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Tuning the Kenkre-Campbell self-trapping transition

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We study the persistence of self-trapping in the presence of arbitrary large perturbations. We obtain the phase diagram for a nonlinear dimer interacting with a third linear impurity site and show that the abrupt Kenkre-Campbell transition is sustained. In addition to the "free" and "self-trapped" regimes we find a "chaotic" regime for some well-defined values of the nonlinearity and linear coupling parameters.

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The discrete nonlinear Schrödinger equation (DNSE), or discrete self-trapping equation, was introduced in 1985 [1] as a generic mathematical model for systems of coupled anharmonic oscillators. It has received considerable attention since due to its applicability in energy transport in molecular crystals [1–3], polyatomic molecules [4], nonlinear switching devices in nonlinear optics [5,6], etc. In the context of the tight-binding model for a one-dimensional solid, the DNSE has the form

$$i\hbar\frac{dc_m}{dt}=E_m c_m+\sum_n V_{mn}c_n-\chi|c_m|^2c_m\ , \tag{1}$$

where $c_m\equiv c_m(t)$ represents the probability amplitude for the excitation to be at a given site m at time t, E_m is the local energy at the mth site, V_{mn} is the intersite transfer matrix element that connects sites m and n, and χ is the nonlinear parameter arising from the excitation-phonon interaction in the antiabatic approximation [3]. Equation (1) can only be solved analytically for a small number of cases, one of which is that for a system with two sites, i.e., a nonlinear dimer. In this system a self-trapping transition occurs for certain values of the nonlinearity parameter and different initial conditions. Eilbeck, Lomdahl, and Scott [1] found a bifurcation in the stationary states of the nonlinear dimer occurring for $\chi=2V$, where $V_{12}=V_{21}\equiv V$. Kenkre and Campbell [7], on the other hand, focused on the time-dependent dimer solutions and showed that the equation for the probability difference in the site occupation $p=|c_1|^2-|c_2|^2$ is that for a classical particle in a quartic potential. For the case where only one of the sites is occupied initially, the solution, written explicitly in terms of Jacobian elliptic functions, shows two distinct regimes: While $0\le\chi/4V\le 1$, $p(t)$ oscillates around zero and there is a complete transfer of the excitation from one site to the other ("free" regime). At $\chi_{cr}=4V$ the trigonometriclike time evolution changes and gives rise to nonperiodic motion while for larger χ values ($\chi|4V>1$) the excitation remains trapped in the original site ("trapped" regime). In this latter case, $p(t)$ has a dc offset and the transfer of the excitation between the two sites is incomplete. The Kenkre-Campbell (KC) self-trapping transition for the nonlinear dimer depends on the initial conditions [8] and for a specific set of the latter can be seen to coincide with the Eilbeck *et al.* transition [9].

It is possible to find completely isolated (nonlinear) dimer systems [10]. There are instances, however, where impurity atoms can be found in close proximity to these nonlinear units or cases where the latter are embedded in a host lattice and are interacting with other nearby sites. In order to investigate the effects of (not necessarily small) perturbations in the KC self-trapping transition for the nonlinear dimer, we introduce the simplest possible "environment," viz. an additional (third) lattice site interacting with each of the other two through the matrix element W ($V_{13}=V_{23}\equiv W$). Equation (1) becomes ($\hbar\equiv 1$)

$$i\frac{dc_1}{dt}=Vc_2+Wc_3-\chi|c_1|^2c_1\ , \tag{2}$$

$$i\frac{dc_2}{dt}=Vc_1+Wc_3-\chi|c_2|^2c_2\ , \tag{3}$$

$$i\frac{dc_3}{dt}=W(c_1+c_2)\ . \tag{4}$$

These equations correspond to a doubly nonlinear trimer (DNT) with the third site being "linear." The exact evolution for the probability amplitudes can only be obtained for a limited set of initial conditions. For the symmetric initial conditions, for example, where $c_1(0)=c_2(0)$, we obtain $c_1(t)=c_2(t)$ at all times, and an explicit solution can be found in terms of ellipitic functions [11]. This solution does not, however, display an abrupt transition (in the sense of KC) and the degree of trapping varies in a continuous fashion with the nonlinear parameter χ [6].

To investigate the effects of the influence of the third

site on the KC self-trapping transition we numerically integrate Eqs. (2)–(4) with $c_m(0)=\delta_{m1}$. Following [7] we calculate $p \equiv |c_1(t)|^2 - |c_2(t)|^2$, the difference in the occupation probability of the nonlinear sites. In the $W=0$ limit we obtain the KC results with the self-trapping transition occurring at $\chi=4(V\equiv 1)$. As W increases (for a given $\chi \leq 4$), the free oscillations of the particle are sustained until a certain boundary is crossed. Then, depending on the actual χ value, the particle becomes either self-trapped or reaches a chaotic regime. For much larger W values, there is another transition from the self-trapping to a free regime. This behavior is shown in Fig. 1.

