Effects of interaction-potential nonlinearities and restoring-force anharmonicities in the discrete nonlinear Schrödinger equation

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The standard discrete nonlinear Schrödinger equation results from an interaction between a moving quasiparticle (such as an electron or an exciton) and lattice vibrations that is linear in the lattice displacements, and a restoring force for the vibrations that is harmonic. We study the effects of nonlinearity in interaction and of anharmonicities in the restoring force on the transport of the quasiparticle. We obtain a generalized transport equation, construct a formalism to solve it, and find explicit solutions appropriate to the evolution of rotational polarons. Rich behavior emerges including saturation of nonlinearities and destruction of self-trapping on increasing the nonlinearity.

I. INTRODUCTION

The discrete nonlinear Schrödinger equation, which describes a number of phenomena in various fields of physics, may be written as

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

where c_m is the amplitude for the system to be in state $|m\rangle$, V_{mn} are intersite transfer-matrix elements describing the linear evolution among the states $|m\rangle$, and χ is the nonlinearity parameter. In the specific system of an electron or exciton in a crystal interacting strongly with phonons or vibrations, $|m\rangle$ denotes the (localized) Wannier state centered on site m, V_{mn} are proportional to the bandwidth of the bare electron or exciton, and χ is the energy lowering due to polaronic effects, often written as a sum of the products of the vibrational energies of the participating modes and the square of their coupling constants with the electron or exciton.

Equation (1.1) or similar equations have been written down or derived by a variety of people in a variety of contexts.[1-7] While the microscopic origin and the precise extent of validity of (1.1) continue to be debated upon actively in the literature,[8-12] it is often assumed that (1.1) may be written down as arising from the following coupled equations of motion for the amplitude c_m of the quasiparticle (electron/exciton), and for the displacement x_m of the molecule which is in strong interaction with the quasiparticle:

$$i\hbar \frac{dc_m}{dt} = \sum_n V_{mn} c_n + E_0 x_m c_m , \tag{1.2}$$

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

The frequency of the molecular vibrations is ω, and the last terms in the right-hand side of (1.2) and the left-hand side of (1.3) describe the interaction of the vibrations with the quasiparticle. In (1.2), the manifestation of the interaction is in the dependence of the energy of the mth

site on the displacement x_m, while in (1.3) it is in the dependence of the force exerted on the molecular oscillator on the probability $|c_m|^2$ that the quasiparticle occupies site m. Here, E_0 and S are appropriate constants. The standard manner (see, e.g., Ref. 7) in which one derives (1.1) from the coupled equations (1.2) and (1.3), is through an argument of time-scale disparity which allows one to neglect the first term in (1.3). On substituting a term proportional to $|c_m|^2$ for x_m in the last term of (1.2), one then obtains (1.1), the nonlinearity parameter χ being equal to $E_0 S / \omega^2$.

At a semimicroscopic level, the interaction terms in (1.2) and (1.3) may be derived from an interaction term in the Hamiltonian of the coupled system which is of the form

$$\mathcal{E}(x_m, c_m) = E_0 x_m |c_m|^2 . \tag{1.4}$$

The respective last two terms of (1.2) and (1.3) are obtained from (1.4) by differentiating $\mathcal{E}(x_m, c_m)$ with respect to c_m^* and x_m, respectively. One then finds that S is nothing other than E_0/M, M being the mass of the oscillator.

We see that there are two assumptions of linearity in the above standard procedure, both of which arise from a Taylor series argument. The interaction term $E_0 x_m |c_m|^2$ in (1.4) is linear in x_m and so is the restoring force which is the product of the oscillator mass M and the term $\omega^2 x_m$ in (1.3). The purpose of the present paper is to investigate the consequences of relaxing these linearity assumptions in the two terms. We are thus interested in generally nonlinear restoring forces $Mf(x_m)$ for the molecular oscillator and in generally nonlinear potentials $E(x_m)|c_m|^2$ for the interaction between the vibrations and the quasiparticle. We will not consider nonlinearities of $\mathcal{E}(x_m, c_m)$ in $|c_m|^2$ in the present paper.

