Time evolution of models described by a one-dimensional discrete nonlinear Schrödinger equation

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The dynamics of models described by a one-dimensional discrete nonlinear Schrödinger equation is studied. The nonlinearity in these models appears due to the coupling of the electronic motion to optical oscillators which are treated in an adiabatic approximation. First, various sizes of nonlinear clusters embedded in an infinite linear chain are considered. The initial excitation is applied either at the end site or at the middle site of the cluster. In both the cases we obtain two kinds of transition: (i) a cluster-trapping transition and (ii) a self-trapping transition. The dynamics of the quasiparticle with the end site initial excitation are found to exhibit (i) a sharp self-trapping transition, (ii) an amplitude transition in the site probabilities, and (iii) propagating solitonlike waves in large clusters. Ballistic propagation is observed in random nonlinear systems. The effect of nonlinear impurities on the superdiffusive behavior of the random-dimer model is also studied. [S0163-1829(96)00922-8]

I. INTRODUCTION

The strong interaction with the lattice vibrations is one of the basic mechanisms influencing the transport of quasiparticles such as electrons or exitons in solids. The consequences have been investigated employing different methods.[1] A recent approach to this problem is based on nonlinear equations.[2–4] One of the simple models with varieties of applications in different areas is the one-dimensional discrete nonlinear Schrödinger equation[5–12]

$$i\frac{dc_m}{dt}=V(c_{m+1}+c_{m-1})+(\epsilon_m-\chi_m|c_m|^2)c_m\,. \qquad (1)$$

Here $c_m(t)$ is the probability amplitude of the quasiparticle at site m at time t, V is the nearest-neighbor transfer matrix element, and ϵ_m and χ_m are the on-site energy and nonlinearity strength of the mth site, respectively. Without any loss of generality we assume $V=1$. Equation (1) arises in the general problem of polaron formation due to the coupling of quasiparticles with optical oscillators in the adiabatic approximation. The simple form of the Eq. (1) with $\epsilon_m=0$ and $\chi_m=\chi$ for all m has been studied numerically.[5] However, in a two-site system which is called the nonlinear adiabatic quantum dimer, the self-trapping transition[4,5] occurs at a critical value of nonlinearity for arbitrary initial conditions.[6–9,11] The applications of the nonlinear dimer analysis have been made to several experimental situations. They are neutron scattering off hydrogen atoms trapped at the impurity sites in metals,[7] fluorescence depolarization,[9] muon spin relaxation,[11] nonlinear optical response of superlattices,[13] etc. The self-trapping transition also occurs in extended nonlinear systems.[12] A possible application is the trapping of hydrogen ions around the oxygen atoms in metal hydrides.[14] All these studies have been performed for a finite number of nonlinear sites by assuming that the quasiparticle is localized within the nonlinear sites. However, the effect of nonlinear sites embedded in a host lattice on the dynamics of quasiparticles has been hardly studied in spite of its importance in real systems. Dunlap *et al.*[15] studied the self-trapping transition at a single nonlinear impurity embedded in a host lattice. Chen *et al.*[16] studied the time-averaged probability at the initial occupation site in an infinite linear chain containing one or many nonlinear impurities. In this study the adiabatic assumption has been removed. They have also studied the adiabatic case, albeit not in detail. So in this paper we plan to study first the dynamics of a quasiparticle in an infinite linear chain containing adiabatic Holstein-type impurities.[1] We use two different kinds of initial conditions. The initial excitation is applied either at the end site or at the middle site of the cluster of the impurities.

If we consider randomness in site energies ϵ_m and $\chi_m=0$ for all m in Eq. (1) Anderson theory[17] predicts that the particle will remain localized within a finite region of the chain after a sufficient time. So it is important to investigate the dynamics of (i) random nonlinear systems (randomness in the nonlinearity parameter) and (ii) systems where disorder in site energies and nonlinearity coexists. Regarding the first question Molina and Tsironis[18] showed the ballistic propagation of the untrapped electronic fraction in a nonlinear random binary alloy. In this paper we study the transport properties of completely random nonlinear systems. Feddersen[19] has studied the effect of nonlinearity on the Anderson localization. Shepelyansky[20] has obtained subdiffusive behavior in on-site-energy-disordered systems only when the nonlinearity parameter exceeds a critical value. It is well known that superdiffusive behavior is obtained in the random-dimer model (RDM).[21] The RDM is characterized by a set of nonscattered states around the dimer energy. This leads to the superdiffusive behavior of the mean square displacement of a particle. We study here the effect of nonlinearity on the superdiffusive behavior of the RDM.

The organization of the paper is as follows. In Sec. II, we study the dynamics of the quasiparticle in a cluster of nonlinear sites embedded in a lattice. The initial excitation is applied either at the end site or at the middle site of the cluster. In Sec. III, we study the dynamics of different kinds of random systems. We end this article by summarizing our main results.