A complete numerical investigation of the W,χ parameter space leads to the W-χ phase diagram of Fig. 2. Three well-defined regions for free, trapped, and chaotic motion are obtained. These dynamic phases where obtained using two different criteria, the spectrum of $p(t)$ as well as its long time average p_{av}. The boundary lines obtained with ether method are in approximate agreement. When crossing, for instance, from the free to self-trapped motion, a center peak appears in the spectrum of $p(t)$ [Figs. 1(e) and 1(f)] accompanied by an *abrupt* change in p_{av} (Fig. 3). In the chaotic regime, on the other hand, the particle motion is erratic and the spectrum gets broadened [Figs. 1(c) and 1(d)]. The latter region is approximately bounded by the $\chi=4$ line where (for $W=0$) the KC transition occurs. Note that the self-trapping regime protrudes to very small χ values for appropriate W values. Self-trapping can now be tuned to occur almost at any desired small χ value, in marked contrast with the KC case.

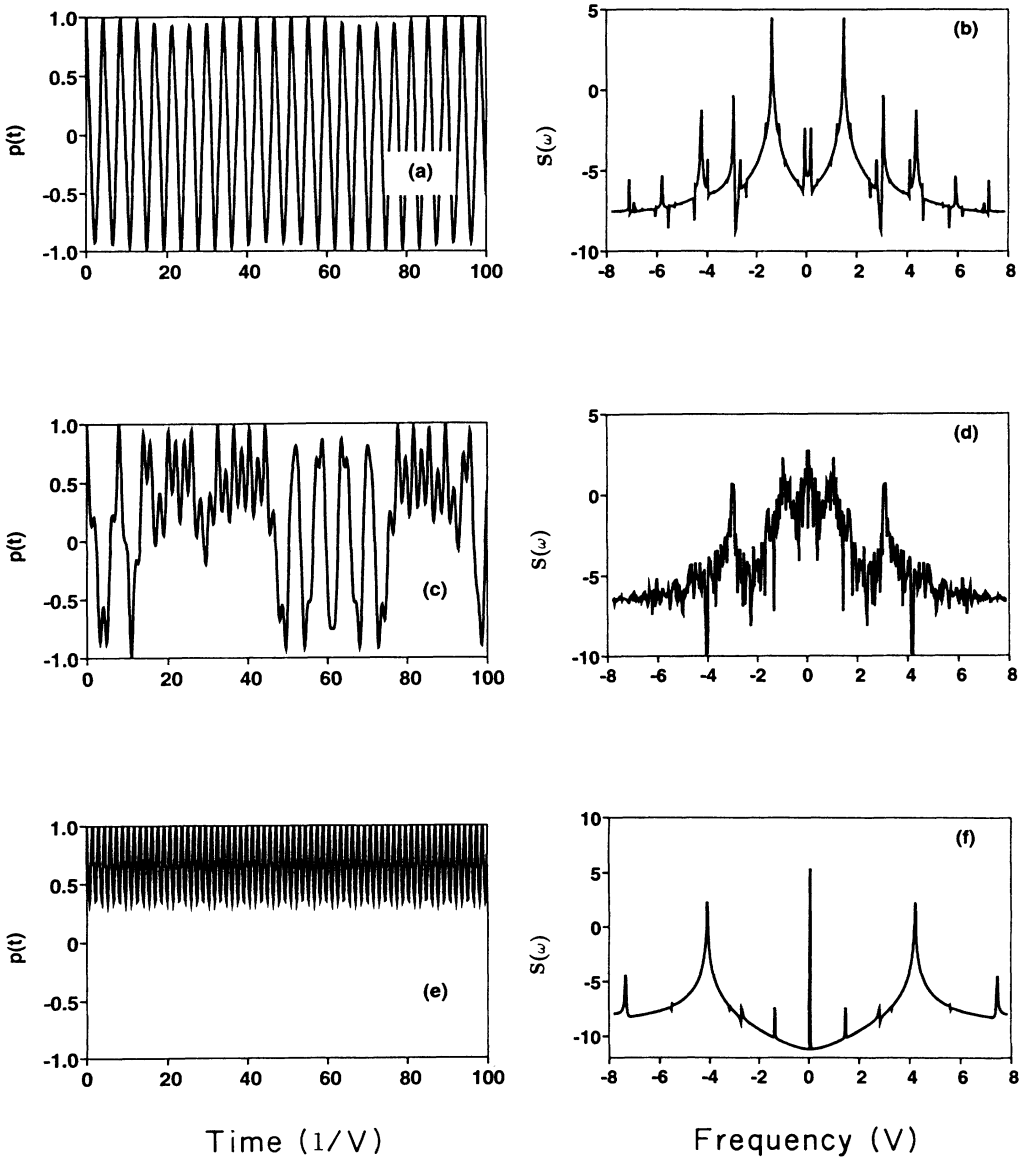

FIG. 1. (a), (c), and (e) probability difference $p(t)$ as a function of time and (b), (d), and (f) the corresponding power spectrum $S(\omega)$ as a function of frequency for $\chi=3.0$ and different values of the impurity matrix element W: (a) and (b) 0.3, (c) and (d) 0.6, and (e) and (f) 1.2. The strong center peak in (f) marks the self-trapped state. The scale for the spectrum (b), (d), and (f) is logarithmic.

