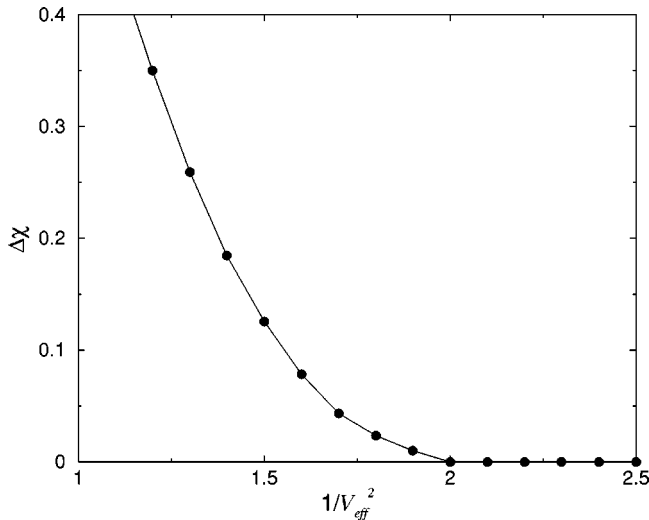


FIG. 7. Plot of the gap $\Delta\chi$ between the peak and the permanent transition point in the time averaged probability of the particle at the initially populated impurity site in a one-dimensional chain with a dimeric nonlinear impurity against the inverse of the square of the hopping element between the impurity sites. Other hopping elements are set to be unity.

for the particle to be at the initially populated impurity site of a one-dimensional chain with a dimeric nonlinear impurity for various values of V_{eff} (the hopping element between the impurity sites) while keeping the other elements unity. We interestingly observed that the gap $\Delta\chi$ between the peak and the permanent transition point reduces as the V_{eff} decreases and eventually vanishes at a critical value of $V_{\text{eff}}=1/\sqrt{2}$ as shown in Fig. 7, i.e., the peak before the permanent transition disappears when the system is equivalent to a Cayley tree with connectivity equal to 2. This implies that the structure of Cayley tree is responsible for the absence of the peak before the permanent transition.

The critical value of χ for various values of the connectivity of the Cayley tree is calculated and found to obey the same power-law behavior as in Eq. (9), but with different values of α and β , i.e., $\alpha\approx 3.554$ and $\beta\approx 0.465$. We note that the critical value of χ for the self-trapping increases due to the presence of one more impurity. For a one-dimensional system the critical value is found to be 4.22 which deviates prominently from the value estimated from Eq. (9) with the

values of α and β mentioned above and $K=1$. This is again due to the different geometry of the host lattice.

We now consider the perfectly nonlinear Cayley tree. The particle is initially placed at any arbitrary site. The sharp self-trapping transition is also observed in this case for various values of K . The critical value of the nonlinear parameter χ_{cr} for self-trapping transition again obeys the same power-law behavior as in Eq. (9) but with $\alpha\approx 3.766$ and $\beta\approx 0.445$. Here we find that the critical values are larger than those for the case of a single and dimeric impurity; however, the difference is not appreciably large. Therefore, it appears that the self-trapping transition is influenced by only few nonlinear neighbors around the initially populated impurity site.

Finally it is worth mentioning that the formation of stationary localized state in the Cayley tree due to a single nonlinear impurity, dimeric nonlinear impurity and also in a perfectly nonlinear Cayley tree has been studied by Gupta and Kundu^{24,25} earlier and in the above three cases the bifurcations in the stationary states were observed which in turn support the occurrence of the self-trapping transitions in the work.

IV. SUMMARY

The self-trapping transition due to a single and a dimeric nonlinear impurity embedded in the Cayley tree is studied. Furthermore, the self-trapping transition in a perfectly nonlinear Cayley tree is observed. Very sharp self-trapping transition is observed for all systems considered here. The geometry of the host lattice is responsible for such a sharp transition. The critical value of the self-trapping transition increases as the number of nonlinear impurities in the host lattice increases. The critical value of χ is found to obey a power law against the connectivity of the Cayley tree for all cases. Results are compared with those for the one-dimensional system.

ACKNOWLEDGMENTS

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