ELSEVIER

18 August 1997

PHYSICS LETTERS A

Physics Letters A 233 (1997) 73–78

Phase–nonlinearity interplay in small quantum systems

S. Raghavan [a], V.M. Kenkre [a], A.R. Bishop [b]

[a] *Center for Advanced Studies and Department of Physics and Astronomy, University of New Mexico, Albuquerque, NM 87131, USA*
[b] *Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, NM 87545, USA*

Received 15 July 1996; revised manuscript received 2 May 1997; accepted for publication 9 June 1997
Communicated by C.R. Doering

Abstract

We report effects of the interplay of quantum phases and nonlinearity in small quantum systems that are characterized by strong interactions between a quasiparticle (an excitation or an electron) and lattice vibrations, and are described by the discrete nonlinear Schrödinger equation. The issue under investigation is the influence that features of the initial placement of a quasiparticle can have on the process of self-trapping. We find that initial phases profoundly control the dependence of self-trapping on initial inhomogeneity. We also find that the only non-trivial stationary state of the system disappears in the presence of *complex* initial site amplitudes and that the amplitude of oscillations, which dips sharply to zero at the stationary state for real initial amplitudes, approaches a nonzero minimum for complex initial amplitudes. © 1997 Published by Elsevier Science B.V.

1. Introduction

The purpose of this article is to report on new findings regarding the interplay of quantum phases and nonlinearity in a nonlinear dimer. The discrete nonlinear Schrödinger equation (DNLSE) [1–9], which describes the adiabatic dynamics of quasiparticle evolution in several systems, is

$$\mathrm{i}\,\mathrm{d}c_m/\mathrm{d}t = \sum_n V_{mn}c_n - \chi|c_m|^2 c_m, \tag{1.1}$$

where c_m is the probability amplitude to find the particle at site m, V_{mn} is the inter-site matrix element, and χ is the nonlinearity parameter describing energy lowering of the particle due to interaction with the lattice.

Eq. (1.1) has been solved for the dimer and some experimentally verifiable observables have been computed [4]. The effect of varying the initial conditions has also been explored [7,8] and two transitions have been observed. One is a "frequency transition" that is a signature of the system becoming self-trapped. The other is an "amplitude transition", characterized by a decrease in the amplitude of oscillations (while in the trapped state), passage through a stationary state, and reversal of amplitude as nonlinearity is increased. Whether self-trapping is aided or hindered by having the quasiparticle occupy a few sites or many sites at the initial time, constitutes a question of considerable relevance [10,11]. The analysis given below addresses this question for the quantum nonlinear dimer. Studies of the dimer have so far concentrated on initial conditions wherein the site amplitudes have been taken to be real [3,4,6–9]. However, for an actual physical system prepared in a pure state, initial conditions will almost always be such that the site amplitudes will be complex. We examine effects of such realistic considerations, including the dependence of trapping on initial inhomogeneity of population and

0375-9601/97/$17.00
PII S0375-9601(97)00451-9

the stability of stationary states. It is important to note that, although the regime of validity of the DNLSE as a consequence of microscopic dynamics is limited [12-14], the problem of the interplay between qunatum phases and nonlinearity studied in this paper is of general interest in quantum nonlinear equations of evolution. The results of the present paper have to be interpreted in this context.

We emphasize that, throughout this paper, as in earlier work [3,4,6-9], by the phrase "quantum phases", we refer only to the quantum mechanical phases associated with the quasiparticle. Clearly, after the semiclassical approximation has been made, there is no meaning to the association of a quantum phase with the vibrational variables.