The physical origin of the nonlinearities in the restoring force and the interaction potential which we investigate here is quite evident. No molecular oscillator is truly Hookian and no interaction energy is truly linear in the oscillator displacement. Indeed, the forms used in (1.2) and (1.3) are simply the lowest terms in any realistic

situation retained through a Taylor expansion. Systems in which the nonlinearities might be particularly interesting are ones in which x_m is a rotation rather than a vibration. For notational purposes, we will therefore denote it by an angle variable θ_m. The system could thus be an electron/exciton moving among the sites m of a chain, there being a rotator (for instance, a dipole) at each site m whose angle from a fixed direction is θ_m. Periodicity in θ_m being essential at least at every interval of 2π, the nonlinear effects could be quite important for rotations which are not too small compared to 2π. We will therefore investigate the consequences for quasiparticle transport which arise on replacing the standard Hooke's linear restoring force by a general nonlinear force proportional to a function $f(\theta_m)$ of the rotational coordinate, and the standard linear interaction potential (1.4) by the general nonlinear potential

$$\mathcal{E}(\theta_m, c_m) = E(\theta_m)|c_m|^2 . \tag{1.5}$$

Equations (1.2) and (1.3) are to be replaced, therefore, by

$$i\hbar\frac{dc_m}{dt} = \sum_n V_{mn}c_n + E(\theta_m)c_m , \tag{1.6}$$

$$\frac{d^2\theta_m}{dt^2} + \omega^2 f(\theta_m) + RE'(\theta_m)|c_m|^2 = 0 . \tag{1.7}$$

It should be clear that, for the rotational case, the constant R is essentially the reciprocal of the moment of inertia of the rotator.

Equations (1.6) and (1.7) are our starting point in this paper. In Sec. II we obtain the discrete nonlinear Schrödinger equation and the discrete nonlinear von Neumann equation which correspond to (1.6) and (1.7), study their form valid in a dimer, i.e., a two-site system, and derive an explicit closed evolution equation for the difference in the probabilities of the occupation of the two sites by the quasiparticle. In Sec. III, this nonlinear equation is solved explicitly, the solution being expressed in quadrature form, and the reduction of the results to earlier linear results is shown. In Secs. IV and V, we explore a specific case appropriate to the rotational polaron, and in Sec. VI, we present concluding remarks.

II. EQUATIONS FOR THE TRANSPORT OF THE QUASIPARTICLE

The application of the standard argument of time-scale disparity to (1.6) and (1.7) yields the closed equation for the amplitude c_m of the electron/exciton:

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

Here $h(|c_m|^2)$ is simply $-E(\theta_m)$, the quantity θ_m being expressed as a function of $|c_m|^2$ obtained as the solution of

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

Henceforth in this paper, we put $\hbar = 1$. Equation (2.1) leads to the density-matrix equation

$$i\frac{d\rho_{mn}}{dt} = \sum_s (V_{ms}\rho_{sn} - V_{sn}\rho_{ms}) - \rho_{mn}[h(\rho_{mm}) - h(\rho_{nn})] . \tag{2.3}$$

The generalized discrete nonlinear Schrödinger equation (2.1) is our generalization of (1.1) to include restoring forces and interaction potential which are nonlinear in the rotational coordinate θ_m. Similarly, the generalized von Neumann equation (2.3) is our corresponding generalization of the equation

$$i\frac{d\rho_{mn}}{dt} = V(\rho_{m+1n} + \rho_{m-1n} - \rho_{mn+1} - \rho_{mn-1}) - \chi\rho_{mn}(\rho_{mm} - \rho_{nn}) \tag{2.4}$$

introduced earlier.[5] Equation (2.4) represents the further assumption of nearest-neighbor transfer interactions, i.e., $V_{mn} = V(\delta_{m,n+1} + \delta_{m,n-1})$, which is often made for simplicity. The linearity assumptions on the restoring force and the interaction potential make the h function linear in the probability as one may see through a comparison of (2.3) and (2.4) or of (2.1) and (1.1).

We shall now specialize our investigation to the case of a dimer, i.e., a two-site system in which m,n can take only the values 1 and 2, and we shall derive an exact closed equation for the difference p, defined through

$$p = \rho_{11} - \rho_{22} \tag{2.5}$$

between the probabilities of occupation of the two sites by the quasiparticle.

