Nature of transitions in augmented discrete nonlinear Schrödinger equations

R. E. Amritkar* and V. M. Kenkre
Center for Advanced Studies and Department of Physics, University of New Mexico, Albuquerque, New Mexico 87131
(Received 15 December 1998)

We investigate the nature of the transitions between free and self-trapping states occurring in systems described by augmented forms of the discrete nonlinear Schrödinger equation. These arise from an interaction between a moving quasiparticle (such as an electron or an exciton) and lattice vibrations, when the effects of nonlinearities in interaction potential and restoring force are included. We derive analytic conditions for the stability of the free state and the crossover between first- and second-order transitions. We demonstrate our results for different types of nonlinearities in the interaction potential and restoring force. We find that, depending on the type of nonlinearity, it is possible to have both first- and second-order transitions. We discuss possible hysteresis effects. [S1063-651X(99)13305-1]

PACS number(s): 64.60.−i, 05.70.Fh, 71.38.+i, 05.45.−a

I. INTRODUCTION

The discrete nonlinear Schrödinger equation,

$$i\hbar\frac{dc_m}{dt}=\sum_n V_{mn}c_n-\chi|c_m|^2c_m, \tag{1.1}$$

has appeared in many contexts in recent years [1–3] in the description of the motion of quasiparticles. Typically, c_m is the amplitude of the system to be in state $|m\rangle$, V_{mn} are intersite transfer-matrix elements describing the linear evolution among states $|m\rangle$, and χ is the nonlinearity parameter. The microscopic origin and the precise extent of validity of Eq. (1.1) have come under close scrutiny recently [4–6]. However, Eq. (1.1) continues to be considered as a useful starting point for transport investigations. It is generally assumed that Eq. (1.1) may be written down as arising from the following coupled equations of motion:

$$i\hbar\frac{dc_m}{dt}=\sum_n V_{mn}c_n+E_0x_mc_m, \tag{1.2}$$

$$\frac{d^2x_m}{dt^2}+\omega^2x_m+S|c_m|^2=0. \tag{1.3}$$

Here, x_m is a vibrational displacement and ω is the frequency of the vibration, and the last terms in the right-hand side of Eq. (1.2) and the left-hand side of Eq. (1.3) describe the interaction of the vibrations with the quasiparticle, E_0 and S being appropriate constants. Time-scale disparity arguments lead to Eq. (1.1), the nonlinearity parameter χ being equal to E_0S/ω^2.

Generalizations of these results have been shown to arise [3,7,8] when account is taken of the fact that molecular oscillators are not generally governed by linear (Hooke's type) restoring forces, and that the interaction energy is generally nonlinear in the oscillator displacement. The generalizations of Eqs. (1.2) and (1.3) lead to [3,7,8]

$$i\hbar\frac{dc_m}{dt}=\sum_n V_{mn}c_n+E(x_m)c_m, \tag{1.4}$$

$$\frac{d^2x_m}{dt^2}+\omega^2f(x_m)+RE'(x_m)|c_m|^2=0. \tag{1.5}$$

The nonlinearities in Eqs. (1.4) and (1.5) can give rise to exotic behavior as shown earlier [3,7,8] including the destruction of self-trapping on increasing nonlinearity. In these cases, as the nonlinearity parameter is increased, we first get a transition to a self-trapping state. But, as the nonlinearity parameter is further increased, the self-trapping state is destroyed with a resulting extended or free quasiparticle.

In the present paper we investigate the *nature* of the free to self-trapping transition for the case of a dimer when generalized forms of the discrete nonlinear Schrödinger equation such as Eqs. (1.4) and (1.5) are operative. We show that, if the transition is of first-order, hysteresis effects will be observed as the nonlinearity parameter is increased and then decreased through the transition point. We derive a general analytic condition for the point in parameter space where the second-order transition turns into a first-order transition as the parameters are varied. We demonstrate this effect by considering several forms of nonlinearities in $f(x_m)$ and $E(x_m)$.