2. The role of initial phases in localization

Following standard analysis of the DNLSE dimer [15], we define the following density matrix combinations,

$$p = |c_1|^2 - |c_2|^2 \qquad q = \mathrm{i}(c_1^* c_2 - c_1 c_2^*),$$
$$r = c_1^* c_2 + c_1 c_2^*, \tag{2.1}$$

where c_1 and c_2 are the amplitudes for the particle to be on either site of the dimer. The above quantities obey the closed equations [3,4]

$$\dot{p} = -2Vq \qquad \dot{q} = 2Vp + \chi pr \qquad \dot{r} = -\chi pq. \tag{2.2}$$

The solution to Eqs. (2.2) is known in general [4,9]:

$$p(t) = C\,\mathrm{dn}[(C\chi/2)(t-t_0)|1/k], \tag{2.3a}$$
$$1/k^2 = 2 + (2/C^2)(\xi^2 - p_0^2)$$
$$C^2 = p_0^2 - \xi^2 + [\xi^4 + (q_0/k_0)^2]^{1/2}, \tag{2.3b}$$
$$\xi^2 = \tfrac{1}{2}(1/k_0^2 + 2r_0/k_0), \tag{2.3c}$$

where $k_0 = \chi/4V$ measures the ratio of the nonlinearity parameter to the inter-site transfer interaction, and p_0, q_0, r_0 are the initial values of p, q, r respectively.

The case of (2.3) where $q_0 = r_0 = 0$, $p_0 = 1$, was studied in Ref. [3]. The case $q_0 = 0, p_0 \neq 0, r_0 \neq 0$, was studied in Ref. [7]. As explained there, for the latter case of $q_0 = 0$, overall probability conservation in a system in a pure state expressed by $p_0^2 + q_0^2 + r_0^2 = 1$ results in

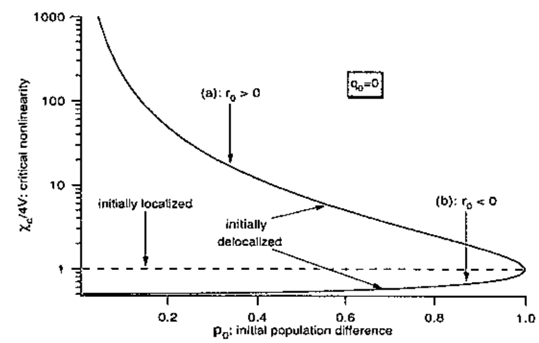

Fig. 1. The critical value of nonlinearity χ_c, i.e. the value required for self-trapping, is plotted logarithmically in units of 4V as a function of the initial population difference p_0 (see Eq. (2.6)). The dashed line $\chi_c = 1$ represents the critical nonlinearity for the completely localized initial condition $p_0 = 1$. In this figure $q_0 = 0$. In (a) $r_0 > 0$ and in (b) $r_0 < 0$.

$$r_0 = \pm(1 - p_0^2)^{1/2}. \tag{2.4}$$

Of the two roots in (2.4), the negative root corresponds to particularly interesting behaviour in that, in addition to the free-trapped transition, an "amplitude transition" occurs. For the case of $q_0 = 0$, the general solution (2.3) becomes

$$p(t) = p_0\,\mathrm{dn}(p_0 \chi t/2|1/k),$$
$$k^2 = k_0^2 p_0^2/(1 + 2k_0 r_0). \tag{2.5}$$

When the system undergoes the "free-trapped" transition, the elliptic modulus k appearing in (2.5) equals 1. We study the dependence of χ_c, the nonlinearity needed to trap the system, on the initial population difference p_0, by noting that (2.5) implies

$$\frac{\chi_c}{4V} = \frac{1 + r_0}{p_0^2} = \frac{1 \pm (1 - p_0^2)^{1/2}}{p_0^2}. \tag{2.6}$$

This dependence of $\chi_c/4V$ on p_0 is shown in Fig. 1 for the (a) positive and (b) negative roots, respectively. There is a profound difference in the two cases, arising from a difference in the initial phases. The positive r_0 case is understood easily. Self-trapping corresponds to unequal population on the two sites in a stationary state, and initial inhomogeneity assists trapping. This is why the amount of nonlinearity needed to trap decreases with increasing p_0. The negative r_0 case is more complex. A larger amount of nonlinearity is needed to trap the system as one increases the initial population difference. While perhaps counterintuitive, this behaviour can be understood easily: reversing the sign of r_0 is synonymous with reversing the sign of χ with respect to the inter-site matrix element V, equivalent to reversing the sign of the population difference. Thus, an enhanced initial population difference counters the trapping tendency of nonlinearity for the negative r_0 case. Similar considerations have appeared elsewhere [17], especially in the context of the different effects that a reversal of the sign of χ has in *discrete* (as opposed to spatially continuous) nonlinear systems.

