# Self-trapping transition for a nonlinear impurity embedded in a lattice

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A nonlinear impurity embedded in a lattice is found to have a self-trapping transition. The system considered is a quantum-mechanical quasiparticle such as an electron or exciton moving via nearest-neighbor interactions among the sites of a chain, one particular site in the chain being such that its site energy is dependent on the occupation probability of the site by the quasiparticle. An integral equation for the quasiparticle amplitude is derived and solved numerically. The numerical results appear to show that a self-trapping transition, which tends to localize the quasiparticle, occurs when the nonlinearity exceeds a critical value relative to the intersite transfer interaction. Analytical arguments are presented to support the numerical findings and additional results are obtained in higher dimensions. The appearance of the transition is found to be more compelling in higher-dimensional lattices.

## I. INTRODUCTION

A lot of recent activity has centered on the analysis of the effect of nonlinear interactions on quasiparticle transport.[1–10] The discrete nonlinear Schrödinger equation has often[4–10] served as the basic transport equation, and exact analytic solutions for small or simple systems, and numerical solutions for larger systems have been obtained, along with applications to experiments such as those on neutron scattering and fluorescence depolarization.

The physical origin of these nonlinear interactions is described in Refs. 4–10 and is, in essence, a strong interaction of the moving quasiparticle with vibrations. The strength of this interaction invalidates perturbation treatments as would be appropriate to the transport of an electron in a metal, and necessitates analysis in terms of equations which are nonlinear in the quantum-mechanical amplitude of the quasiparticle. The nonlinearity has fascinating new consequences whose elucidation has occupied a large number of investigators recently.[4–10]

In an effort to apply these ideas to phenomena such as energy transfer in photosynthetic units,[11–13] attempts have been started[10,14] to analyze the effects of nonlinearity in transport on excitation *capture*. A recent analytic calculation[14] on a representation of an antenna reaction center complex in a photosynthetic system is an example of such work. In the light of the renewed interest that we see in this field, we report some features of a nonlinear impurity embedded in a lattice that we have found through numerical simulations.

This paper is set out as follows. In Sec. II, we introduce our model and write down the basic integral equation of motion obeyed by the amplitude for the quasiparticle to be at the nonlinear trap site embedded in a linear lattice. In Sec. III, we show, on the basis of a numerical solution of the integral equation, that a transition from self-trapped to free behavior appears to occur in our system at a certain value of the ratio of the nonlinearity to the transfer interaction. In Sec. IV, we present analytical arguments which support our findings and justify our suggestion that the numerically observed crossover in the behavior of the quasiparticle signifies a true transition rather than a numerical artifact. Section V contains a generalization to higher dimensions and Sec. VI constitutes a summary and discussion. A discussion of the relation of our problem to that of the stationary aspects of the linear defect is presented in the Appendix.

## II. MODEL AND THE INTEGRAL EQUATION

In its simplest form, our system consists of a quasiparticle which moves on a chain via nearest-neighbor interactions $V$ and is trapped by a site which has nonlinear behavior arising from strong interactions with vibrations leading to the nonlinearity described by the cubic term in the so-called discrete nonlinear Schrödinger equation. Perhaps the simplest possible model of capture is one in which one of the sites in the chain is itself the trap site and possesses the cubic nonlinearity. The equation of motion is

$$i\frac{\partial}{\partial t}C_m = V(C_{m+1}+C_{m-1})-\delta_{m,0}\chi|C_0|^2C_0 \ , \qquad (2.1)$$

at time $t$, $\chi$ is the nonlinearity parameter which measures the amount by which the site energy is lowered at a site if the quasiparticle occupies that site, and where $m=0$ denotes the trap site. In (2.1) and in the rest of the paper, we put $\hbar=1$.

We consider the initial condition that the quasiparticle is placed completely at the impurity site. With the help of the defect technique, the amplitude $C_0$ can then be written down as

$$C_0(t)=J_0(2Vt)+i\chi\int_0^t dt'|C_0(t')|^2C_0(t')J_0(2V(t-t')) \ , \qquad (2.2)$$

 

where $J_0$ is the ordinary Bessel function of the first kind and of order zero. An analytic solution of Eq. (2.2) does not appear possible. For this reason, we solve it numerically. We discuss our results below.