If we define the function $g(p)$ up to an arbitrary constant through

$$\frac{dg(p)}{dp} = h(\rho_{11}) - h(\rho_{22}) , \tag{2.6}$$

and notice that $\rho_{11} = (1+p)/2$ and $\rho_{22} = (1-p)/2$, the dimer case of (2.4) can be written as

$$\frac{dp}{dt} = 2Vq , \tag{2.7}$$

$$\frac{dq}{dt} = -2Vp + \frac{dg(p)}{dp}r, \tag{2.8}$$

$$\frac{dr}{dt} = -\frac{dg(p)}{dp}q, \tag{2.9}$$

for the density-matrix element contributions defined through $q = i(\rho_{12} - \rho_{21})$, $r = (\rho_{12} + \rho_{21})$, and (2.5). The solution of (2.9), its substitution in (2.8) and the substitution of the result in the differential form of (2.7) yield the desired closed equation for p. With the definition

$$\phi(p) = \frac{d}{dp}\left[\frac{1}{2}g^2(p) - g(p)[2Vr_0 + g(p_0)]\right], \tag{2.10}$$

where p_0 is the initial value of the probability difference, the dynamic equation for $p(t)$ is

$$\frac{d^2p}{dt^2} + 4V^2p + \phi(p) = 0 . \tag{2.11}$$

We see that the fictitious classical oscillator whose dis-

placement represents the probability difference in the dimer sites is subjected to two forces. One is the linear force $4V^2p$ corresponding to the linear dimer. The other is $\phi(p)$. As will be seen explicitly below, the latter takes on substantially different forms for the generalized nonlinearities discussed in the present paper but reduces, as expected, to a difference of a cubic term and a linear term in the standard case[5] of cubic nonlinearity.

III. EXPLICIT SOLUTION OF THE TIME-DEPENDENT DYNAMICS

The solution of (2.11) is straightforward. On multiplying it by dp/dt and integrating, one obtains the solution for p up to quadratures. With the definition of the effective potential

$$U(p)=2V^2(p^2-p_0^2)+\tfrac{1}{2}[g(p)-g(p_0)]^2$$
$$-2Vr_0[g(p)-g(p_0)], \qquad (3.1)$$

the solution of p to quadratures is

$$t-t_0=\int_{p_0}^p \frac{dz}{\sqrt{2[U(z)-U(p_0)]}}=\int_{p_0}^p \frac{dz}{\sqrt{2U(z)}}, \qquad (3.2)$$

where we have written t_0 explicitly as the initial value of the time t, and where we use the fact, evident from (3.1), that $U(p_0)$ vanishes by construction. The "energy conservation equation" for the fictitious classical oscillator whose motion obeys (2.11) is

$$\frac{p^2}{2}+U(p)=\frac{p_0{}^2}{2}+U(p_0)=\frac{p_0{}^2}{2}. \qquad (3.3)$$

Contact with earlier results for the case of linear harmonic interactions[5] is made immediately on noticing that, in that case,

$$h(|c_m|^2)=\chi|c_m|^2 , \qquad (3.4)$$

$$g(p)=\frac{\chi}{2}p^2 , \qquad (3.5)$$

$$\phi(p)=\frac{\chi^2}{2}p^3-\chi p\left[2Vr_0+\frac{\chi}{2}p_0^2\right], \qquad (3.6)$$

$$U(p)=\frac{\chi^2}{8}(p^2-p_0^2)^2+V(2V-r_0\chi)(p^2-p_0^2), \qquad (3.7)$$

and this reduces solution (3.2) to that given in Refs. 5 and 6. Thus, for the further simplified initial condition that the quasiparticle is on one of the two sites, one recovers the elliptic function solution for the probability difference[5]

$$p(t)=\mathrm{cn}(2Vt|\chi/4V) \qquad (3.8)$$

as expected.

IV. SINUSOIDAL RESTORING FORCE AND SINUSOIDAL INTERACTION

While we are in a position to use our quadrature solution (3.2) to analyze any system with given restoring force $f(\theta)$ and given interaction energy $E(\theta)$, we shall explicitly examine here the simplest nontrivial case, viz. on wherein both these functions are sinusoidal functions of θ:

$$f(\theta)=\frac{\sin(\Lambda\theta)}{\Lambda}, \qquad (4.1)$$

$$E(\theta)=\frac{E_0}{\Lambda}\sin(\Lambda\theta). \qquad (4.2)$$

The limit $\Lambda\to0$ gives the standard linear harmonic case. Our interest is in examining our solution with (4.1) and (4.2) for nonzero Λ. With the definitions

$$\Delta=\frac{E_0}{\Lambda}; \quad \chi=\frac{E_0{}^2R}{\omega^2}, \qquad (4.3)$$

straightforward calculations give

$$h(|c_m|^2)=\frac{\chi|c_m|^2}{\sqrt{1+(\chi/\Delta)^2|c_m|^4}}. \qquad (4.4)$$

The substitution of (4.4) in the generalized discrete nonlinear Schrödinger equation (GDNLSE), i.e., Eq. (2.1), yields

$$i\hbar\frac{dc_m}{dt}=\sum_n V_{mn}c_n-\frac{\chi|c_m|^2}{\sqrt{1+(\chi/\Delta)^2|c_m|^4}}c_m. \qquad (4.5)$$