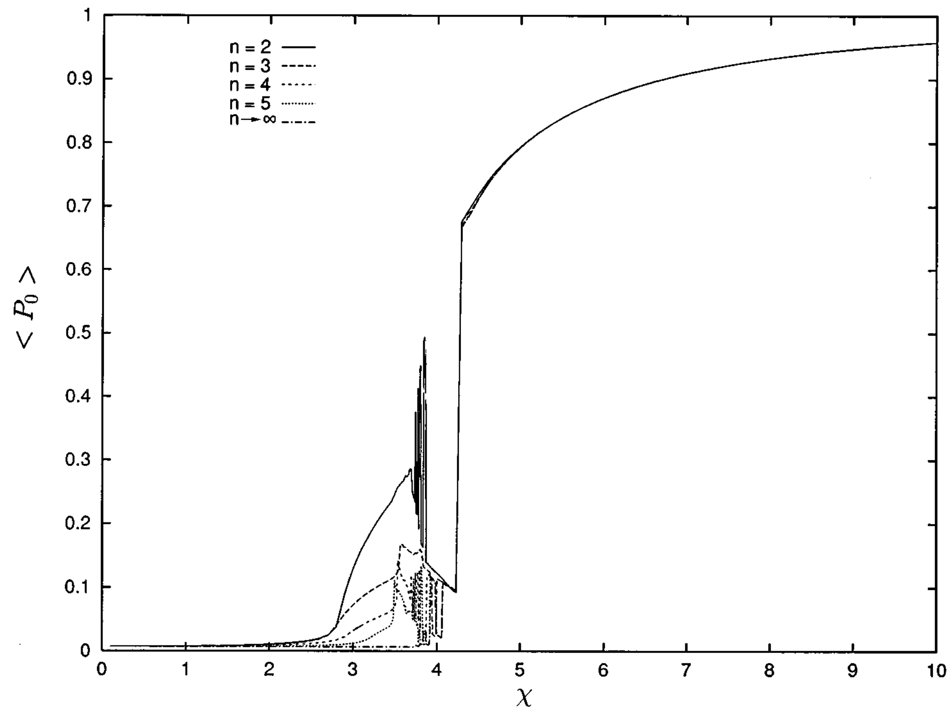

FIG. 1. Time-averaged probability at the initial excitation site ($\langle P_0\rangle$) as a function of χ for different sizes (n) of the nonlinear cluster. The initial excitation is applied at the end site ($m=0$) of the cluster.

II. CLUSTER OF NONLINEAR IMPURITIES EMBEDDED IN A LATTICE

A. Initial excitation at the end of the cluster

We consider a system containing a cluster of n number of nonlinear impurity sites of equal strength χ embedded in a host lattice. All the site energies are assumed to be zero. The initial excitation is applied at left end site of the nonlinear cluster. We call this the zeroth site. The sites on the left and right of the initial occupation site are numbered as $m=-1,-2,-3,\ldots$ and $m=1,2,3,\ldots$, respectively. We first study here the time-averaged probability of the nonlinear sites. For the mth site it is defined as

$$\langle P_m\rangle = \lim_{T\to\infty}\frac{1}{T}\int_0^T |c_m(t)|^2 dt, \tag{2}$$

with $|c_m(0)|^2=\delta_{m,0}$. Here, $|c_m(t)|^2$ is the probability of the quasiparticle at the mth site at time t. We solve the first-order coupled nonlinear differential equations numerically by using a fourth-order Runge-Kutte method. The system is taken as a self-expanding lattice to avoid boundary effects. For time averaging we have taken $T=200$ with an interval $\Delta T=0.01$. The accuracy of the numerical integration is checked through the total probability. Here, we consider the cases for $n=2,3,4,5$ and an asymptotically large value of n ($n\to\infty$). For $n\to\infty$ we mean that the system contains two semi-infinite chains. The perfect chain without any nonlinearity is connected to the other one which is a perfect nonlinear chain. The initial excitation is applied at the junction where the nonlinear impurity exists. In Fig. 1 we have plotted the time-averaged probability at the initial occupation site, $\langle P_0\rangle$, as a function of χ for different values of n. In all these cases we find that $\langle P_0\rangle$ starts increasing significantly from $\chi=\chi_{\rm cr1}$. For $n=2$ the value of $\chi_{\rm cr1}$ is ~ 2.8. In general the value of $\chi_{\rm cr1}$ increases with increasing the size of the nonlinear cluster. A sharp transition in $\langle P_0\rangle$ occurs at $\chi_{\rm cr2}\sim 4.23$ for all values of n. In the region between $\chi_{\rm cr1}$ and $\chi_{\rm cr2}$ we obtain fluctuations in $\langle P_0\rangle$. For a better understanding of this behavior we study next the time-averaged probability of the unoccupied nonlinear sites.