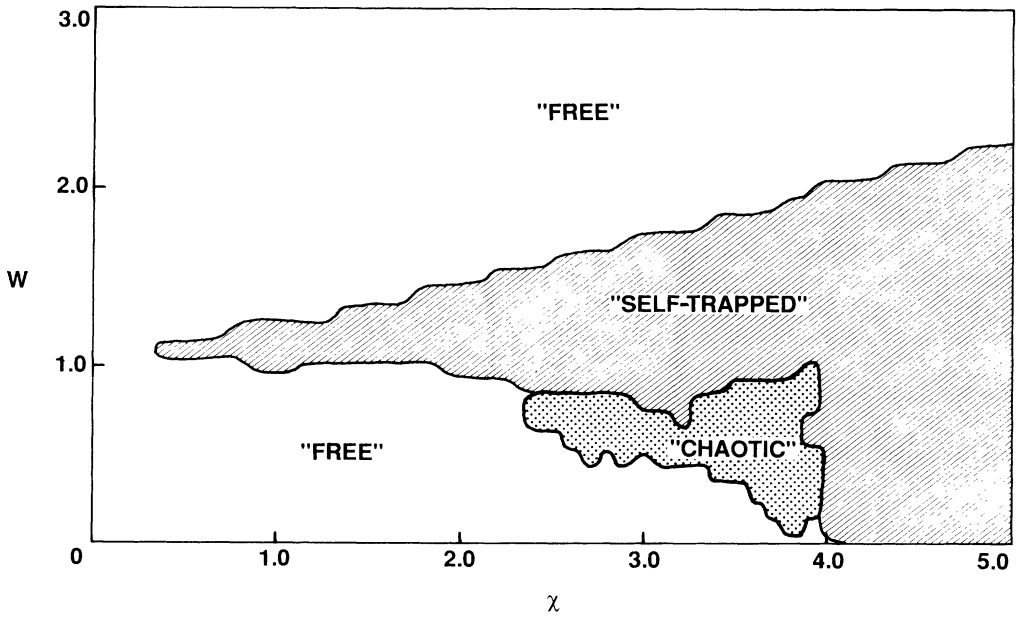

FIG. 2. Dynamical phases for the doubly degenerate trimer as a function of the impurity matrix element W and the nonlinearity parameter χ. The regimes labeled "free," "chaotic," and "self-trapped" designate complete, chaotic, and incomplete energy transfer, respectively. The boundary lines between the phases represent the approximate location where a discontinuous change in the dynamical behavior of the trimer occurs.

In order to ascertain the precise nature of the self-trapping transition, we investigate $p_{\rm av}$, the time-averaged probability difference for the nonlinear sites as a function of χ. We choose several different values of the linear coupling W and compare with the dimer as well as the completely linear case ($\chi=0$). For the latter (linear trimer with two nonequal transfer matrix elements) we obtain the exact solution for p:

$$p(t)=\tfrac{1}{4}[(1+8W^2)^{-1/2}-1]\cos\left[\frac{3-(1+8W^2)^{1/2}}{2}t\right] +\tfrac{1}{4}[(1+8W^2)^{-1/2}+1]\cos\left[\frac{3+(1+8W^2)^{1/2}}{2}t\right]. \tag{5}$$

In the linear trimer, $p_{\rm av}$ is always zero except for the "singular" case $W=1$, i.e., when all three overlap integrals are identical. Then, two of the energy eigenvalues are degenerate leading to maximum "linear" localization on the initial site that results in the largest possible probability difference, $p_{\rm av}=\frac{1}{3}$.