This GDNLSE reduces to (1.1), i.e., the standard discrete nonlinear Schrödinger equation (DNLSE), for small χ/Δ but predicts substantially different transport features for non-negligible values of χ/Δ. Thus, whereas the increase of the nonlinearity χ leads in the DNLSE (1.1) to merely stronger nonlinear effects, it leads in (4.5) first to stronger nonlinear effects but eventually to a total *disappearance* of nonlinear features. For large values of χ/Δ, (4.5) reduces to a *linear* equation which, unlike (1.1) can exhibit no self-trapping. In the light of the occurrence of this saturation of nonlinearity, we term Δ, the saturation energy or the saturation parameter. It measures the (static) site energy lowering that every site in the crystal feels for high values of nonlinearity.

The counterpart of the DNSLE results (3.4) for this rotational polaron is

$$h(|c_m|^2)=\chi|c_m|^2(1+(\chi/\Delta)^2|c_m|^4)^{-1/2} \qquad (4.6)$$

and that of (3.5) is

$$g(p)=\Delta[\sqrt{(p+1)^2+(2\Delta/\chi)^2}+\sqrt{(p-1)^2+(2\Delta/\chi)^2}$$
$$-2\sqrt{1+(2\Delta/\chi)^2}]. \qquad (4.7)$$

We choose the arbitrary constant in $g(p)$ as to make $g(0)=0$. Expressions for $\phi(p)$ and $U(p)$ corresponding to (3.6) and (3.7) can also be written down explicitly[14] but they are tedious and have therefore not been shown here. It is straightforward to show that (4.7) reduces to (3.5) for large values of Δ/χ, i.e., for sufficiently small values of nonlinearity. In Fig. 1, we plot the function $g(p)$ appropriate to the GDNLSE [Eq. (4.7)] for several values of Δ/χ. The value of $\chi/2V$ taken is 2. For the large value 6 of Δ/χ, the function $g(p)$ coincides for all practical purposes with that for the ordinary DNLSE [Eq. (3.5)].
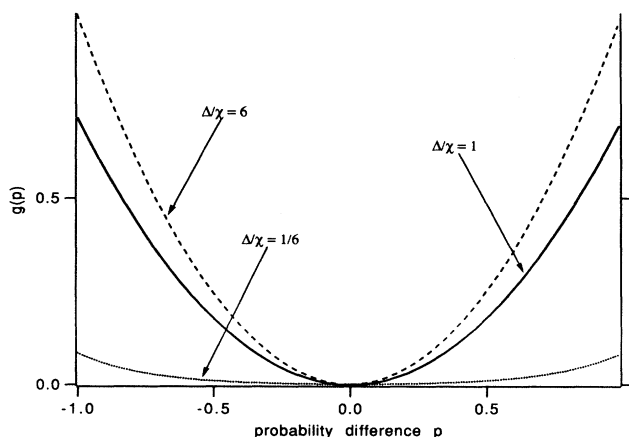
FIG. 1. The function $g(p)$ as given by the GDNLSE (4.7) plotted versus the probability difference p for $\chi = 4V$ and for several values of the saturation energy. For the case $\Delta/\chi = 6$, and for all larger values of Δ/χ, the function $g(p)$ coincides for all practical purposes with that for the ordinary DNLSE [Eq. (3.5)]. Smaller values of Δ/χ are seen to result in smaller $g(p)$ for a given nonlinearity.
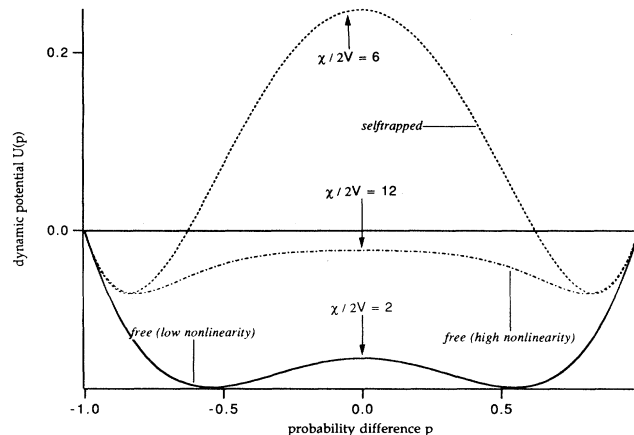