## III. NUMERICAL SOLUTION AND THE SELF-TRAPPING TRANSITION

In Fig. 1, we show a graph of the probability to remain on site zero as a function of time for various values of the nonlinear coupling constant. For $\chi=4V$, we see that the probability to remain at the initial site decreases from 1 and oscillates around a value which is about 0.67. The oscillations eventually die away. Similar behavior is observed for all values of $\chi$ larger than $4V$. In contrast, for smaller coupling, of the size $\chi \lesssim 3V$, the probability appears to decay to zero. Clearly, the latter case signifies that the quasiparticle escapes the trap site while the former case represents some self-trapping. Thus, the system exhibits what appears to be a transition as a function of $\chi/V$.

Of the large number of values of nonlinearity for which we have carried out numerical studies of the transition, we have chosen to display in Fig. 1 only those in the neighborhood of the transition. We note that, when the nonlinear coupling constant is $\chi/V=3.20$, the probability at the initially occupied site decreases rapidly as a function of time. More careful study, e.g., for the case of $\chi/V=3.22$, shows that, while the probability decreases initially and drops to about 0.13, it then *increases* to a value of 0.30 at $Vt=90$, before again decreasing and once again increasing at $Vt=160$. These recurrences repeat at regular intervals, as is especially evident for slightly larger values of $\chi/V$. The recurrences eventually die out, leaving a nonzero value of the probability at long times. There is thus no doubt that there is self-trapping for values of $\chi \gtrsim 3.22$ V. While the curves in Fig. 1 suggest strongly that the self-trapping behavior disappears when $\chi/V$ is less than some finite value, it is not possible to make that assertion with certainty. The question must be asked whether the probability that appears to have decayed on some time scale might not rise again for larger times, signifying that self-trapping is still effective. It is not easy to answer this question when numerical analysis is our only tool.

To investigate the existence of the transition, we studied the recurrence period of the probability oscillations. On approaching the suspected transition value from the self-trapped side ($\chi/V>3.205$), we found that the period