II. TRANSITION BETWEEN EXTENDED AND SELF-TRAPPING STATES

Following the steps described in Ref. [7], one may write, under the assumption of time-scale disparity in Eqs. (1.4) and (1.5), a closed equation for the quasiparticle amplitude c_m,

$$i\hbar\frac{dc_m}{dt}=\sum_n V_{mn}c_n-h(|c_m|^2)c_m, \tag{2.1}$$

where $h(|c_m|^2)$ is simply $-E(x_m)$, the quantity x_m being expressed as a function of $|c_m|^2$ obtained as a solution of

*Permanent address: Physical Research Laboratory, Navrangpura, Ahmedabad 380009, India.

$$f(x_m) = -(R/\omega^2)E'(x_m)|c_m|^2. \tag{2.2}$$

Further, for the case of a dimer ($m=1,2$), a closed evolution equation for the probability difference $p=|c_1|^2-|c_2|^2$ results [7]:

$$\frac{d^2p}{dt^2} = -\frac{dU(p)}{dp}, \tag{2.3}$$

$$U(p) = 2V^2p^2 + g(p)[\tfrac{1}{2}g(p) - g(p_0) + 2Vr_0]. \tag{2.4}$$

The function $U(p)$ can be viewed as the potential energy of a fictitious classical oscillator whose displacement is the probability difference p. In Eq. (2.4), the function $g(p)$ is given, up to an arbitrary constant, by

$$\frac{dg(p)}{dp} = h\left(\frac{1+p}{2}\right) - h\left(\frac{1-p}{2}\right), \tag{2.5}$$

and p_0, q_0, and r_0 are the initial values of p, and of $q = i(c_1^*c_2 - c_2^*c_1)$ and $r = c_1^*c_2 + c_2^*c_1$, respectively, and we have put $\hbar = 1$.

The stationary states can be analyzed [8] in a simpler manner. Thus, p_s, the value of the probability difference in the stationary states obeys

$$2Vp_s = \pm\sqrt{1-p_s^2}\left[\frac{dg(p)}{dp}\right]_{p=p_s}. \tag{2.6}$$

We would now like to point out that the stability of the stationary solutions of Eq. (2.6) with $q=0$ can be decided simply by considering the eigenvalues of the matrix,

$$\begin{pmatrix} 0 & 2V & 0 \\ -2V-g''r & 0 & g' \\ 0 & g' & 0 \end{pmatrix}, \tag{2.7}$$

where the primes refer to derivatives with respect to the argument. This stability matrix is obtained using the following equations for p, q, and r [7]:

$$\frac{dp}{dt} = 2Vq,$$

$$\frac{dq}{dt} = -2Vq - r\frac{dg}{dp},$$

$$\frac{dr}{dt} = q\frac{dg}{dp}.$$

The stationary solution is stable provided the real parts of all the eigenvalues of the matrix (2.7) are negative or zero.

Consider the extended or free polaron solution, which corresponds to $p_s=0$, and is always a solution of Eq. (2.6). The stability of this solution can be studied by considering the eigenvalues of the matrix (2.7). An equivalent procedure is to equate the slopes of the two sides of Eq. (2.6) at $p_s = 0$. The condition for the transition between the stable and unstable free polaron states is given by

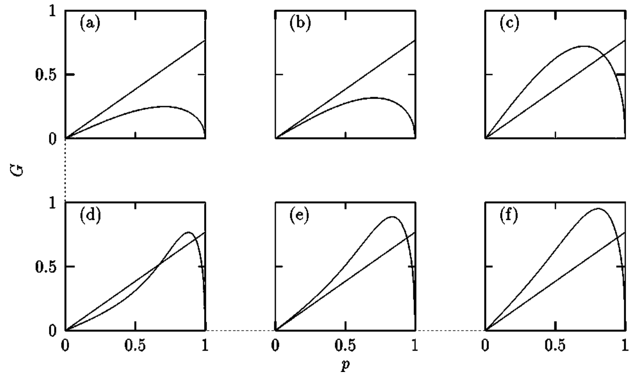

FIG. 1. Schematic plots of the graphical solution to Eq. (2.6). The plots (a), (b), and (c) show the graphs of $G(p_s)$ and $2Vp_s$ as a function of p_s near a second-order transition from a free to a self-trapping state. (a) shows the situation when the free state is stable while (c) shows the situation when the self-trapping state is stable. (b) shows the plot at the transition. The plots (d), (e), and (f) correspond to the situation near a first-order transition when the free state changes from a stable to an unstable state. (d) shows the plot when the free state is stable while (f) shows the plot when it is unstable. (e) represents the transition. Note that the condition (2.8) is satisfied in both (b) and (e). The crossover between (b) and (e) is given by the condition (2.12).