In Fig. 2 we have plotted the time-averaged probability of the initially unoccupied nonlinear site ($\langle P_1\rangle$) of the dimer as a function of χ. For comparison we have also plotted $\langle P_0\rangle$. When the nonlinearity strength χ exceeds $\chi_{\rm cr1}$ we observe both a $\langle P_0\rangle$ and $\langle P_1\rangle$ increase with increasing χ and their values are almost equal. This implies that the particle oscillates with a finite probability among the dimer sites. This partial localization or trapping within the cluster can be understood from the following. At $t=0$ the energy level of the sites $m=-1,0$, and 1 are $0,-\chi$, and 0, respectively. With increasing the time the site probability of $m=0$ decreases and of $m=1$ increases. Consequently, the energy level of the sites $m=0$ and 1 moves upward and downward from the original positions, respectively. Thus, the energy gap between the sites $m=0$ and 1 becomes smaller than the gap between $m=-1$ and 0. So the initially localized particle at site $m=0$ favors the nearest-neighbor nonlinear site (i.e., $m=1$) and the energy level of that site decreases. At the same time the energy gap between the sites $m=1$ and 2 increases. Thus the particle feels a quantum well and it oscillates within the well with a finite probability. Of course, some probability will escape along the leads in both directions of the dimer. Now the leakage of the probability through the leads reduces with the increase of χ due to the increase in the energy gaps between the sites $m=0$ and -1 and between $m=1$ and 2. When χ attains a critical value, say, $\chi_{\rm cr1}$, these gaps become sufficiently large to trap the particle within the cluster. So $\chi_{\rm cr1}$ marks the onset of the cluster-trapping transition of the particle. With a further increase in χ, the competition among the nonlinear sites to trap

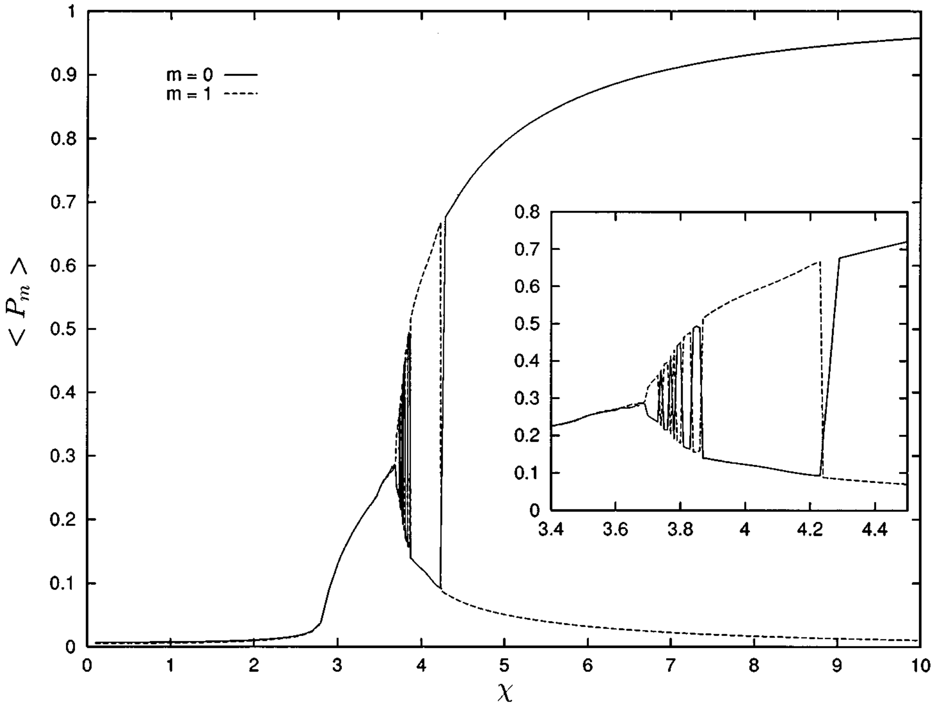

FIG. 2. Time-averaged probability of initially occupied ($\langle P_0 \rangle$) and unoccupied ($\langle P_1 \rangle$) sites of the nonlinear dimer embedded in a host lattice as a function of χ. The inset shows details of the $\langle P_0 \rangle$ and $\langle P_1 \rangle$ with χ in the fluctuation regime. The initial excitation is applied at the end site $(m=0)$ of the dimer.

the particle starts. Depending on the strength of the nonlinearity the particle is preferentially trapped either at the initially occupied site or at the unoccupied site (see the inset of Fig. 2). When χ is just below χ_{cr2}, the value of $\langle P_1 \rangle$ is much larger than $\langle P_0 \rangle$. But when χ crosses χ_{cr2}, we find a sharp fall in $\langle P_1 \rangle$ and an increase in $\langle P_0 \rangle$. For a further increase of χ, $\langle P_0 \rangle$ increases and $\langle P_1 \rangle$ decreases gradually. We do not obtain any further transition. So χ_{cr2} is called the critical value of χ for the self-trapping transition.

To understand the behavior in the fluctuation regime of time-averaged site probabilities we study their temporal behavior. This is shown in Fig. 3. After a few oscillations, we observe a transition where the amplitude of the two oscillations decreases suddenly and the phases are just opposite to each other [see Fig. 3(a)]. The amplitude transition in the site probabilities always occurs simultaneously. Furthermore, the transition occurs from a peak of the oscillation in one case and from a dip in the other one. Consequently, one of the site

