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ANALYSIS OF THE INTERPLAY OF QUANTUM PHASES AND NONLINEARITY APPLIED TO DIMERS WITH ANHARMONIC INTERACTIONS

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ABSTRACT

We extend our analysis of the effects of the interplay of quantum phases and nonlinearity to address saturation effects in small quantum systems. We find that initial phases dramatically control the dependence of self-trapping on initial asymmetry of quasiparticle population and can compete or act with nonlinearity as well as saturation effects. We find that there is a minimum finite saturation value in order to obtain self-trapping that crucially depends on the initial quasiparticle phases and present a detailed phase-diagram in terms of the control parameters of the system: nonlinearity and saturation.

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1 Introduction

We analyze here some features of a quasiparticle interacting with lattice vibrations that are strongly anharmonic in nature. An example of such an oscillator is to be found in liquid crystals where the vibration is rotational [1]. Work done on these lines by Kenkre and collaborators on *rotational polarons* has shown the existence of fascinating phenomena like saturation of selftrapping on *increasing* nonlinearity beyond a characteristic value [2–4]. Further work on a different kind of oscillator, one which is harmonic for small displacements from equilibrium but subjected to a restoring force, which is logarithmic for large displacements also showed similar behaviour [5]. In a study of the more commonly encountered harmonic systems, it was shown [6] that the initial quantum phases can profoundly control the process of self-trapping in nonlinear quantum dimers where the interacting vibrations were assumed to be harmonic (see also [13]). The purpose of this note is to report some interesting behaviour that occurs when the initial quantum phases can interact with the nonlinearity in the system as well as the saturation effects of anharmonic vibrations. We point out here that throughout this paper, we shall assume the vibrations to be classical. It is important to note that, although the regime of validity of the DNLSE as a consequence of microscopic dynamics is limited [7–9], the problem of the interplay between quantum 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 [2,10–14], 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.

We begin here with the following coupled equations [2–4] for the generalized displacement x_m of the oscillator at site m, and for the quasiparticle amplitude c_m at site m,

$$i\hbar\frac{dc_m}{dt} = \sum_n V_{mn}c_n + E(x_m)c_m, \tag{1.1}$$

$$\frac{d^2x_m}{dt^2} + \omega^2 f(x_m) + RE'(x_m)|c_m|^2 = 0, \tag{1.2}$$

where V_{mn} is the intersite matrix element between sites m and n, R is a proportionality constant related to the geometry of the system, $E(x_m)$ is a generally nonlinear function of the coordinate x_m describing the quasiparticle-vibration interaction, and $\omega^2 f(x_m)$ is a general nonlinear function giving the restoring force on the vibrational coordinate.

For the rotational polaron, as noted elsewhere [2–4], the restoring force and the interaction are described as

$$f(x) = \frac{\sin(\Lambda x)}{\Lambda}, \quad E(x) = \frac{E_0}{\Lambda}\sin(\Lambda x). \tag{1.3}$$

2

Following the analysis of Kenkre et al. [3,4], one obtains the amplitude equation

$$i\hbar \frac{dc_m}{dt} = \sum_n V_{mn} c_n - \frac{\chi |c_m|^2}{\sqrt{1 + (\chi/\Delta)^2 |c_m|^4}} c_m. \tag{1.4}$$

in general, and for the two-site system (dimer) in particular,

$$\dot{p} = -2Vq \ , \ \dot{q} = 2Vp + \frac{dg(p)}{dp} r \ , \ \dot{r} = -\frac{dg(p)}{dp} q, \tag{1.5}$$

where

$$g(p) = \Delta \left[\sqrt{(p+1)^2 + \left(\frac{2\Delta}{\chi}\right)^2} + \sqrt{(p-1)^2 + \left(\frac{2\Delta}{\chi}\right)^2} - 2\sqrt{1 + \left(\frac{2\Delta}{\chi}\right)^2} \right]. \tag{1.6}$$

with the definitions

$$p = |c_1|^2 - |c_2|^2 \ ; \ q = i(c_1^* c_2 - c_1 c_2^*) \ ; \ r = c_1^* c_2 + c_1 c_2^*. \tag{1.7}$$

and where p_0, r_0 refer to the initial values of p, r respectively. Here the nonlinearity $\chi = E_0^2 R/\omega^2$ and the saturation energy $\Delta = E_0/\Lambda$.