The above effects can be shown to arise quite simply from (2.6). Differentiating (2.6) with respect to p_0^2, we get

$$\frac{\mathrm{d}\chi_c}{\mathrm{d}p_0^2} = \mp \frac{2V}{p_0^4\sqrt{1-p_0^2}}\left(\sqrt{1-p_0^2} \pm 1\right)^2, \tag{2.7}$$

where the upper signs are to be taken for positive r_0, and the lower signs for negative r_0. Since the right hand side is a positive quantity except for the $\mp$ sign, it is clear that for positive (negative) r_0, as p_0 is increased, one needs less (more) nonlinearity to trap the quasiparticle.

A study of the stationary states of the system helps one to understand the trapping dependence shown in Fig. 1. In Eq. (2.1), r is the population difference of the *stationary states* of the system with *no* nonlinearity. Negative r implies that the eigenstate of energy $-V$ is more populated than the eigenstate of energy V. It can be shown that, in the presence of nonlinearity, the state that evolves from the $-V$ state is the self-trapped state. For $r_0 < 0$, greater initial population in this state leads to trapping. Increasing p_0 leads to a decrease in the population in the $-V$ state. Therefore, self-trapping requires greater nonlinearity when p_0 is increased. This behaviour is intimately related to the existence, in a linear disordered system, of a mobility edge [18] which separates higher-energy delocalized k-states from lower energy trapped states. In our two-site system, the $+(-)$ state, in which the site amplitudes have identical (opposite) phases, is the higher (lower) energy k-state.

3. Effect of complex initial site amplitudes

The above considerations apply to the case of real initial site amplitudes. We now relax that constraint,

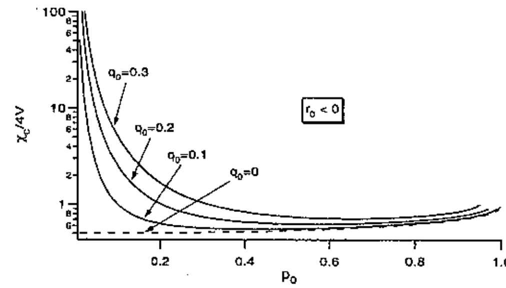

Fig. 2. χ_c plotted logarithmically in units of $4V$ as a function of p_0 (see Eq. (3.2)). Treated here is the case of $r_0 < 0$ and general $q_0 \neq 0$. Values of q_0 considered are 0.3, 0.2, 0.1 and 0. The last case ($q_0 = 0$) shown here by the dashed line, corresponds to Fig. 1b.

and replace (2.4) by

$$r_0 = \pm(1 - p_0^2 - q_0^2)^{1/2}. \tag{3.1}$$

The condition for the particle to be trapped is that the elliptic parameter k, defined in (2.3), must exceed 1. The critical value of the nonlinearity is given by

$$\chi_c/4V = (1 + r_0)/p_0^2$$
$$= [1 \pm (1 - p_0^2 - q_0^2)^{1/2}]/p_0^2. \tag{3.2}$$

If $\chi < \chi_c$, the particle executes periodic motion, and $p(t)$ follows the dn function. When χ exceeds χ_c, the particle is trapped. Eq. (3.2) reduces to (2.6) for the case ($q_0 = 0$) of real initial site amplitudes. As in the $q_0 = 0$ case, the negative root in (3.2) corresponds to particularly interesting behaviour. We restrict our analysis to that case and plot the dependence of the critical nonlinearity χ_c on initial inhomogeneity in Fig. 2. The existence of a minimum χ_c for nonzero q_0 implies that, for small values of p_0, if the system starts out free, an increase in p_0 causes self-trapping.