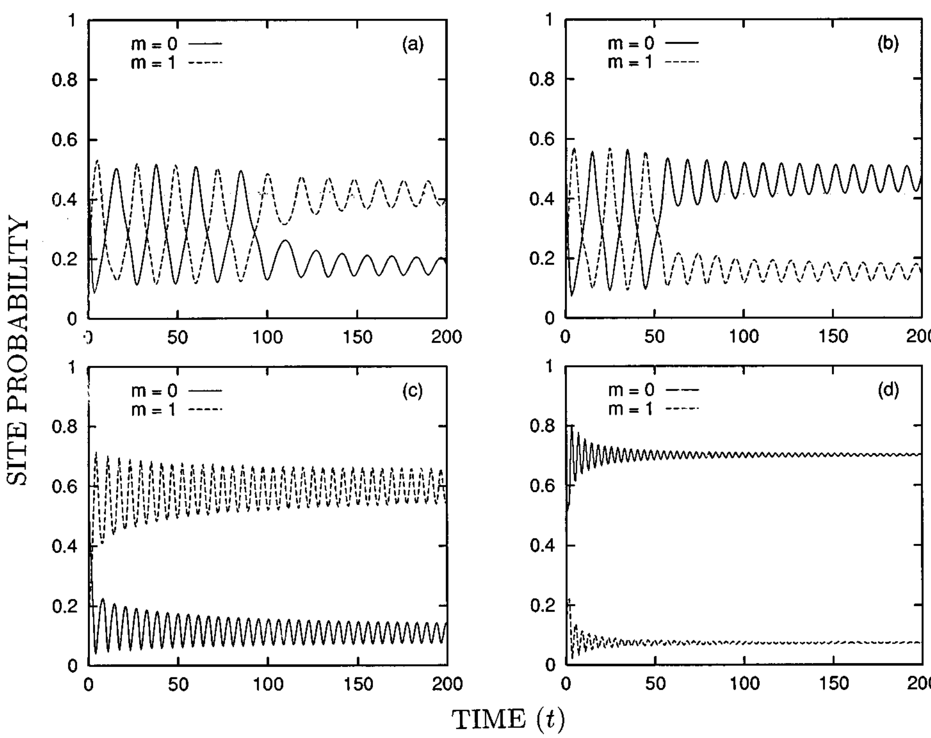

FIG. 3. Plot of site probabilities of the dimer sites embedded in a host lattice as a function of time (t) for different values of nonlinearity parameter χ as follows: (a) $\chi=3.72$, (b) $\chi=3.77$, (c) $\chi=4$, and (d) $\chi=4.4$. In all these cases the initial excitation is applied at the end site $(m=0)$ of the dimer.

probabilities oscillates with a more mean probability than the other. Thenceforth, the amplitude of the oscillation of the probabilities decreases with time. This kind of transition is obtained in the nonadiabatic nonlinear quantum dimer problem in the presence of rapid vibrational relaxation caused by the damping in the lattice vibration.[22] Two transitions are observed, a static transition at $\chi = 2V$ (Ref. 5) and a dynamic transition at $\chi = 4V$.[6] The static transition is governed by the relaxation term of the lattice vibration. Here, it seems that the leads at both ends of the nonlinear dimer introduce effectively a damping term in the lattice vibration. This effect appears through the escape probability from the dimer cluster. However, the main difference here is that the transition occurs at different values of χ. The transition time as well as the number of the dynamical adiabatic dimer type oscillations decreases with increasing χ [compare Figs. 3(a) and 3(b)]. Furthermore, near χ_{cr2} the number of dynamical adiabatic dimer kind oscillations does not reduce for a wide range of χ. Consequently, we do not find any fluctuation in the time-averaged probability in this region (see the region $3.87 < \chi < 4.23$ of the inset of Fig. 2). The amplitude transition in the site probabilities occurs after half a period of the oscillation [see Fig. 3(c)]. Thus, just below χ_{cr2}, $\langle P_1 \rangle$ is found to be much larger than $\langle P_0 \rangle$. When χ just crosses χ_{cr2} the transition occurs at a time which is even less than the half period [see Fig. 3(d)]. As there is no dynamical adiabatic dimer-type oscillation we do not find any further transition in the amplitude of the site probabilities with the increase of χ. So in contrast to Ref. 16, we find that the quasiparticle recognizes both the nonlinear impurities just above χ_{cr1} and for a further increase of χ, the amplitude transition of the site probabilities occurs. Furthermore, we obtain damped oscillation in the site probabilities for $\chi > \chi_{cr2}$. This has to be contrasted with the regular oscillation above $\chi = 4$ in an isolated nonlinear dimer.[6] We also study the time-averaged probability at the nonlinear sites for $n = 3$, 4, and 5. In all these cases we observe the same behavior as observed in the dimer embedded in a host lattice.

For a relatively large size nonlinear cluster (e.g., $n = 30$) the partial localization of the particle is found to occur at different regions of the cluster. We study the particle propagation in a lattice for the case of $n = 30$ for different values of χ. For small values of χ ($\leqslant 3.1$) we obtain the delocalization behavior of the particle. For a further increase of χ we find that a solitonlike wave, extended over a few sites, moves through the nonlinear cluster. Thus, we obtain an oscillation of the solitonlike wave in the cluster. This is shown for $\chi = 3.51$ in Fig. 4. It should be noted that the maximum probability is found within this solitonlike wave. The time period of the oscillation of the wave within the cluster is increased with time. This indicates that if we increase the time, the oscillation will cease and the solitonlike wave will be localized within a few sites of the nonlinear cluster. This is exactly obtained (see Fig. 4). The number of oscillations decreases before localization with increasing χ. The position of the localization of the wave, however, depends on the value of χ but the pattern is not discerned here. For a further increase of χ we do not find any oscillation. It moves along the cluster and gets trapped within a few sites of the nonlinear cluster. With increasing the value of χ the trapping region in general moves towards the initial excitation site and we obtain a sharp self-trapping transition at $\chi_{cr2} \sim 4.23$. It should be noted that the width and peak value of the solitonlike wave decrease and increase, respectively, with increasing the value of χ. Though we are not able to probe the value of χ where the solitonlike wave starts to form, it is within $\chi = 3.1$ and 3.2. It should also be noted that the movement of the solitonlike wave is obtained only when the size of the nonlinear cluster is much larger than the width of the wave.