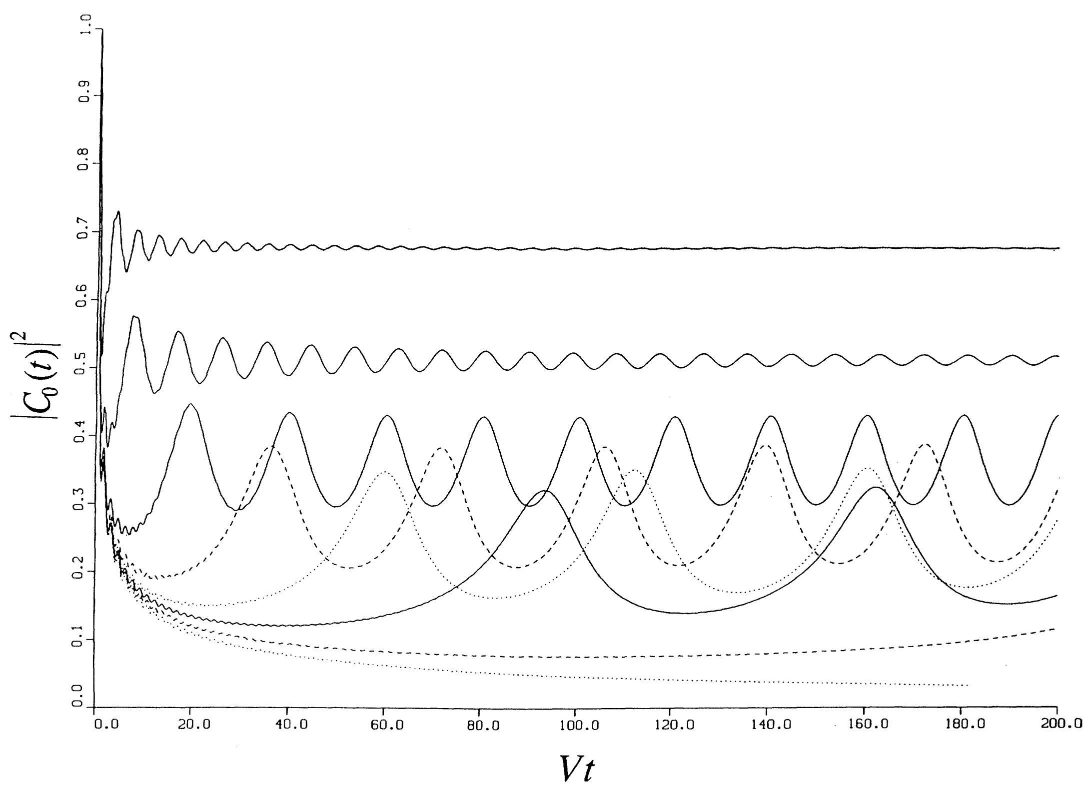


FIG. 1. The probability to remain at the initially occupied site $|C_0(t)|^2$ plotted vs dimensionless time $Vt$ for several values of $\chi$ in the neighborhood of the apparent trapping-detrapping transition. The top curve, which shows self-trapping such that $|C_0(t)|^2 \sim 0.67$, has been calculated for $\chi=4.00V$. As the value of $\chi$ is reduced, the probability remaining at long times also decreases. The next lower curve has been calculated for $\chi=3.50V$, and the next for $\chi=3.30V$. As we continue to reduce $\chi$, it becomes more difficult to determine which curve corresponds to which value of $\chi$. For this reason, we have distinguished between them with different line types. They are as follows: the next lower dashed line has been calculated for $\chi=3.25V$; the next dotted line has been calculated for $\chi=3.23V$; the next solid line, for $\chi=3.22V$; the next dashed line, for $\chi=3.21V$; the lowest dashed line, for $\chi=3.20V$.

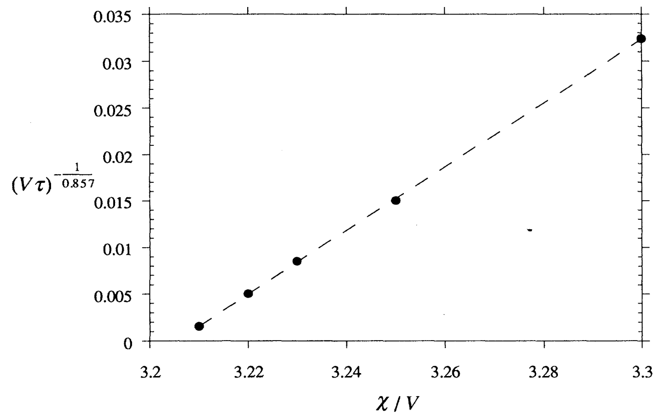


FIG. 2. The quantity $(1/V\tau)^{1/0.857}$ plotted as a function of $\chi/V$ to show agreement with the empirically found formula (3.1). The first recurrence time $\tau$ was obtained for values of $\chi$ near $3.20V$ by inspection of Fig. 1. Relation (3.1) suggests an abrupt transition to infinite recurrence time (and detrapping) when $\chi \sim 3.20V$.

becomes very long as $\chi/V$ tends to 3.205. A true transition would be described by the recurrence becoming infinite. However, such behavior is difficult to pin down numerically. For example, for the value of $\chi/V=3.21$, it appears at short times that there might be complete decay of the probability, with no recurrences. However, a much longer iteration shows this not to be the case. The first recurrence is at $Vt=254$, and the probability increases to 0.28. As we have already mentioned, for $\chi/V=3.20$, we observe only a steady decay, at least out to $Vt=800$, which is as far as we have iterated. It is not possible to state whether or not there will be a recurrence for this value of $\chi/V$ if we look at still longer times. We can only report that, for times such that $Vt \lesssim 800$, we have observed an apparent trapping-detrapping transition which occurs at a value of $\chi/V$ between 3.20 and 3.21.