As has been shown in Refs. [2–4], one obtains from Eq. (1.6) an equation of motion for a fictitious conservative oscillator whose displacement is p, and that moves in a potential given by

$$U(p) = 4V^2 p^2 + g^2(p) - 2g(p)[g(p_0) - 2Vr_0], \tag{1.8}$$

2 Rotational polaron

We start this section with the elementary observation that as long as $g(p)$ in Eq. (1.8) is an even function of p, the potential will also be one. Furthermore, if $g(0) = 0$, $U(0) = 0$. This implies that the critical condition to determine the transition between free evolution to self-trapped behaviour can be found by examining the condition $U(p_0) \leq 0$. This condition combined with Eq. (1.8) gives

$$|g(p_0) - 2Vr_0| \geq 2V. \tag{2.1}$$

It is therefore instructive to view the condition expressed in Eq. (2.1) in terms of a phase-diagram with the saturation ratio Δ/V and the critical nonlinearity ratio χ_c/V as the parameters for different values of p_0, r_0 marking regions of free and self-trapped evolution. We first examine the case for real initial conditions, i.e., $q(0) \equiv q_0 = 0$. In the next section, we shall generalize to complex initial conditions.

Figure 1 shows the phase diagram for the case when $r_0 < 0$. It is to be interpreted in the following manner. For a given value of the saturation ratio Δ/V, as one increases the value of nonlinearity ratio χ_c/V, one traverses regions of free-evolution. As soon as one encounters the boundary (for the relevant value of p_0), one enters the region of self-trapped evolution. This is the region where Eq. (2.1) is satisfied. Note that upon increasing the value of nonlinearity beyond a certain value one crosses this region and passes into free evolution again. This is as expected and is in accordance with the observation in Refs. [3,4] that self-trapping can be destroyed by increasing the nonlinearity. Note also that for the initial phase chosen so that $r_0 < 0$, for a given value of saturation, it requires less nonlinearity to enter the self-trapped phase if the amount of initial asymmetry (measured by p_0) is less. This is in consonance with the observation of Ref. [6]. It is interesting that this interplay between choice of initial phase and initial asymmetry remains qualitatively unaffected even in the presence of saturation effects. It is important, also, to note that one gets out of this self-trapped phase for correspondingly lower values of nonlinearity. It is interesting to see that as one moves to lower values of p_0, the system tolerates lesser values of saturation to enter the self-trapped phase, the most stringent limit being posed at the value $p_0 = 1$. It is straightforward to estimate the least saturation ratio required (and the corresponding value of critical value of nonlinearity ratio): $\Delta_c/V = \sqrt{27/4}, \chi_c/V = \sqrt{27/2}$. It occurs for $p_0 \to 0$ and is in agreement with what is obtained in Ref. [4]. There are several features of interest in the phase diagram. For fixed p_0, the phase boundary exhibits two asymptotes. The first of these occurs for finite χ_c/V and $\Delta/V \to \infty$. This is the standard DNLSE limit and it corresponds to $\chi \ll \Delta$. The value of this asymptote is given by $\chi_c/V = 4(1 - \sqrt{1 - p_0^2})/p_0^2$ and is the result of Ref. [6]. The second asymptote is actually more interesting since it marks the boundary marking the destruction of self-trapping. The behaviour along this boundary is given by the relationship

$$\frac{\chi_c}{V} = \left[\frac{\Delta}{V}\right]^{3/2} \alpha(p_0), \qquad (2.2)$$

where $\alpha(p_0) = p_0\sqrt{2}/[(1 - p_0^2)(1 - \sqrt{1 - p_0^2})]^{1/2}$. Equation (2.2) shows that for small and intermediate values of p_0, the dependence of χ_c/V on Δ/V is of power-law type with an exponent of 1.5. The case of $p_0 = 1$ has to be dealt with carefully, however, and an analysis shows that when $p_0 \to 1$, the equation for the boundary becomes $\chi_c/V = (\Delta/V)^2$. The exponent thus changes from 1.5 to 2 and this explains the clear gap in the upper phase boundary between small and large values of p_0.