In asymptotic limit (i.e., $n \to \infty$) we also obtain the formation of a solitonlike wave extended over a few sites in the nonlinear cluster. Here, we do not find any oscillation of the wave as obtained in the case of $n = 30$. For lower values of χ the wave moves along the lattice but finally it is trapped in a region as shown in Fig. 5. If we increase the value of χ, the localization regime of the wave moves towards the initially occupied site and thus we obtain a sharp self-trapping transition at $\chi_{cr2} \sim 4.23$. The width and the peak value of the wave decrease and increase, respectively, with increasing χ. However, we did not probe the region of χ where the solitonlike wave starts to form.

B. Initial excitation at the middle of the cluster

We study here the same system but the initial excitation is given at the middle site ($m = 0$) of the cluster. The cluster

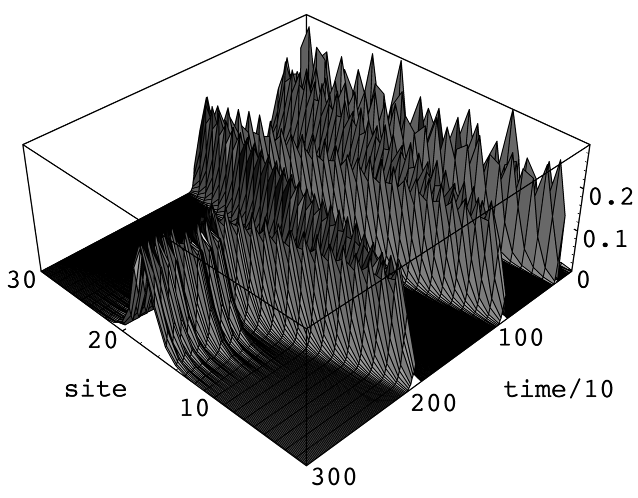

FIG. 4. Electronic probability propagation profile as a function of time (t) for $\chi = 3.51$. Here, $n = 30$ and the initial excitation is applied at the end site ($m = 0$) of the nonlinear cluster.

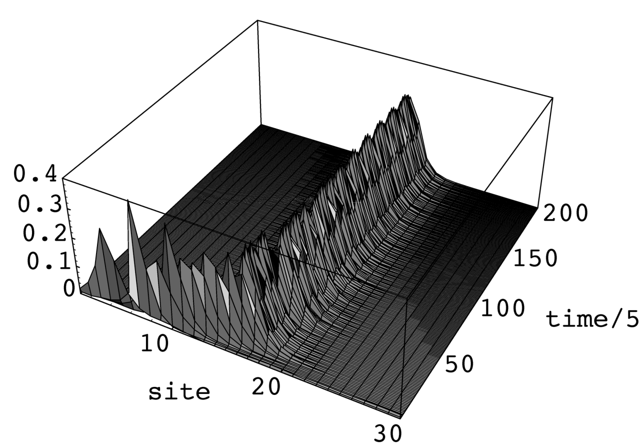

FIG. 5. Same as Fig. 4 but $n \to \infty$ and $\chi = 3.6$.