FIG. 2. The counterintuitive phenomenon of destruction of self-trapping on increasing nonlinearity illustrated through plots of the effective dynamic potential $U(p)$ for a given saturation energy $\Delta = 6V$. The case $\chi/2V = 2$ shows free motion resulting from a low value of nonlinearity. A higher value of nonlinearity, viz. $\chi/2V = 6$, shows the occurrence of self-trapping. A further increase in nonlinearity, $\chi/2V = 12$ shows the destruction of self-trapping. By contrast, the result of the standard DNLSE are to make self-trapping always more effective as nonlinearity is increased.

Large saturation energy, equivalently slow variation in the sinusoidal functions representing the restoring force and the interaction energy [see Eqs. (4.1) and (4.2)], obviously results in the linear harmonic case being recovered. Smaller saturation energies result in smaller $g(p)$ for a given nonlinearity as is clear from Fig. 1.

V. DYNAMICS AND STATIONARY STATES OF THE ROTATIONAL POLARON

Our studies of the rotational polaron have uncovered several new phenomena and we have commented upon some of them earlier.[6,13,14] Here we describe the most striking of them which involves the disappearance of self-trapping on increasing the nonlinearity. In order to illustrate this phenomenon, we plot in Fig. 2, the effective dynamic potential $U(p)$, obtained from (3.1) with (4.7). For simplicity, we consider the initial condition of complete localization at one of the two sites. We then have $p_0 = 1$, $r_0 = 0$. We have taken a fixed saturation energy Δ in Fig. 2. In units of $2V$, it equals 3. Whether the motion is self-trapped or free is clear from the vertical location of the horizontal line depicting the "constant energy" of the fictitious oscillator representing the evolution. If it lies always above $U(p)$, the motion is free. Otherwise, the motion is self-trapped, the intersection of the horizontal line with the $U(p)$ curve being indicative of the extent of values that the probability difference p can take. For small values of the nonlinearity there is free motion as is clear from the $\chi/2V = 2$. An increase in the nonlinearity χ results in self-trapping as expected: the $\chi/2V = 6$ curve shows that the probability difference oscillates between 1 and about 0.6. The surprising new consequence of our analysis is evident from the $\chi/2V = 12$ curve. We see that a further increase of nonlinearity *frees* the quasiparticle rather than self-trapping it more effectively, as

would happen in the DNLSE, i.e., in the limit that Δ/χ tends to infinity.

This phenomenon of destruction of self-trapping is obviously due to a saturation effect. In order to explain the saturation more clearly, we provide $U(p)$ plots along with the corresponding probability evolution plots in Fig. 3. The latter are obtained from the exact solution (3.2). In units of $2V$, the saturation energy has the respective values 100 [Fig. 3(a)], 2.5 [Fig. 3(b)], and 2 [Fig. 3(c)]. As expected, the first of these cases shows behavior as in the standard DNLSE, since Δ is large. When χ is small (solid line), the potential is near harmonic and the quasiparticle is able to oscillate between $p = -1$ and $p = 1$. As χ increases, the center of the potential starts to rise (dashed and dotted lines). Eventually the maximum of the potential exceeds the value of the initial potential which is equal to zero. In this case, the quasiparticle is self-trapped at its initially occupied site. In Fig. 3(b), increasing the nonlinearity from $\chi = V$ (solid line) to $\chi = 10V$ (dashed line) raises the center of the potential above $U = 0$, and thus localizes the quasiparticle. However, the potential is lowered as χ takes the value of $18V$. The quasiparticle is now free again. Self-trapping is thus destroyed for large enough nonlinearities. The disappearance of self-trapping can also occur for *all* values of nonlinearity if the saturation energy is small enough since, as Fig. 1 has shown, the self-trapping effect, represented by $g(p)$, becomes smaller over the entire range as the saturation energy becomes smaller. This case is seen in Fig. 3(c), which represents the smallest value of the saturation energy in the set shown. The center of the potential never exceeds the value of the initial potential, and thus no

self-trapping ever occurs for any values of nonlinear parameter χ.