Let us now examine the case $r_0 > 0$. Figure 2 is the $r_0 > 0$ counterpart of Fig. 1. One immediately notices the profound difference between the two cases $r_0 < 0$ and $r_0 > 0$. For instance, one has the largest available area of parameter space for the self-trapped phase when $p_0 = 1$ and this area progressively decreases when p_0 decreases from this value. In contrast to the case where $r_0 < 0$, the phase boundaries for different values of p_0 lie embedded within one another in a non-overlapping fashion. It is instructive and straightforward to calculate asymptotic values of the various features of the phase diagram especially in the region of small p_0. In this limit, the turning point of the phase boundary (marking the mininum amount of saturation allowed for self-trapping) scales with the initial population difference as $\Delta_c/V \sim 6\sqrt{3}/p_0^2$ and the corresponding value of critical

nonlinearity is $\chi_c/V = \sqrt{2}\Delta_c/V$. Again, in this limit, there are two asymptotes for the phase-boundary. The first occurs when one is in the standard DNLSE regime and $\chi \ll \Delta$. Here, one recovers the standard result that the critical value of nonlinearity needed to trap, $\chi_c/V = 8/p_0^2$ and $\Delta/V \to \infty$. The second asymptote marks the boundary where one gets out of the self-trapped phase to the freely evolving phase. This is in the strongly anharmonic phonon regime. The relationship between the parameters at this boundary is markedly different from the asymptote discussed above and the following equation for the boundary holds: $\chi_c/V \approx p_0(\Delta/V)^{3/2}$. It is important to note that this power-law dependence of χ_c/V on Δ/V is similar to the one found for the case $r_0 < 0$. However, the crucial point is that when $r_0 < 0$, the dependence of χ_c/V and Δ/V on p_0 is quite weak, particularly for p_0 far from 1. On the other hand, for $r_0 > 0$, both χ_c/V and Δ/V diverge as $1/p_0^2$. This explains why, whereas for $r_0 < 0$, on the upper phase boundary, the curves seem to merge for different values of p_0, the corresponding curves are well-separated for $r_0 > 0$. There is thus a clear quantitative difference between the two quantum phases $r_0 < 0$ and $r_0 > 0$.

3 Complex initial amplitudes

Thus far, we have only examined the case where the initial conditions for the quasiparticle are real, i.e., $q_0 = 0$. However, it is important to understand the effect of arbitrary initial quantum phases. To this end, we write the basic condition for examining the self-trapped-free phase boundary (2.1) as

$$|g(p_0) \pm 2V\sqrt{1 - p_0^2 - q_0^2}| \geq 2V. \tag{3.1}$$

Using the expression (1.6) in Eq. (3.1) above, we plot in Fig. 3, the parameter space indexed by the saturation ratio Δ/V and the nonlinearity χ_c/V separating the self-trapped regions from the free region. For both Fig. 3(a) and Fig. 3(b), $r_0 < 0$. In Fig. 3(a), $p_0 = 0.1$ and in Fig. 3(b), $p_0 = 0.8$. The primary observation is that relaxing the constraint of reality of the initial quantum amplitudes results in a loss of parameter space available for self-trapping. For small values of p_0 (illustrated by Fig. 3(a)), the phase boundary is much more sensitive to changes in q_0. In fact, for large and intermediate values of q_0 and for small values of p_0, the diagram looks very much like the one obtained in Fig. 2 for $r_0 > 0$. This can be understood very easily by analyzing the expression (1.6) in conjunction with the equality condition of Eq. (3.1) that results in

$$\frac{\Delta}{V} = \frac{2(1 - [1 - p_0^2 - q_0^2]^{1/2})}{\sqrt{(p_0 + 1)^2 + \left(\frac{2\Delta}{\chi}\right)^2} + \sqrt{(p_0 - 1)^2 + \left(\frac{2\Delta}{\chi}\right)^2} - 2\sqrt{1 + \left(\frac{2\Delta}{\chi}\right)^2}}. \tag{3.2}$$

For small values of p_0 and nonzero values of q_0, the right-hand side of Eq. (3.2) tends to diverge as $1/p_0^2$ just as would happen for $r_0 > 0, q_0 = 0$ because the numerator does not vanish in the limit $p_0 \to 0$. Furthermore, the values for the turning point marking the end of the self-trapped region also have the same qualitative behaviour as in the $r_0 > 0, q_0 = 0$

case. Specifically, when $q_0 \neq 0, r_0 < 0$, the values of the parameters at the turning point are: $\Delta/V = 3\sqrt{3}(1 - \sqrt{1 - q_0^2})/p_0^2, \chi_c/V = \sqrt{2}\Delta/V$. Thus we see that the values of the turning point diverge as $1/p_0^2$, similar to the case when $r_0 > 0, q_0 = 0$.