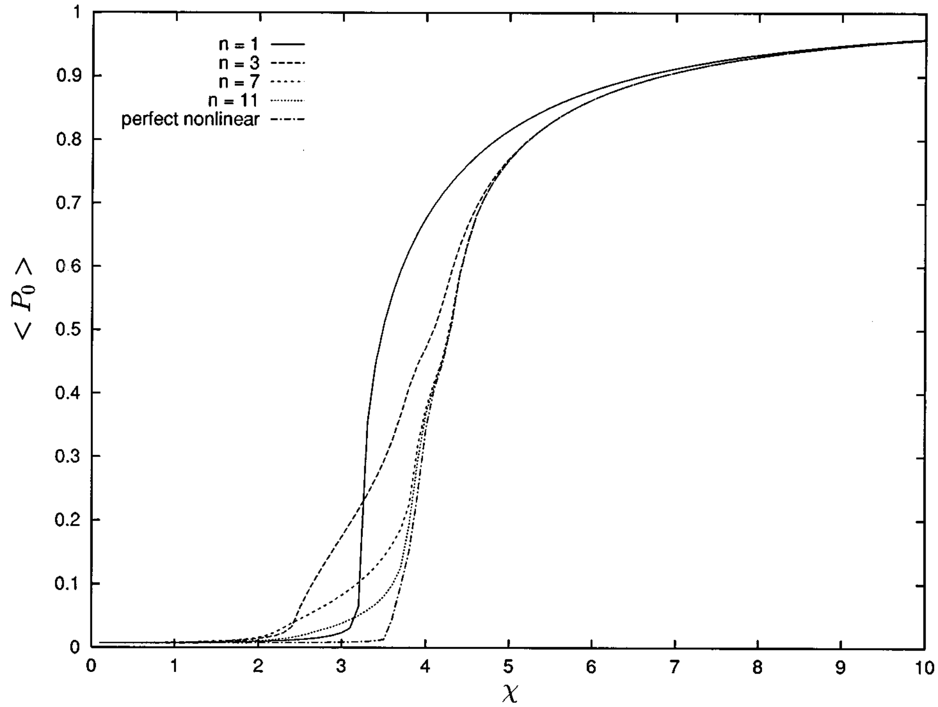

FIG. 6. Time-averaged probability of the initial excitation site ($\langle P_0\rangle$) as a function of χ for different values of n. The initial excitation is applied at the middle site ($m=0$) of the nonlinear cluster.

contains an odd number of sites. As the system is symmetric around the initial occupation site we do not find the asymmetric probability distribution. So the properties in this system should be different from the earlier cases. The time-averaged probability at the initial excitation site is shown in Fig. 6 for different values χ and n. In the case of a single nonlinear impurity system we obtain the self-trapping transition at $\chi_{\rm cr1}\sim 3.2$.[15,16] For higher values of n we find that $\langle P_0\rangle$ increases significantly from $\chi=\chi_{\rm cr1}$ and it characterizes the cluster-trapping transition. The value of $\chi_{\rm cr1}$ for $n=3$ is ~ 2.4 which is much less than the self-trapping transition value of χ for $n=1$. The value of $\chi_{\rm cr1}$ in general increases with increasing the size of cluster. In the asymptotic limit (i.e., a perfect nonlinear system) the value of the transition point is $\chi_{\rm cr1}^{\rm asy}\sim 3.5$.[23] We further study the time-averaged probability of the neighboring nonlinear sites of the zeroth site for $n=5$ (see Fig. 7). We find that the time-averaged probability of the other nonlinear sites also starts increasing from $\chi_{\rm cr1}$. The value of $\langle P_m\rangle$ decreases as we go away from the initial occupation site, i.e., as $|m|$ increases. This means that beyond $\chi_{\rm cr1}$ the particle lies within a few sites of the cluster with center at the initial excitation site. Again, as both sides of the zeroth site contain nonlinearity the particle is attracted by the nonlinear sites in both directions. Thus, with increasing the size of the cluster we find that $\langle P_0\rangle$ decreases and consequently the value of $\chi_{\rm cr1}$ increases. Beyond $\chi_{\rm cr1}$ we find that the time-averaged probability of the nonlinear sites (except the zeroth site) first increases and then decreases with increasing the value of χ. But $\langle P_0\rangle$ gradually increases with increasing the value of χ. Thus, we obtain the localization of the particle at $m=0$ with maximum probability which is called self-trapping. However, in this case we do not obtain any sharp self-trapping transition as seen in the previous case. In the study of particle propagation we observe a localized solitonlike wave with the peak value at $m=0$. The width and peak value of the wave decrease and increase, respectively, with increasing the value of χ. This is obtained in all cases discussed here.

III. RANDOM SYSTEMS

The ballistic motion of an initially localized particle in a one-dimensional nonlinear random binary alloy has been observed recently.[18] Here we also show the ballistic motion of a particle in completely random nonlinear systems. The random nonlinear systems are characterized by random distribution of the nonlinearity parameter, χ with the values $0<\chi_m<\chi_{\rm max}$. All the site energies are assumed to be zero. The initial excitation is applied at the zeroth site. Furthermore, we assume that the value of χ_0 is $\chi_{\rm max}$. The mean square displacement (MSD) is defined as

$$\langle m^2\rangle=\sum_{m=-\infty}^{\infty} m^2|c_m(t)|^2, \tag{3}$$

with the initial condition $|c_m(0)|^2=\delta_{m,0}$. After some initial transient behavior the speed ($\sqrt{\langle m^2\rangle}/t$) of the particle settles down to a constant which depends on $\chi_{\rm max}$. The speed of the particle decreases with increasing $\chi_{\rm max}$. Around a critical value of $\chi_{\rm max}$ the speed decreases drastically and beyond this region we observe the slow decay of the speed. The untrapped portion of the probability leads to the ballistic motion of the particle above the critical value of $\chi_{\rm max}$.[18] To obtain the critical value of $\chi_{\rm max}$ we have plotted the time-averaged probability of the initial excitation site for different realizations in Fig. 8. The critical values of $\chi_{\rm max}$ are found to be in the range between ~ 3 and ~ 3.5. Beyond the critical value, $\langle P_0\rangle$ in general increases very fast with increasing χ but with a certain degree of sample-to-sample variation.