$$g''(0) = h'(\tfrac{1}{2}) = 2V. \tag{2.8}$$

The function h and its derivatives will, in general, depend on the nature of nonlinearities. As $h'(1/2)$ increases with the nonlinearity parameter, and crosses the value $2V$, we get a transition from a free to a self-trapping state. As the nonlinearity parameter further increases, it is possible that the self-trapping state is destroyed if $h'(1/2)$ decreases again and falls below the value $2V$. An interesting situation arises if $h'(1/2) < 2V$ for all values of the parameters. In this case the free state is always stable and, in general, the self-trapping state will not be obtained except in some special cases to be discussed afterwards.

An alternative way of expressing Eq. (2.8), although perhaps not particularly transparent, is

$$\frac{R(E'(x))^2}{\omega^2 f'(x) + \dfrac{R}{2}E''(x)} = 2V, \tag{2.9}$$

where x is given by the solution of $\omega^2 f(x) = -(R/2)E'(x)$.

What is the nature of the transition when condition (2.8) is satisfied? To answer this question it is necessary to consider the nature of the plot of the right-hand side of Eq. (2.6), say $G(p_s)$, as a function of p_s.

$$G(p_s) = \sqrt{1-p_s^2}\left[\frac{dg(p)}{dp}\right]_{p=p_s}. \tag{2.10}$$

Schematic plots of G and $2Vp_s$ versus p_s near the first-order and second-order transitions in the vicinity of the point where condition (2.8) is satisfied, are shown in Fig. 1. Expanding the function G in Taylor series for small p_s, we get

$$G\sim g''(0)p_s+\left(\frac{g''''(0)}{6}-\frac{g''(0)}{2}\right)p_s^3+\ \ldots, \quad (2.11)$$

where we have used $g'(0)=g'''(0)=0$ [see Eq. (2.5)]. The crossover between the second-order and first-order transitions is obtained when the second term on the right-hand side of the above Taylor expansion is zero. Using Eqs. (2.8) and (2.11), the condition for the crossover is given by

$$g''''(0)=\frac{h'''(1/2)}{4}=6V, \quad (2.12)$$

where the relation between the derivatives of g and h is obtained using Eq. (2.5). Note that the condition (2.12) obtained above corresponds to the crossover between Figs. 1(b) and 1(e). When both the conditions (2.8) and (2.12) are satisfied, we get a crossover from a second-order transition between the free and self-trapping states to a first-order transition between these states. The second-order transition is obtained when $h'''(1/2)<24V$ and $h'(1/2)=2V$.

For the case of a first-order transition, experimental manipulation of hysteresis effects is possible in principle if the nonlinearity parameter can be controlled experimentally. One end of the hysteresis loop is given by Eq. (2.8) while the other end is obtained as the simultaneous solution of Eq. (2.6) and of

$$2V=\frac{1}{2}\left[h'\left(\frac{1+p_s}{2}\right)+h'\left(\frac{1-p_s}{2}\right)\right](1-p_s)^{3/2}. \quad (2.13)$$

Within these two extremes both the free and self-trapping states will be stable. The point at which the actual first-order phase transition occurs can be calculated by equating the potential energies of the free and self-trapping states using Eq. (2.4) for the fictitious oscillator with displacement p_s.

III. EXAMPLES

We now consider several examples that illustrate how the nonlinearities affect the transition between free and self-trapping states and how interesting crossover aspects occur between the first- and second-order transitions.