It is possible to understand the qualitative similarity between the $r_0 > 0, q_0 = 0$ and $r_0 < 0, q_0 \neq 0$ cases. In doing so, we can understand a general similarity between the results here and those of Ref. [6]. The point is that when $r_0 < 0, q_0 \neq 0$, in order to trap the system (either the DNLSE one or its generalized cousin), one has to bring the system to a state that is further away in character from the stationary state of the system, marked by $r_0 < 0, q_0 = 0$, and thus closer to one denoted by $r_0 > 0, q_0 = 0$. Thus both the cases $r_0 < 0, q_0 \neq 0$ and $r_0 > 0, q_0 = 0$ are similar. What is interesting is that this similarity is very deep and persists right through into the strongly anharmonic regime.

4   Logarithmic oscillator

Along lines identical to those discussed above, we have analyzed the free-self-trapped phase boundary for the system of a quasiparticle in strong interaction with a logarithmic oscillator discussed earlier in Ref. [5]. The counterpart of Eq. (1.6) is given by

$$g(p) = \frac{8\chi_0^2}{\chi}e^{-\chi/2\chi_0}\sinh^2\left(\frac{\chi p}{4\chi_0}\right), \tag{4.1}$$

where χ_0 is a saturation parameter. The DNLSE limit is recovered in the limit $\chi/\chi_0 \ll 1$. The phase-boundary in the parameter space $\chi_0/V, \chi_c/V$ marking the transition from free evolution to self-trapped behaviour is given then by the expression

$$\frac{8\chi_0^2}{\chi_c}e^{-\chi_c/2\chi_0}\sinh^2\left(\frac{\chi_c p}{4\chi_0}\right) = 2V(1 + r_0) \tag{4.2}$$

Since the phase-diagrams obtained for this system are qualitatively similar to the ones obtained for the rotational polaron, we do not discuss them in detail here. The logarithmic oscillator, besides possessing qualitatively features (similar to the rotational polaron) like saturation of nonlinearity also exhibits the same asymptotic forms for the phase boundaries and turning points. For example, the least saturation value required to support self-trapping occurs for $r_0 < 0, p_0 \to 0$ for $\chi_0/V = e/(2\sqrt{2}), \chi_c = 4\chi_0$. The asymptotes corresponding to $\chi_c/V, \chi_0/V \to \infty$, are a bit different for $p_0 \ll 1$. In contrast to the power-law type behaviour (with exponent 1.5) exhibited for the rotational polaron case, the dependence of critical nonlinearity χ_c on saturation parameter χ_0 is a bit more complicated and numerical evidence seems to indicate the exponent is only slightly greater than 1. However, for $p_0 = 1$, we obtain a result similar to that obtained for the rotational polaron, viz., that $\chi_c/V \sim (\chi_0/V)^2$. For the case, $r_0 > 0$, the available parameter space for self-trapping again shrinks like the counterpart for the rotational polaron. It is particularly simple to calculate the asymptotic properties and turning point of the phase boundary (marking the minimum saturation required for self-trapping) in the limit of small values

6

of p_0. In this regime, the turning point is marked by $\chi_0/V = 8e/p_0^2, \chi_c = \chi_0$. The lower asymptote (in the DNLSE regime) is recovered: $\chi_c/V = 8/p_0^2, \chi_0/V \to \infty$ whereas the upper asymptote in the anharmonic regime is given by the implicit relation:

$$\chi_0 = \frac{4\chi_c}{\log(\chi_c/V)p_0^2} \, , \; \chi_c \to \infty. \qquad (4.3)$$

5 Conclusion

We have extended our analysis [6] of the effect of quantum-mechanical quasiparticle phases on self-trapping by treating saturating dimers [2-5]. We find that initial quasiparticle phases can compete or act with nonlinearity as well as saturation effects. For the case $r_0 < 0$ (in contrast to $r_0 > 0$), the region of available parameter space for self-trapping increases with decreasing asymmetry of initial population, p_0. In particular, as reported in Ref. [4], there exists a minimum value of saturation ratio Δ/V below which no self-trapping can occur for any value of nonlinearity. What is interesting, however, is that this critical value is the least when $r_0 < 0, p_0 \to 0$ and increases for all other regimes. The diametrically opposite case of $r_0 > 0, q_0 = 0, p_0 \to 0$ yields a starkly different condition, viz., that this critical value of saturation diverges as $1/p_0^2$. A generalization to the case of complex initial amplitudes gives results similar to the case when $r_0 > 0, q_0 = 0$. We have also analyzed the logarithmic oscillator and obtained qualitatively similar features as those shown by the rotational polaron. We are thus led to conjecture that these features are perhaps universal to dimers interacting with oscillator potentials that have saturating nonlinearity.