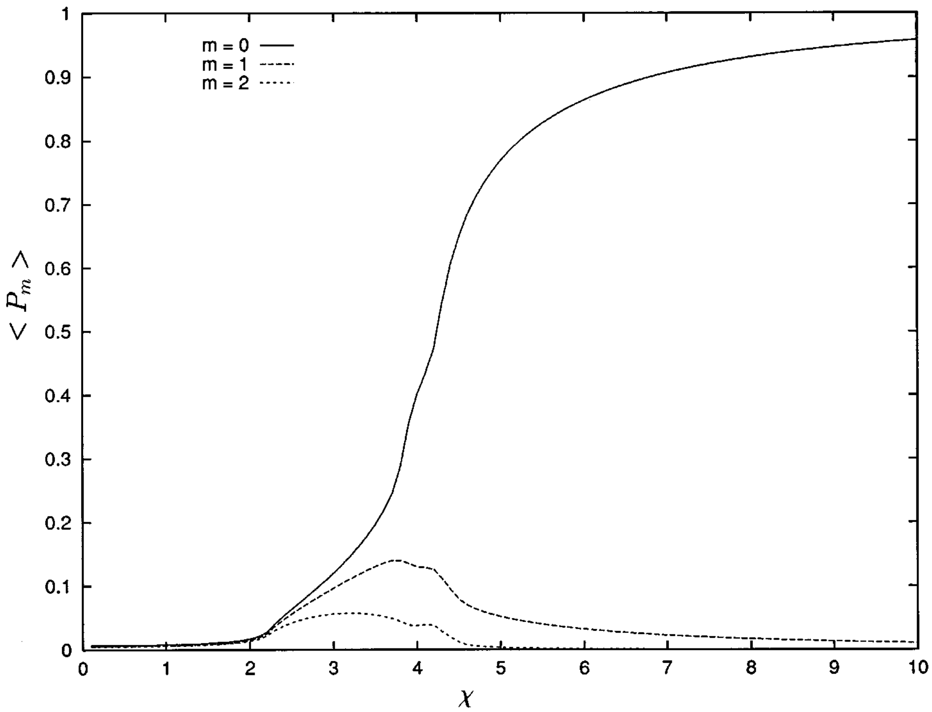

FIG. 7. Time-averaged probability ($\langle P_m \rangle$) of the nonlinear sites of the cluster of size $n=5$ embedded in a host lattice as a function of χ. The initial excitation is applied at the middle site ($m=0$) of the cluster. As the system is symmetric around the zeroth site $\langle P_{-1}\rangle=\langle P_1\rangle$ and $\langle P_{-2}\rangle=\langle P_2\rangle$.

Within the region between $\chi\sim 3$ and $\chi\sim 4.5$ we obtain a large deviation in $\langle P_0\rangle$ for different realizations. Beyond this region $\langle P_0\rangle$ increases slowly as $\chi_{\max}$ goes up and the probability of all other sites decreases. In this limit the random nonlinear lattice to a good approximation can be replaced by a perfect lattice with a single nonlinear defect of strength $\chi_{\max}$. This is also true for perfect nonlinear system. It can be shown that beyond the transition region of χ the speeds of the particles in random nonlinear systems, in perfect nonlinear systems, and in single nonlinear defect systems are almost equal. We study next the effect of nonlinearity in the superdiffusive motion of the random-dimer model (RDM).

The RDM is a binary alloy containing two types of atoms with site energies ϵ_a and ϵ_b. The restriction on the randomness is that the site energy ϵ_a appear in a pair which is called a dimer. So the system is the random distribution of the dimer and other site energy ϵ_b. If we assume $\epsilon_b=0$ and $V=1$, then we obtain $\sim\sqrt{N}$ number of nonscattered states around ϵ_a.[24] Here, N is the length of the sample. The MSD goes as $\langle m^2\rangle\sim t^{3/2}$.[21] This is obtained only when $|\epsilon_a|<2$. We now study the effect of nonlinearity on the transport properties of the RDM. We assume that all the sites have equal nonlinearity strength and it is χ. It should be noted that by adding the nonlinearity the effective site energies are al-

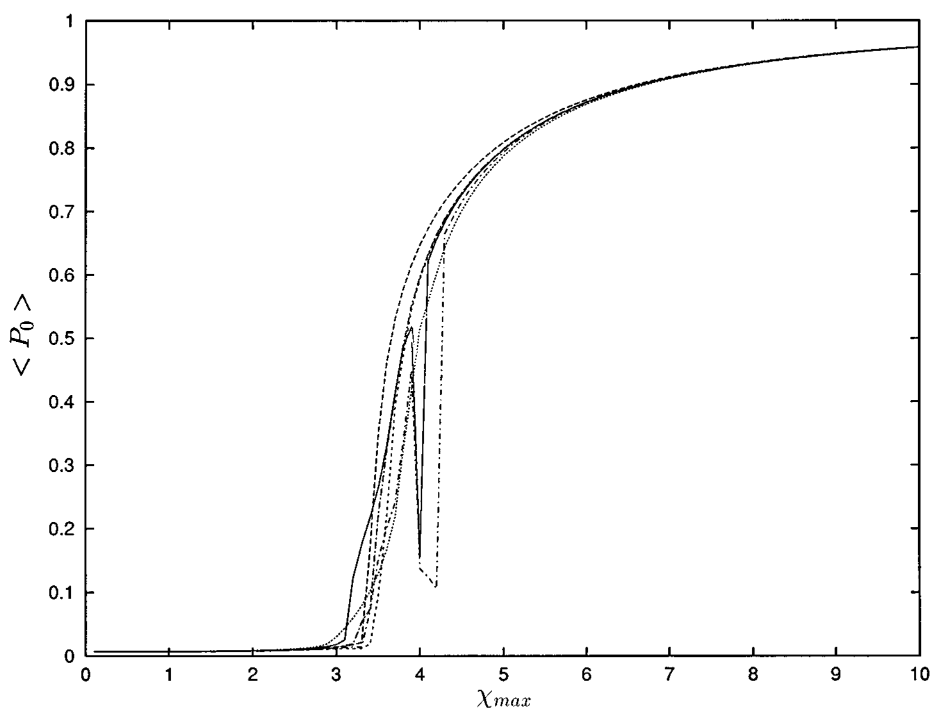

FIG. 8. Time-averaged probability of the initial excitation site ($\langle P_0\rangle$) as a function of $\chi_{\max}$ for different realizations of random nonlinear systems.