A. Harmonic linear case

For the case of harmonic potential and linear interaction [see Eq. (1.1)],

$$h(|c|^2)=\chi|c|^2. \quad (3.1)$$

Condition (2.8) gives $\chi=2V$. Thus the free state becomes unstable giving a self-trapping state as χ is increased beyond $2V$ and remains in the self-trapping state for larger values of χ. Condition (2.12) is never satisfied (except for $V=0$) and hence the transition to self-trapping state is always second-order.

B. Rotational polaron

Consider the system termed a rotational polaron by Kenkre *et al.* [7] wherein x is a rotation rather than a vibration and, therefore, denoted by an angle variable θ. The system could be an electron/exciton moving among the sites m of a chain, there being a rotator (for example, a dipole) at each site m whose angle from a fixed direction is θ. The choice of an identical sinusoidal dependence on θ for both the restoring force and the interaction energy,

$$f(\theta)=\frac{\sin(\Lambda\theta)}{\Lambda},$$

$$E(\theta)=\frac{E_0}{\Lambda}\sin(\Lambda\theta), \quad (3.2)$$

are known [7] to lead to

$$h(|c|^2)=\frac{\chi|c|^2}{\sqrt{1+(\chi/\Delta)^2|c|^4}}. \quad (3.3)$$

where $\Delta=E_0/\Lambda$ and $\chi=E_0^2R/\omega^2$. The limit $\Lambda\to 0$ gives the standard linear harmonic case. Here the oscillator potential is $[1-\cos(\Lambda\theta)]/\Lambda^2$.

We apply our condition (2.8) for the transition to self-trapping state and obtain

$$h'\left(\frac{1}{2}\right)=\frac{\chi}{\left[1+\left(\frac{\chi}{2\Delta}\right)^2\right]^{3/2}}=2V. \quad (3.4)$$

First we note that the maximum of $h'(1/2)$ occurs at $(\chi/\Delta)^2=2$. If the maximum value of $h'(1/2)$ is less than $2V$, the self-trapping state is *never* obtained. This gives the condition for the existence of self-trapping state as $(\Delta/V)^2>27/4$. This is the same condition as obtained by Wu and Kenkre [8] through a more elaborate procedure of solving a cubic equation. We also note that, for $(\Delta/V)^2>27/4$, Eq. (3.4) has two solutions as the nonlinearity parameter χ is varied. To determine the order of the transition, we use our second condition (2.12) to obtain

$$h'''\left(\frac{1}{2}\right)=3\chi(\chi/\Delta)^2\frac{(\chi/\Delta)^2-1}{[1+(\chi/2\Delta)^2]^{7/2}}=24V. \quad (3.5)$$

Using Eqs. (3.4) and (3.5), we find that the crossover between first-order and second-order transitions is obtained when

$$(\chi/V)^2=4(1+a)^2, \quad (\Delta/V)^2=(1+a)^3/a,$$

$$a=(3+\sqrt{21})/6. \quad (3.6)$$

Figure 2 shows the phase-space plot of the system (3.2) in the Δ/V versus χ/V plane. The solid lines represent the second-order transition while the dashed line corresponds to the first-order transition. We notice that the free to self-trapping transition as χ is increased, is always second order while the self-trapping to free transition (reentrant transition) can be first-order *or* second-order. The two dash-dot lines on either side of the first-order transition show the parameter range where both the free and self-trapping states are stable and thus hysteresis effects may be observed as the nonlinearity parameter χ is varied.

Figure 3 shows the plot of the stationary solutions p_s as a function of the nonlinearity parameter χ/V for two different

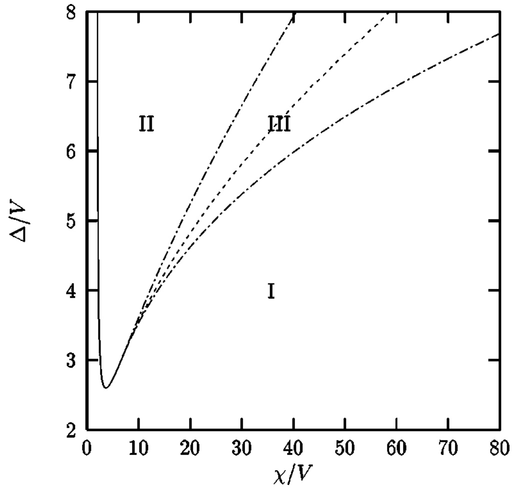

FIG. 2. Plot of the phase diagram for the rotational polaron with sinusoidal nonlinearities in the parameter space, V/Δ versus χ/Δ, showing the regions of free and self-trapping states denoted by I and II, respectively. The solid line corresponds to a second-order transition while the dashed line corresponds to a first-order transition. The dash-dot lines on either side of the first-order transition enclose the region of hysteresis effects (denated by III) where both free and self-trapping states are stable.