The $q_0 = 0$ analysis reported in Ref. [7] has shown that, for $r_0 < 0$, the initial state can become a stationary state for a certain value of the nonlinearity, viz. for $\chi/4V = \frac{1}{2}(1 - p_0^2)^{1/2}$. At that value, the elliptic modulus k becomes infinite. Further increase in the nonlinearity makes k^2 negative, and the imaginary argument transformation [16] shows the appearance of the "amplitude transition" [7]. Our present analysis shows that when $q_0 \neq 0$, there is no possibility of an occurrence of the stationary state discussed above. The plot of the elliptic parameter k^2 as a function of $\chi/4V$ in Fig. 3 shows that, for $q_0 \neq 0$, the elliptic pa-

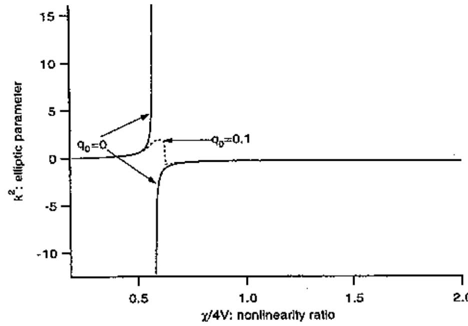

Fig. 3. The elliptic parameter k^2 as a function of the nonlinearity ratio $\chi/4V$ for $p_0 = 0.5$ and two values of q_0 as shown. As in Fig. 2, $r_0 < 0$.

rameter never becomes infinite. However, it exhibits the characteristic discontinuity observed for $q_0 = 0$, signalling the change of $p(t)$ from evolution given by the dn function to one given by

$$p(t) = C \times \mathrm{nd}(C\chi(1+|k^2|)^{1/2}t/2|k| \,|(1+|k^2|)^{-1/2}) \tag{3.3}$$

where C is given by (2.3). In Fig. 3, the dashed line represents $q_0 = 0$ and the solid line represents $q_0 = 0.1$. For $q_0 = 0$, the evolution changes markedly in character at the transition across the stationary state. On the other hand, for $q_0 \neq 0$, there is no dramatic change in character in the evolution across the transition. This corresponds to the the absence of a stationary state, and to the fact that the derivative of $p(t)$ initially is nonzero.

Potential plots can facilitate the present analysis. It is straightforward [3] to write down a closed equation in p from (2.2),

$$\dot{p}^2 + U(p) = U_0, \tag{3.4a}$$

$$U(p) = \tfrac{1}{2}Bp^4 - Ap^2, \tag{3.4b}$$

$$U_0 = \tfrac{1}{2}Bp_0^4 - Ap_0^2 + (2V)^2q_0^2, \tag{3.4c}$$

$$A = \tfrac{1}{2}\chi^2p_0^2 - 4V^2 - 2V\chi r_0, \quad B = \tfrac{1}{2}\chi^2. \tag{3.4d}$$

Eq. (3.4) is the equation of motion for a fictitious oscillator whose displacement is described by $p(t)$ and whose potential is given by $U(p)$. Fig. 4 shows the plot of $U(p)$ defined in (3.4b) with the horizontal line showing U_0 of (3.4c). The dot (a) marks the value of p_0 for negative r_0 and the dot (b) denotes the value of p_0 for positive r_0. One sees that for positive r_0, the displacement of the fictitious particle can only have values less than the initial value p_0, whereas for negative r_0, it always has values greater than p_0. One can associate this behaviour with the observation that in the former case, the slope of $U(p)$ with respect to p near p_0 is positive, whereas in the latter case, it is negative. Combining (2.2) and (3.4) one has

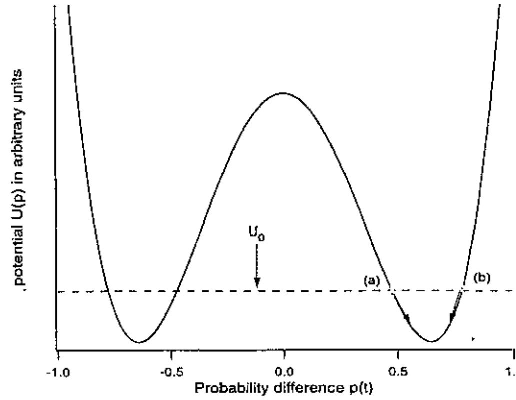

Fig. 4. Potential plot to explain the "amplitude transition" of Ref. [7]. The dashed line represents U_0 defined in (3.4). Initial locations at (a) and (b) correspond to $r_0 < 0$ and $r_0 > 0$ respectively. The arrows depict the initial motion of the fictitious oscillator.