Acknowledgement

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Figure Captions

(i) The critical value of nonlinearity ratio χ_c/V, i.e., the value required for self-trapping is plotted logarithmically against the saturation ratio Δ/V for various values of initial population difference p_0. Here, $r_0 < 0, q_0 = 0$.

(ii) χ_c/V is plotted logarithmically against Δ/V for different values of p_0. In this figure, $r_0 > 0, q_0 = 0$.

(iii) χ_c/V is plotted logarithmically against Δ/V for non-zero values of q_0. In (a), $p_0 = 0.1$ and in (b), $p_0 = 0.8$. For both (a) and (b), $r_0 < 0$.
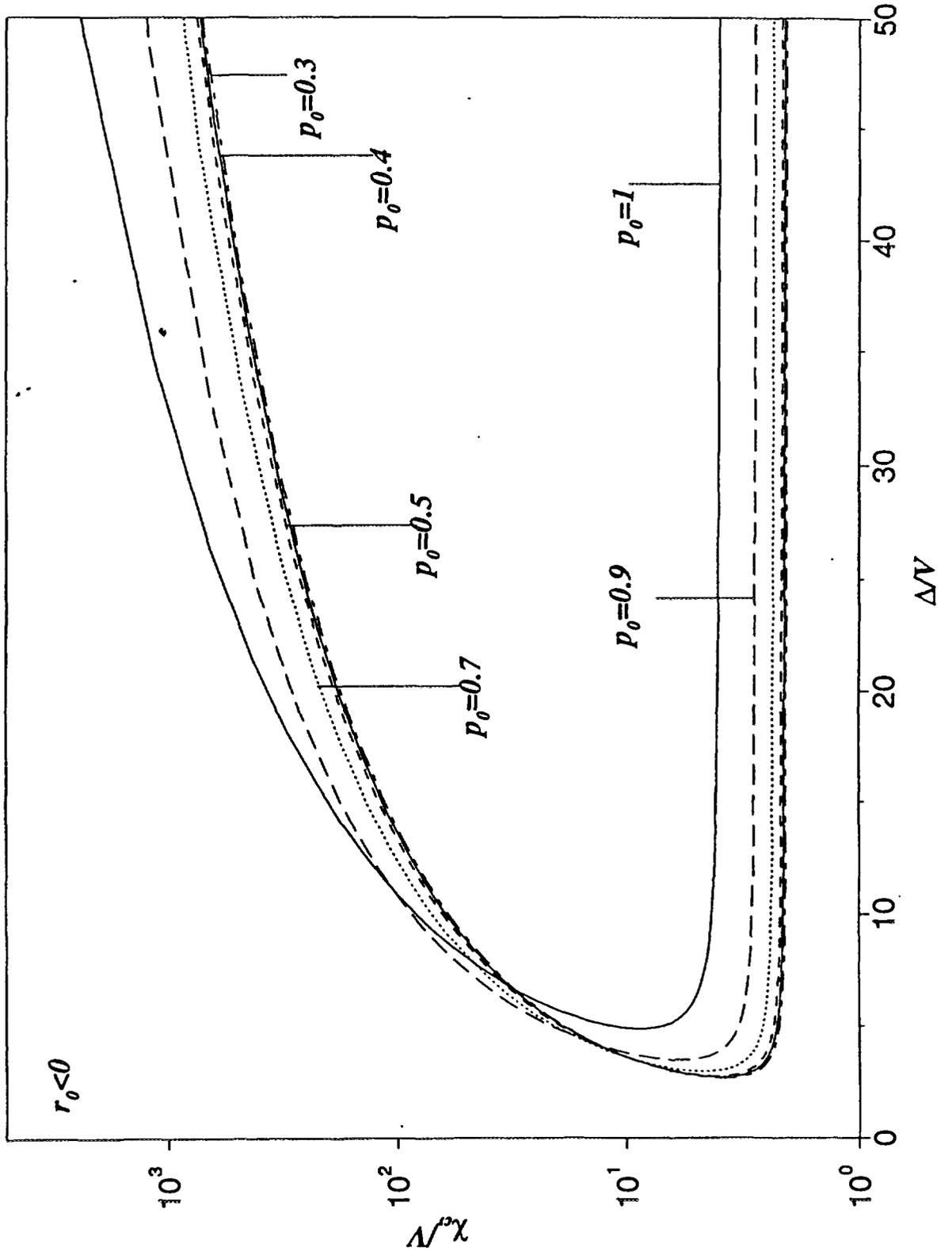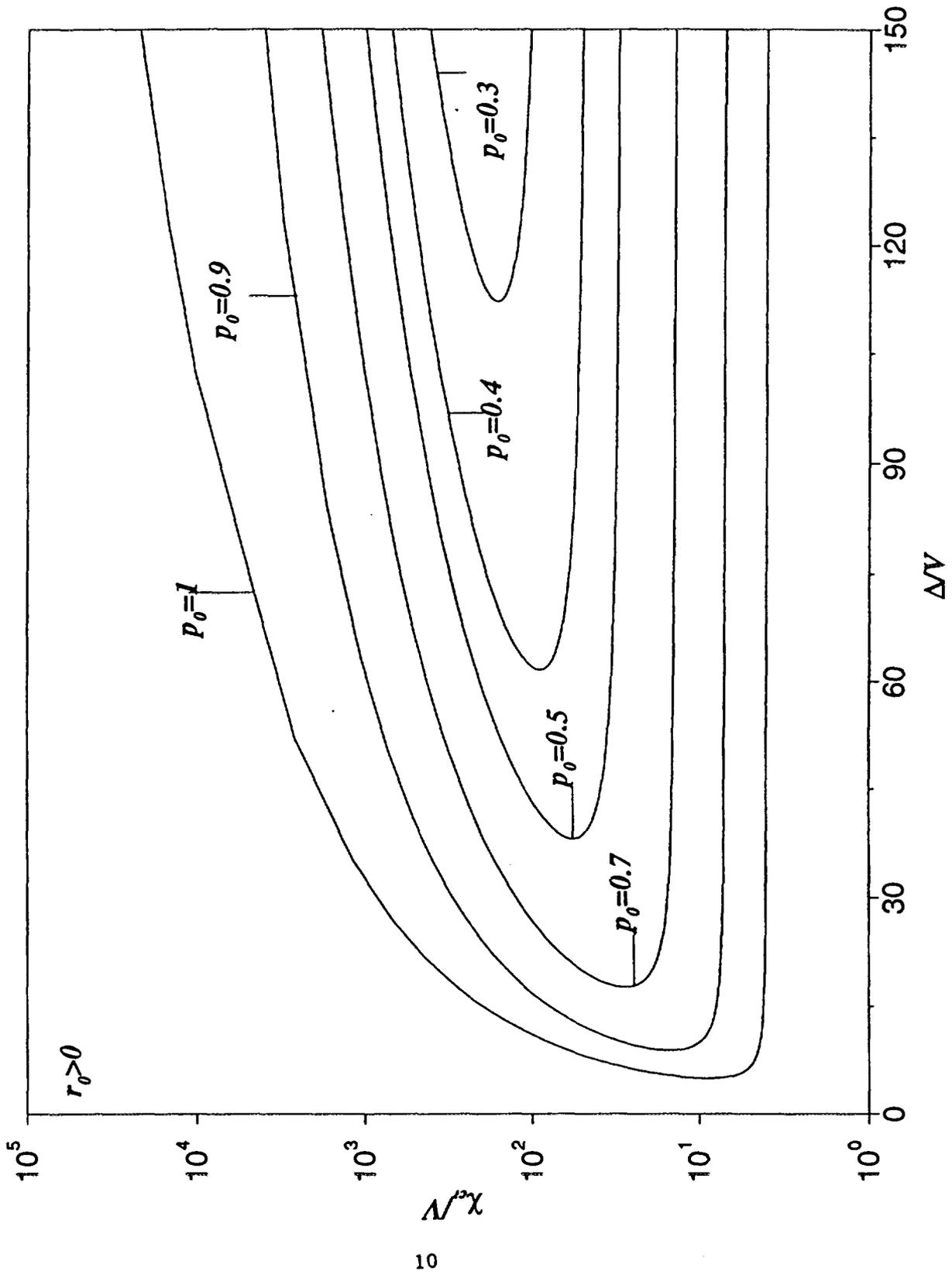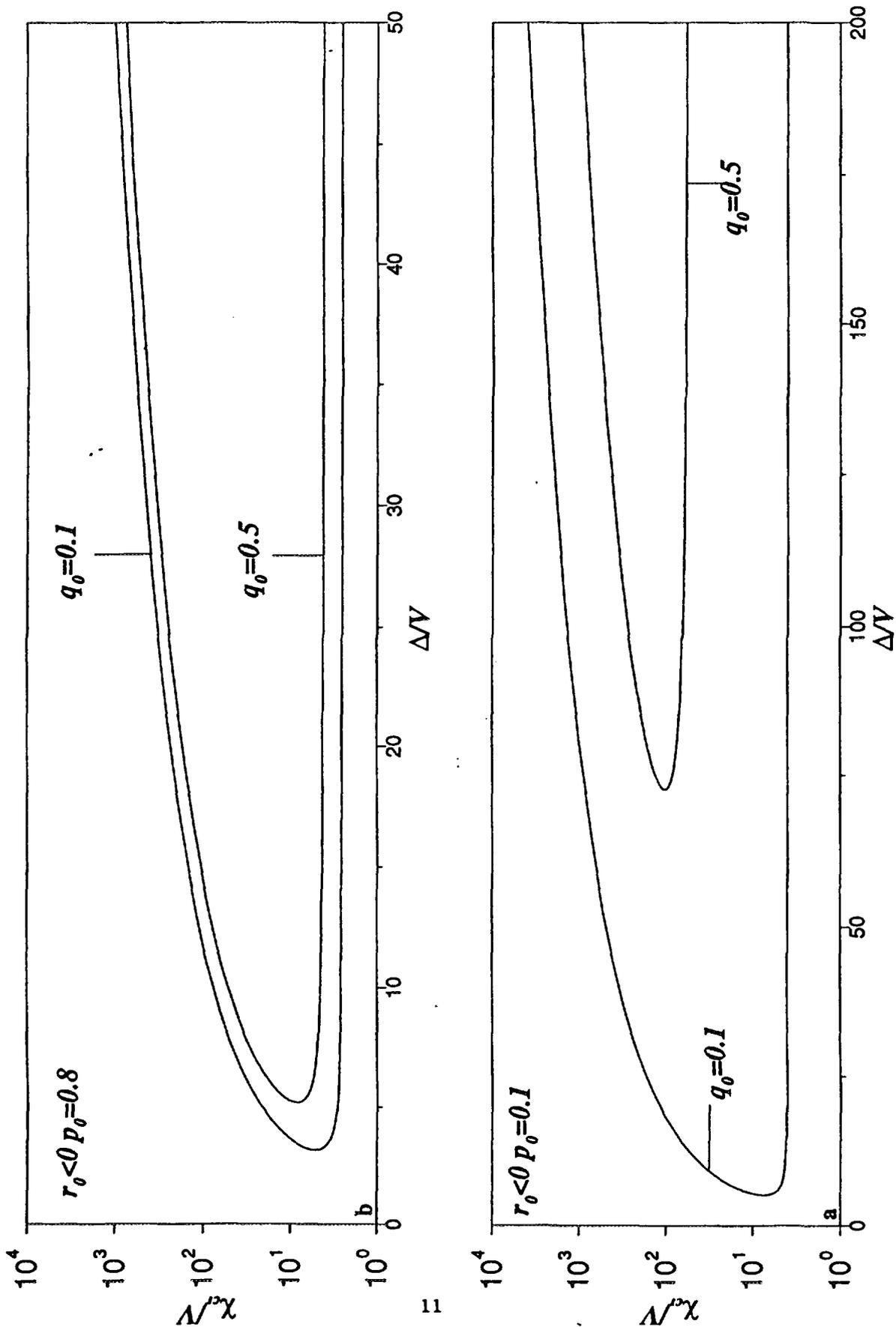
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Fig. 1

Fig. 2

10

Fig.3

11