values of Δ/V showing both first-order and second-order transitions. Note that, for the first-order transition, we will observe a hysteresis loop as the nonlinearity parameter is varied.

It is interesting to note that the form of the function $h(|c|^2)$ in Eq. (3.3) is very general and can be obtained for other types of nonlinearities also. Consider the case where the oscillator potential is $[1-\mathrm{sech}(\Lambda x)]/\Lambda^2$, and

$$f(x)=\frac{1}{\Lambda}\mathrm{sech}(\Lambda x)\tanh(\Lambda x),$$

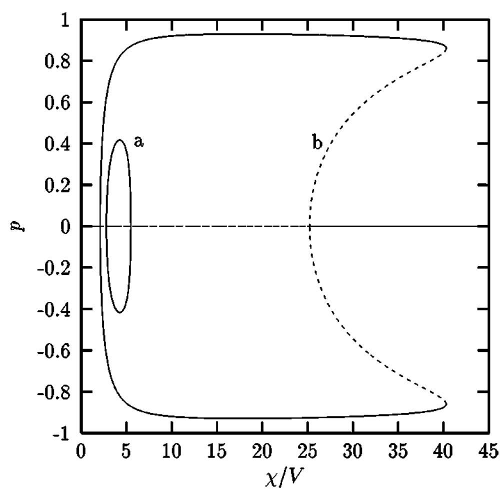

FIG. 3. Plot of the stationary-state probability difference p_s versus the parameter χ/V showing the onset of self-trapping followed by its disappearance on increasing nonlinearity for the rotational polaron. Curves (a) and (b) correspond to $\Delta/V=2.8$ and 6, respectively. In (a) the transition corresponding to the disappearance of self-trapping is of second order while in (b) it is of first order. The stable states are shown by solid line while the unstable states are shown by dashed lines. The region of stability of the free state ($p_s=0$) is shown only for $\Delta/V=6$ (curve b).

$$E(x)=\frac{E_0}{\Lambda}\tanh(\Lambda x). \tag{3.7}$$

It is easy to verify that the form of the function $h(|c|^2)$ is the same as Eq. (3.3). More general nonlinear functions may be written with the oscillator potential $[1-\mathrm{cn}(\Lambda x|k)]\Lambda^2$, and

$$f(x)=\frac{1}{\Lambda}\mathrm{sn}(\Lambda x|k)\mathrm{dn}(\Lambda x|k),$$

$$E(x)=\frac{E_0}{\Lambda}\mathrm{sn}(\Lambda x|k), \tag{3.8}$$

where cn and sn are Jacobian elliptic functions with the elliptic modulus k. If $k=0$, the functions cn and sn are, respectively, cos and sin [Eqs. (3.2]. If $k=1$, they are, respectively, sech and tanh. Again, using the properties of Jacobian elliptic function, it is possible to show that $h(|c|^2)$ has the same form as in Eq. (3.3). Thus the phase diagram is similar to that of Fig. 2.