$$U'(p_0) = Vp_0(2V + \chi r_0), \tag{3.5}$$

which implies that, if r_0 is positive, the slope is always positive (for positive p_0) whereas, if r_0 is negative, the sign of the slope reverses once $r_0 < -2V/\chi$. We have given here an explanation, based on the "effective potential" method, of the "amplitude transition" observed in Ref. [7], wherein it was seen that for $q_0 = 0, r_0 < 0$, once $r_0 < -2V/\chi$, the population difference $p(t)$ never decreased below the initial population difference p_0 and that this behaviour was absent for positive r_0.

We have found it instructive to study the behaviour of the amplitude of the oscillations of $p(t)$ as a function of nonlinearity. The amplitude a of the oscillations is given by

$$a = \sqrt{\frac{A+f}{B}} - \sqrt{\frac{A-f}{B}}, \tag{3.6a}$$

$$f = \sqrt{A^2 + 2Bm}, \quad m = \tfrac{1}{2}Bp_0^4 - Ap_0^2 + (2V)^2q_0^2, \tag{3.6b}$$

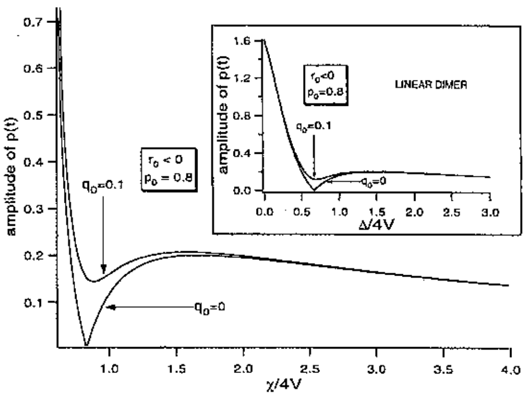

Fig. 5. The amplitude of oscillations for the nonlinear dimer as a function of $\chi/4V$ (see Eq. (3.6)) for $r_0 < 0$ and $p_0 = 0.8$, for two values of q_0: 0 and 0.1, respectively. The inset shows the amplitude of oscillations for a linear non-degenerate dimer plotted as a function of $\Delta/4V$, where the energy difference (non-degeneracy) between the two sites is Δ (see Eq. (3.7)). We also take $r_0 < 0$, $p_0 = 0.8$ and $q_0 = 0$, 0.1 in the inset.

and A and B are given by (3.4). The plot of the amplitude as a function of nonlinearity is displayed in the main figure in Fig. 5. The main figure shows the case when $q_0 = 0, 0.1$. The sharp fall in amplitude at the stationary state should be noted when $q_0 = 0$. When $q_0 = 0.1$, there is no stationary state, and consequently the amplitude never drops to zero. Instead, it smoothly approaches a local minimum. In terms of the fictitious p oscillator, this corresponds to the energy of the p particle being a minimum.

It is useful to compare the amplitude plots with those of the linear non-degenerate dimer. In the latter situation, the amplitude a between the two sites is given by

$$a = \frac{2}{\Omega}\left[m_0 + \left(\frac{b}{2\Omega}\right)^2\right]^{1/2}, \tag{3.7a}$$

$$m_0 = (2V)^2 q_0^2 + \Omega^2 p_0^2 + b p_0,$$

$$b = 2(2V\Delta r_0 - \Delta^2 p_0), \tag{3.7b}$$

$$\Omega = \sqrt{\Delta^2 + (2V)^2}, \tag{3.7c}$$

where Δ is the energy difference between the two sites.