The above analysis addresses the time evolution of the dimer for given initial conditions. The stationary states of the dimer also show interesting variation with non-linearity. The appearance of self-trapping, its disappearance for higher values of the nonlinearity, and the occurrence of multiple stationary states have been discussed elsewhere.[6,13,14] Here we explain only the basic method for those investigations. The simplest manner of examining the stationary states of the dimer is to set the right-hand sides of (2.7)–(2.9) equal to zero or to put the force on the fictitious oscillator given in (2.10) and (2.11) equal to zero, and then to replace p_0 and r_0 by p and r, respectively, in the resulting equations. Since q_0 equals zero from (2.7) in the stationary states, and the squares of p,q,r add up to 1 from their definition, one has

$$r = \pm \sqrt{1-p^2}. \qquad (5.1)$$

The stationary state probability differences are thus obtained as the solutions of

$$2Vp \pm \sqrt{1-p^2}\,\frac{d}{dp}g\,(p)=0. \qquad (5.2)$$

Nonzero solutions signify self-trapping. It is possible to construct a potential $W(p)$ whose derivative is given by the left-hand side of (5.2). The minima in such a plot obviously signify stationary states. The disappearance of self-trapping (as manifested in the stationary states) on increasing the nonlinearity has been described in Ref. 6 where the probability difference p in the stationary state has been shown to exhibit a bifurcation signifying self-trapping above a critical value of the nonlinearity, and then a destruction of the self-trapping above another critical value of the nonlinearity.[6] A complete study of the multiple stationary states of the rotational polaron, and their stability, will be found elsewhere.[14]
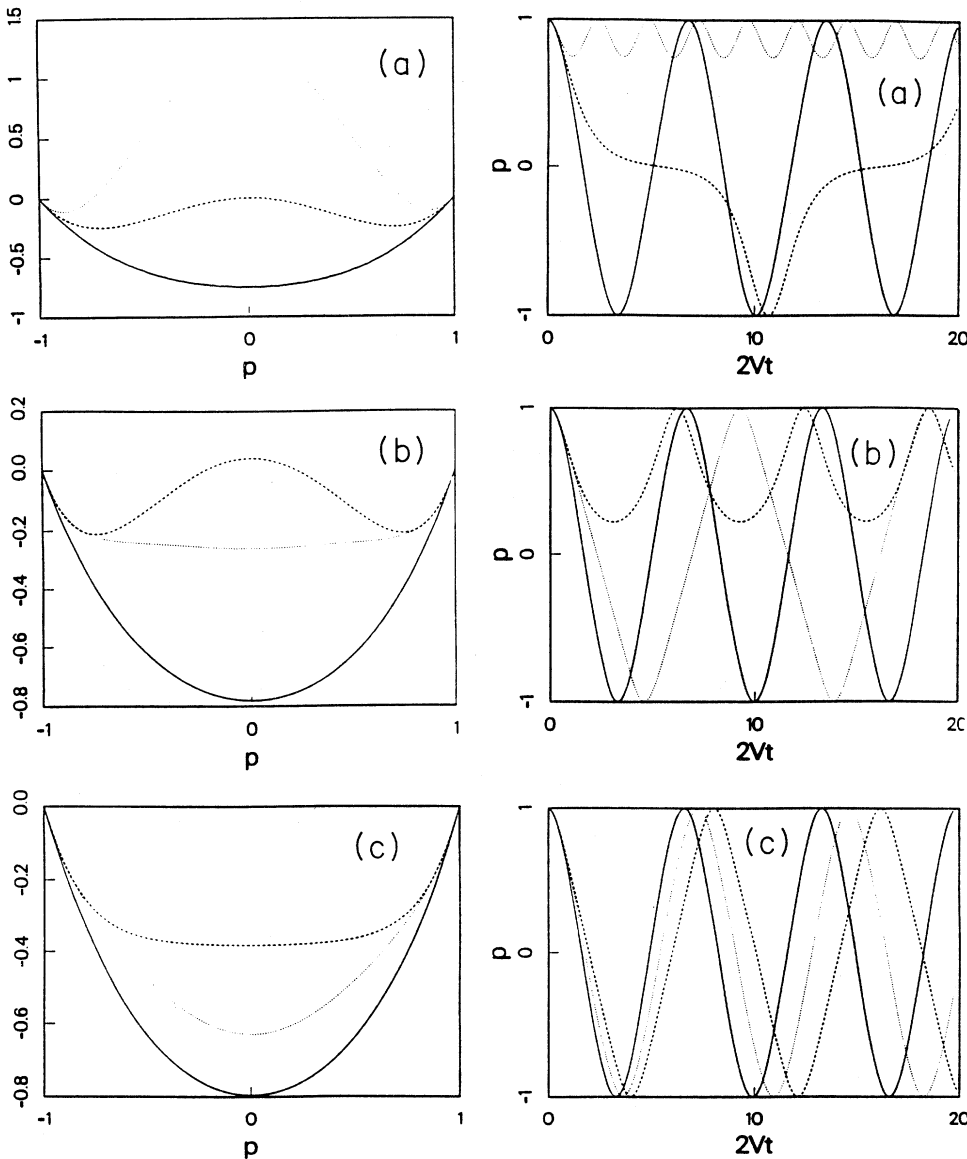