C. Logarithmically hard oscillator

Consider an oscillator, which behaves normally for small displacements x (simple harmonic), while it has a hard spring force for large displacements. Such an oscillator has been modeled by the following oscillator potential $\mathcal{U}(x)$ [9,10]:

$$\mathcal{U}(x)=ka(a-|x|)\left[\ln\left(1-\frac{|x|}{a}\right)+|x|\right]. \tag{3.9}$$

Note that this potential is defined only for $|x|<a$ and it reduces to the harmonic potential $\frac{1}{2}kx^2$ for small x. As $|x|\to a$, the potential diverges. The nonlinear function $f(x)$ is given by

$$f(x)=\begin{cases}-ka\ln\left(1-\frac{x}{a}\right) & \text{for} \quad x>0\\ ka\ln\left(1+\frac{x}{a}\right) & \text{for} \quad x<0,\end{cases} \tag{3.10}$$

and the interaction will be taken to be linear, i.e., $E(x)=E_0x$. The function h has then an exponential form [9,10]:

$$h(|c|^2)=\chi_0(1-e^{-(\chi/\chi_0)|c|^2}), \tag{3.11}$$

where the nonlinearity parameter χ and the saturation parameter χ_0 are given by

$$\chi=\frac{GE_0}{k},\quad \chi_0=E_0a. \tag{3.12}$$

Condition (2.8) for the transition to self-trapping state gives

$$h'(\tfrac{1}{2})=\chi e^{-\chi/2\chi_0}=2V. \tag{3.13}$$

The results are very similar to the sinusoidal nonlinearities considered in the previous subsection. By considering the maxima of $h'(1/2)$ we find that the self-trapping state does not exist if $(\chi_0/V)<e$. For $(\chi_0/V)>e$, Eq. (3.13) has two

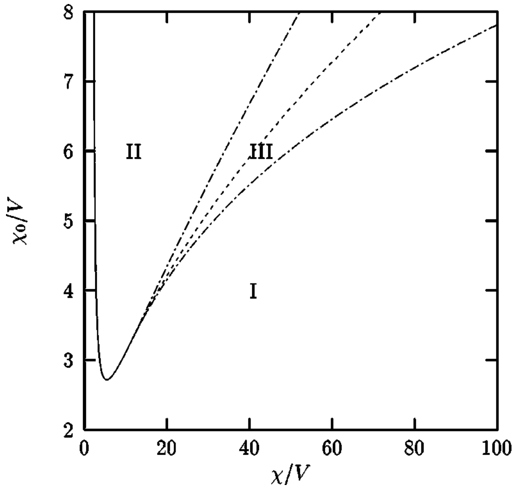

FIG. 4. Plot of the phase diagram for the logarithmically hard potential in the parameter space, χ_0/V versus χ/V, showing the regions of free and self-trapping states shown by I and II, respectively. The solid line corresponds to a second-order transition while the dashed line corresponds to a first-order transition. The dash-dot lines on either side of the first-order transition enclose the region of hysteresis effects (region III).

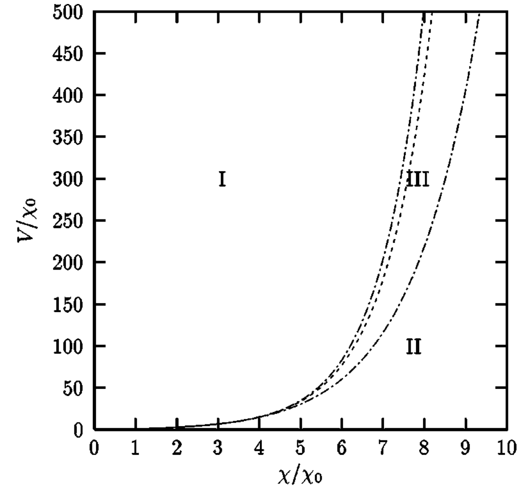

FIG. 5. Plot of the phase diagram for the logarithmically soft potential in the parameter space, V/χ_0 versus χ/χ_0, showing the regions of free and self-trapping states shown by I and II, respectively. The solid line corresponds to a second-order transition while the dashed line corresponds to a first-order transition. The dash-dot lines on either side of the first-order transition enclose the region of hysteresis effects (region III).

solutions as the nonlinearity parameter χ is varied. The second condition (2.12) which determines the order of the transition, gives

$$h'''(\tfrac{1}{2})=\frac{\chi^3}{\chi_0^2}\,e^{-\chi/2\chi_0}=24V. \tag{3.14}$$

Equations (3.13) and (3.14) give us the following condition for the crossover between first-order and second-order transition:

$$\frac{V}{\chi_0}=\sqrt{3}e^{-\sqrt{3}},\quad \frac{\chi}{\chi_0}=2\sqrt{3}. \tag{3.15}$$

Figure 4 shows the phase-space plot in the χ_0/V versus χ/V plane. The behavior is very similar to the one observed for the sinusoidal potential case treated in the previous subsection (Fig. 2).