The comparison of the amplitude for the nonlinear dimer (3.6a) with that of the linear non-degenerate dimer (3.7a) is made clear in Fig. 5. The inset refers to the linear non-degenerate dimer. The similarity between the linear non-degenerate dimer and the nonlinear, degenerate dimer suggests that we may able to understand many aspects of the behaviour of the nonlinear dimer by replacing the nonlinearity χ by an energy difference or on-site disorder Δ in a *linear* degenerate dimer. Thus presence or absence of the discontinuity lies not so much in the nonlinear nature of the dimer but in the fact that a nonlinearity produces an effective energy mismatch, and, that by appropriate adjustments in the initial conditions or the amount of energy mismatch, it is possible or not to arrive at a stationary state according as whether q_0 is zero or not. In particular, the similarity can be understood in the following fashion. For small oscillations, *once the particle is trapped*, the potential $U(p)$ in which $p(t)$ moves is approximately the same as a harmonic oscillator potential, which is the potential for a linear non-degenerate dimer with appropriate energy disorder. At the stationary state (when $q_0 = 0$), the potentials are practically identical. Thus, the amplitude plots are very similar especially in the region around the stationary state where the amplitude of oscillations is small.

4. Summary

We have examined the effects of the interplay of quantum phases and nonlinearity in small quantum systems. We find that the initial phases have a strong influence on the dependence of self-trapping on the initial population difference between the two sites of the quantum nonlinear dimer. In studying the analogy between the degenerate nonlinear dimer and the non-degenerate dimer, we find that many of the nonlinear effects can be understood as originating from an effective disorder in a linear system [7,19]. Ongoing work includes investigation of spatially extended systems, focussing on the analogy with mobility edges in linear disordered systems [18].

Acknowledgement

Work at Los Alamos is supported by the U.S. Department of Energy. We thank the referees for their useful and insightful comments.

References

[1] A.S. Davydov, J. Theor. Biol. 38 (1973) 559; Phys. Usp. 25 (1982) 898, and references therein.
[2] J.C. Eilbeck, P.S. Lomdahl and A.C. Scott, Physica D 16 (1985) 318.
[3] V.M. Kenkre and D.K. Campbell, Phys. Rev. B 34 (1986) 4959.
[4] V.M. Kenkre and G.P. Tsironis, Phys. Rev. B 35 (1987) 1473.
[5] D.K. Campbell, A.R. Bishop and K. Fesser, Phys. Rev. B 26 (1982) 6862.
[6] V.M. Kenkre, G.P. Tsironis and D.K. Campbell, in: Nonlinearity in Condensed Matter, eds. A.R. Bishop, D.K. Campbell, P.Kumar and S. Trullinger (Springer, Berlin).
[7] G.P. Tsironis and V.M. Kenkre, Phys. Lett. A 127 (1988) 209.
[8] V.M. Kenkre and G.P. Tsironis, Chem. Phys. 128 (1988) 219.
[9] V.M. Kenkre, in: Singular Behaviour and Nonlinear Dynamics, Vol.II, eds. St. Pnevmatikos, T. Bountis and Sp. Pnevmatikos (World Scientific, Singapore, 1989).
[10] V.M. Kenkre and H.-L.Wu, Phys. Lett. A 135 (1989) 120.
[11] R.S. Knox, in: Bioenergetics of photosynthesis, ed. Govindjee (Academic Press, New York, 1975) p.183.
[12] D.Vitali, P.Allegrini and P.Grigolini, Chem. Phys. 180 (1994) 297, and references therein.
[13] M.I. Salkola, A.R. Bishop, V.M. Kenkre and S. Raghavan, Phys. Rev. B 52 (1995) R3824, and references therein.
[14] V.M. Kenkre, S. Raghavan, A.R. Bishop and M.I. Salkola, Phys. Rev. B 53 (1996) 5407.
[15] R.P. Feynman, F.L. Vernon and R.W. Hellwarth, J. Appl. Phys. 28 (1957) 49.
[16] P.F. Byrd and M.D. Friedman, Handbook of elliptic integrals for engineers and scientists, 2nd Ed. (Springer, Berlin, 1971).
[17] R. Scharf and A.R. Bishop, Phys. Rev. A 43 (1991) 6535; V.M. Kenkre and St. Pnevmatikos, unpublished.
[18] J.M. Ziman, Models of Disorder, (Cambridge, 1979); P.W. Anderson, Phys. Rev. 109 (1958) 1492.
[19] D.H. Dunlap, V.M. Kenkre and P. Reineker, Phys. Rev. B 47 (1993) 14842.