For $W=0$ we have the original KC problem with an abrupt self-trapping transition at $\chi_{\rm cr}=4$. When this nonlinear dimer interacts weakly (small W) with the linear impurity, the original KC picture is approximately preserved except for the additional small, well-localized chaotic regime that acts as a precursor to the self-trapping transition. As W increases, the chaotic regime extends to smaller nonlinearity values. For W values larger than approximately $W\approx 0.8$, chaos gives in to self-trapping. As W increases further, the KC self-trapping transition is being attracted to smaller and smaller χ values reaching a minimum at $W\approx 1.1$. Further increase of W repeals the transition to larger nonlinearity parameter values (Figs. 2 and 3).

The minimum in the $\chi_{\rm cr}$ value, which signals the occurrence of the self-trapping transition for $W\approx 1.1$, is a result of two oppositely "moving" localization phenomena [11]. The first is the attraction of the genuine KC transition to smaller χ values where the linear impurity state becomes more dominant. The other is related to the degeneracy found in the linear trimer for $W=1$. This degeneracy leads effectively to (linear) localization, which, in the presence of small energy mismatch (χ) is being shifted to slightly larger W values. The two localization tendencies in DNT meet at $W\approx 1.1$ leading to the aforementioned minimum in $\chi_{\rm cr}$. This ability to tune the occurrence of the self-trapping transition by changing,

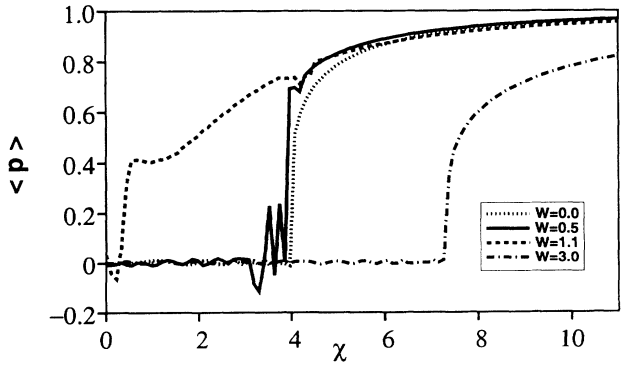

FIG. 3. Time-averaged probability difference $p_{\rm av}\equiv\langle p\rangle$ as a function of the nonlinearity parameter χ for different W values: 0.0 (dotted line), 0.5 (solid line), 1.1 (dashed line), and 3.0 (dash-dotted line). The critical nonlinearity $\chi_{\rm cr}$ for the abrupt self-trapping transition initially decreases as a function of W, reaches a minimum at approximately $W\approx 1.1$, and subsequently increases.

for instance, the distance of the impurity site from the nonlinear dimer can have important experimental ramifications in spectroscopic studies [12], as well as in nonlinear optics. The tunability of the dimer transition depends sensitively on the initial conditions used. A complete study will be presented elsewhere [11].

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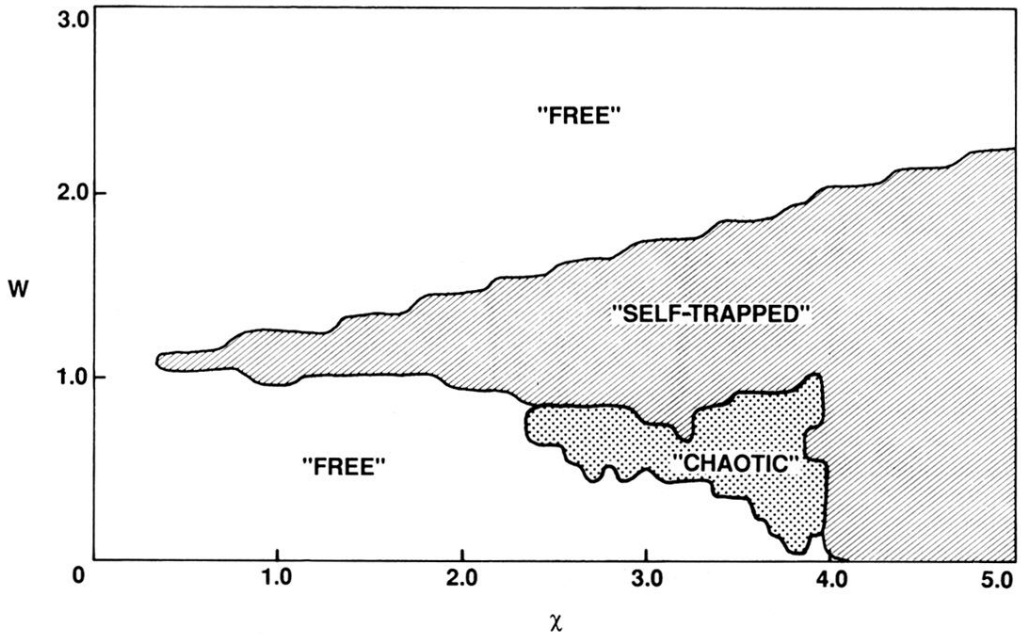

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