D. Logarithmically soft oscillator

Consider an oscillator, which behaves normally for small displacements x (simple harmonic), while it has a *soft* spring force for large displacements. We model this by the following oscillator potential $\mathcal{U}(x)$:

$$\mathcal{U}(x)=ka(a+|x|)\left[\ln\left(1+\frac{|x|}{a}\right)-|x|\right]. \tag{3.16}$$

The nonlinear function $f(x)$ is given by

$$f(x)=\begin{cases} ka\ln\left(1+\dfrac{x}{a}\right) & \text{for}\quad x>0\\ -ka\ln\left(1-\dfrac{x}{a}\right) & \text{for}\quad x<0. \end{cases} \tag{3.17}$$

We take the interaction to be linear, i.e., $E(x)=E_0x$. The function h has the form,

$$h(|c|^2)=\chi_0(e^{(\chi/\chi_0)|c|^2}-1), \tag{3.18}$$

where we have introduced the nonlinearity parameter $\chi=GE_0/k$ and the saturation parameter $\chi_0=ka$. Condition (2.8) for the transition to self-trapping state gives

$$h'(\tfrac{1}{2})=\chi e^{\chi/2\chi_0}=2V. \tag{3.19}$$

We note that $h'(1/2)$ is a monotonically increasing function of χ and has a solution for all values of V. This is similar to the case of simple harmonic oscillator. However, unlike the simple harmonic oscillator, the transition in this case can be *both first- and second-order*. The second condition (2.12), which determines the order of the transition, gives

$$h'''(\tfrac{1}{2})=\frac{\chi^3}{\chi_0^2}e^{\chi/2\chi_0}=24V. \tag{3.20}$$

Equations (3.19) and (3.20) give us the following condition for the crossover between first-order and second-order transition:

$$\frac{V}{\chi_0}=\sqrt{3}e^{\sqrt{3}},\quad \frac{\chi}{\chi_0}=2\sqrt{3}, \tag{3.21}$$

Figure 5 shows the phase-space plot in the V/χ_0 versus χ/χ_0 plane. Figure 6 shows the plot of the stationary states p_s as a function of χ/χ_0 for two different values of V/χ_0 showing both the second- and the first-order transitions.

Before we conclude this section, we note that in the cases when the free state never loses its stability as the nonlinearity parameter is varied, it is still possible that the self-trapping state is stable in some parameter range. As an example, consider the following form of the function h:

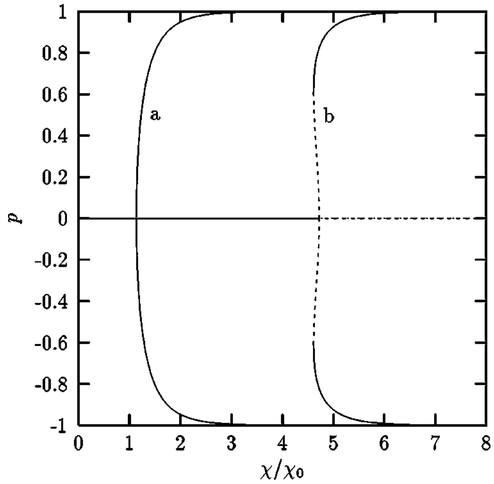

FIG. 6. Plot of the stationary-state probability difference p_s versus the parameter χ/χ_0 showing the onset of self-trapping for the logarithmically hard potential. Curves (a) and (b) correspond to $V/\chi_0=1$ and 25, respectively. In (a) the transition corresponding to the free to self-trapping state is of second-order while in (b) it is of first-order. The stable states are shown by solid lines while the unstable states are shown by dashed lines. The region of stability of the free state ($p_s=0$) is shown only for $V/\chi_0=25$ (curve b).