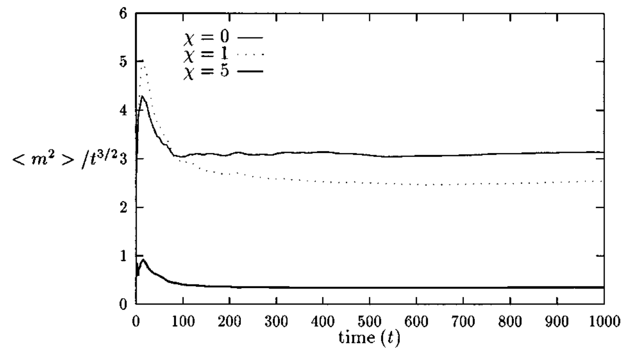

FIG. 9. Plot of $\langle m^2\rangle/t^{3/2}$ as a function of time (t) for the RDM with different values of χ. Here, $\epsilon_a=1$.

tered. Thus initially the dimer correlation is distorted. As the system contains an escape probability, the distortion of the dimer correlation decreases with increasing time. So we expect the superdiffusive behavior in the MSD. This is exactly obtained (see Fig. 9). The exponent of the MSD is $\sim$1.5. We also study the time-averaged probability of the initial excitation site which is one of the dimer sites. We obtain a sharp self-trapping transition at different values of $\chi_{\rm cr2}$ which increases as ϵ_a increases. Thus, by increasing the site energy we can alter the value of $\chi_{\rm cr2}$. For negative values of ϵ_a the value of $\chi_{\rm cr2}$ remains almost constant. If the initial excitation is applied at the site where dimer is absent, we obtain the opposite behavior. That is, for positive values of ϵ_a the $\chi_{\rm cr2}$ almost remain constant and for negative values of ϵ_a, and $\chi_{\rm cr2}$ changes significantly. Above $\chi_{\rm cr2}$ we also obtain the superdiffusive behavior in the MSD.

IV. SUMMARY

We have studied the dynamics of quasiparticles in different kinds of nonlinear systems. We first studied the dynamics of the quasiparticle in a cluster of nonlinear impurities embedded in a perfect linear host lattice. The initial excitation is applied either at the end site or at the middle site of the nonlinear cluster. In both the cases we studied the time-averaged site probabilities and the particle propagation. In the former case we observed the cluster-trapping transition at $\chi_{\rm cr1}$ due to the localization of the quasiparticle within the nonlinear cluster. For $\chi>\chi_{\rm cr1}$ the amplitude transition in the probabilities of the nonlinear sites is obtained, showing that the escape probability through linear sites is analogous to a damping term in the oscillator equation of motion. The absence of any well-defined transition in the amplitude of the site probabilities beyond $\chi_{\rm cr2}$ indicates the self-trapping at this value of χ. This value of $\chi_{\rm cr2}$ is $\sim$4.23 for any size of the clusters of the nonlinear sites. This clearly indicates that a single mechanism is responsible for self-trapping. For relatively large size clusters we observed that the localization of the quasiparticle occurs in the cluster in the form of a solitonlike wave extending over a few sites. This cluster localization starts between $\chi=3.1$ and 3.2. In the asymptotically large size of the nonlinear cluster we also find that the solitonlike wave moves along the cluster but after some time it localizes in a region. This localization time and the trapping region depend on χ. When the initial excitation is applied at the middle site of the cluster, cluster localization also occurs. The critical value in general increases with increasing the size of the cluster. However, here we do not find any sharp self-trapping transition as well as the transition in the amplitude of site probabilities.

The MSD in random nonlinear systems shows that the ballistic motion and the speed decreases significantly in the transition regime. The initial excitation is applied in this case at the site with maximum nonlinearity. The time-averaged probability of the initial excitation site is also studied for different realizations. In each case we obtained a rapid increase in $\langle P_0\rangle$ within a range of χ. It should be noted that beyond this region of χ the dynamics of the quasiparticle in the single nonlinear impurity system, in random nonlinear systems, and in the perfect nonlinear system are similar. The effect of nonlinearity on the superdiffusive behavior of the RDM has also been studied. The exponent of the MSD remains almost same. With increasing the strength of the nonlinearity the prefactor of the MSD decreases with the increase in χ. The self-trapping transition also occurs in this case. The self-trapping value of χ increases with increasing ϵ_a provided χ and ϵ_a both are positive quantities. For negative values of ϵ_a, this value of χ remains almost constant with increasing χ. This aspect will be studied later.

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