FIG. 3. Dynamics of the rotational polaron described through probability evolution plots (right side of the figure) along with corresponding $U(p)$ plots (left side of the figure) for several values of the nonlinearity and the saturation energy. The ordinate on all the left plots is $U(p)$. In units of $2V$, the saturation energy has the respective values 100 (a), 2.5 (b), and 2 (c). The nonlinearity χ is small for the solid lines ($\chi=V$), larger for the dashed lines ($\chi=10V$), and largest for the dotted lines (18V). Oscillations of $p(t)$ favoring one of the sites signify self-trapping. Of particular interest is (c) in which it is seen that the disappearance of self-trapping can occur for *all* values of nonlinearity if the saturation energy is small enough: the center of the potential never exceeds the value of the initial potential, and no self-trapping ever occurs for any values of χ.

VI. CONCLUDING REMARKS

We have investigated the effect of nonlinearities in the interaction potential and anharmonicities in the restoring force on the evolution of a system consisting of a quasiparticle interacting with vibrations. We have obtained a generalized transport equation for the quasiparticle which we have called the generalized discrete nonlinear Schrödinger equation (GDNLSE). We have given a practical prescription for obtaining the equation explicitly from the nonlinearity in the interaction potential and anharmonicity in the restoring force, and for solving the equation for the time evolution in a dimer. We have illustrated the general formalism by applying it to a system we have called the rotational polaron, which is appropriate to the oscillatory coordinate being a rotation. We have discovered new effects including a saturation of nonlinearity, destruction of self-trapped states, and occurrence of multiple stationary states.

The physics behind what we have called a rotational polaron is that of an electron, or electronic or vibrational excitation, in strong interaction with an oscillator subject to a sinusoidal potential. A rotator provides the simplest example of such an oscillator. Our analysis is of interest in the study of liquid crystals, which consist of partially ordered aggregates of molecules possessing directed shapes such as rods or discs.[15] The angular oscillations that such molecules can perform around their equilibrium directions provide an example of the coordinate θ that we have discussed in the present paper. The rotational polaron would be encountered generally in any system in which a quasiparticle (an electron, or electronic or vibrational excitation) interacts with the angular oscillations so strongly that the presence of the quasiparticle has an appreciable effect on the equilibrium direction of the molecule.

Our starting equations are (1.6) and (1.7) for the coupled evolution of the quantum quasiparticle and the classical vibrations. They involve the generalization of the more common (1.2) and (1.3) which lead to the standard DNLSE. We have carried out that generalization in order to introduce nonlinear and anharmonic effects. The latter appear through a replacement of the linear interaction energy expression (1.4) by the general expression (1.5), and by the replacement of linear restoring forces by more general counterparts. The coupled equations (1.6) and (1.7) lead to our generalized transport equation for the quasiparticle amplitudes, viz. the GDNLSE (2.1), and the corresponding von Neumann equation for the density matrix, viz. (2.3).

We obtain soluble equations for the two-site system. The density-matrix elements lead to (2.7)–(2.9), and to the closed evolution equation (2.11) for the probability difference. General force and potential expressions are (2.10) and (3.1) and the explicit solution to quadratures is (3.2). The application to the system of rotational polarons is made through (4.1) and (4.2), leads to the specific transport equation (4.5). Figures 2 and 3 show the effects of saturation on the dynamics. We explain a useful method to study stationary states leading to (5.2). The application of the general formalism to a variety of nonlinearities and anharmonicities will form the content of a future publication.

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