$$h(|c|^2)=\chi_0(e^{(\chi/\chi_0)[|c|^2-0.05(\chi/\chi_0)]}-1). \qquad (3.22)$$

Let $V/\chi_0=9$. In this case, the free state is always stable since condition (2.8) is not satisfied for any value of the nonlinearity parameter χ. The self-trapping state is stable between $\chi/\chi_0=7.238\ldots$ to $11.520\ldots$. The plot of the stationary states p_s as a function of χ/χ_0 will show two closed loops on either sides of $p_s=0$ axes. However, we expect that the types of function h as in Eq. (3.22) correspond to exotic forms of nonlinearities in the interaction potential and anharmonicities of vibrations and are unlikely to be physically relevant. For example, the unharmonic potential, which gives the function h in Eq. (3.22), is a sum of a linear term proportional to $|x|$ and a logarithmically soft potential.

IV. CONCLUDING REMARKS

We have investigated the nature of the free to self-trapping transition relevant to the effect of nonlinearities in the interaction potential and anharmonicities in the restoring force in a system consisting of quasiparticles interacting with vibrations. We have given explicit calculations for the two-site system. We have determined the phase diagram of the system in parameter space. The regions of free and self-trapping states have been clearly identified. We have shown how the nature of the transition between these states can be determined. The first-order transition shows hysteresis effects as the parameter is varied. We have illustrated our results using several examples. For the rotational polaron with sinusoidal interaction we have found that the transition involving the onset of the self-trapping state is second-order but that the one corresponding to the destruction of the self-trapping state could be first-order or second-order. The same conclusions emerge for the logarithmically hard oscillator potential. For the logarithmically soft potential we have found that the transition for the onset of the self-trapping state can be both first order or second order. There is no destruction of the self-trapping state in this case.

ACKNOWLEDGMENT

This work was supported in part by the National Science Foundation under Grant no. DMR-9614848.

[1] J.C. Eilbeck, P.S. Lomdahl, and A.C. Scott, Physica D **16**, 318 (1985); V.M. Kenkre and D. Campbell, Phys. Rev. B **34**, 4959 (1986); V.M. Kenkre, G.P. Tsironis, and D. Campbell, in *Nonlinearities in Condensed Matter*, edited by A.R. Bishop, D.K. Campbell, P. Kumar, and S. Trullinger (Springer-Verlag, Berlin, 1987).

[2] J.C. Eilbeck and A.C. Scott, in *Structure, Coherence, and Chaos in Dynamical Systems*, edited by P.L. Christiansen and R.D. Parmentier (Manchester University Press, Manchester, 1989), p. 139, and references therein; J.C. Eilbeck, in *Davydov's Soliton Revisited: Self-trapping of Vibrational Energy in Protein*, edited by P.L. Christiansen and A.C. Scott (Plenum, New York, 1990), and references therein.

[3] V.M. Kenkre, in *Singular Behaviour and Nonlinear Dynamics*, edited by S. Pnevmatikos, T. Bountis, and Sp. Pnevmatikos (World Scientific, Singapore, 1989), Vol. II; Physica D **68**, 153 (1993), and references therein.

[4] D. Vitali, P. Allegrini, and P. Grigolini, Chem. Phys. **180**, 297 (1994).

[5] M.I. Salkola, A.R. Bishop, V.M. Kenkre, and S. Raghavan, Phys. Rev. B **52**, 3824 (1995); V.M. Kenkre, S. Raghavan, A.R. Bishop, and M.I. Salkola, *ibid.* **53**, 5407 (1996).

[6] V.M. Kenkre, J. Lumin. **76**, 511 (1998).

[7] V.M. Kenkre, H.-L. Wu, and I. Howard, Phys. Rev. B **51**, 15 841 (1995).

[8] H.-L. Wu, Ph.D. thesis, University of New Mexico, 1989; H.-L. Wu and V.M. Kenkre, Phys. Lett. A **199**, 61 (1995).

[9] V.M. Kenkre, M.F. Jørgensen, and P. Christiansen, Physica D **90**, 280 (1996).

[10] V.M. Kenkre, Physica D **113**, 233 (1998).