To quantify our observations, we recorded the time $\tau$ for the first recurrence in probability as a function of $\chi/V$. In Fig. 2 we have plotted $\tau$ for values of $\chi/V$ in the neighborhood of 3.2. Assuming that the results can be fit by a power law, we have found a best fit. The power law fit is described by the relation

$$V\tau = \left[\frac{2.924}{\chi/V-3.205}\right]^{0.857} . \tag{3.1}$$

Although the result of numerical rather than analytic calculations, (3.1) is extremely suggestive. The equation implies that the recurrence period becomes infinite for $\chi/V=3.205$, and thus signifies an abrupt transition from self-trapping to free behavior.

## IV. ANALYTIC ARGUMENTS IN SUPPORT OF THE TRANSITION

An analytical solution of (2.2), if available, could lend complete credence to our suggestion that a transition does occur in this system. In the absence of such an exact solution, we investigate (2.2) through what we consider a reasonable approximation. If the factor $|C_0(t')|^2$ in the integrand of (2.2) were absent, i.e., if it were replaced by 1, an exact solution could be written down immediately. Thus, if we replace $\chi|C_0(t')|^2$ by the time-independent quantity $\Delta$, we have

$$C_0(t)=J_0(2Vt)+i\Delta\int_0^t dt' C_0(t')J_0[2V(t-t')] , \tag{4.1}$$

which is the solution of

$$i\frac{\partial}{\partial t}C_m = V(C_{m+1}+C_{m-1})-\delta_{m,0}\Delta C_0 , \tag{4.2}$$

rather than that of (2.1). Equation (4.2) describes a *linear* defect. The analytic solution of (4.1) is straightforward via Laplace transforms. Thus, if tildes denote Laplace transforms, and $s$ is the Laplace variable, (4.1) gives

$$\tilde{C}_0(s)=\frac{1}{\sqrt{s^2+4V^2}-i\Delta} \equiv \tilde{G}(s) , \tag{4.3}$$

where we have introduced the quantity $\tilde{G}(s)$ for future use. The explicit inversion of (4.3) gives

$$C_0(t)=J_0(2Vt)+i\Delta\int_0^t ds e^{i\Delta s}J_0(2V\sqrt{t^2-s^2}) . \tag{4.4}$$

What makes our original problem analytically difficult is the presence of $|C_0(t')|^2$ in the integrand of (2.2). Let us therefore replace it by a known function and treat (2.2) via a self-consistent procedure. The choice of the function to represent $|C_0(t')|^2$ should surely be determined by what we have learned about the evolution of the trap site probability through the numerical work described in Sec. III. We have seen that $|C_0(t)|^2$ starts at the value 1 at the initial time and then decays to a value which may or may not be zero. Let us tacitly assume that as $t\to\infty$, the trap probability does tend to a constant. The product of that constant and the nonlinearity parameter $\chi$ is the limiting value of the energy lowering, which we will call $\Delta$. If $\Delta$ is nonzero, there is self-trapping. If $\Delta$ vanishes, the quasiparticle is free. If we can show that the ratio of the nonlinearity to the transfer interaction controls $\Delta$ in that the latter is zero for values of $\chi/V$ which are smaller than a critical value, but nonzero for $\chi/V$ larger than the critical value, we will have supported the numerical finding of the trapping-detrapping transition.

We represent the essential behavior of the factor $\chi|C_0(t)|^2$ in the integrand of (2.2) by replacing it as follows:

$$\chi|C_0(t)|^2 \to \Delta+(\chi-\Delta)f(t) , \tag{4.5}$$

where $f(t)$ varies from 1 to 0 as $t$ goes from 0 to infinity. A possible candidate for $f(t)$ is $e^{-\alpha t}$, where $1/\alpha$ is the time constant over which the trap probability decays from 1 to its eventual value. The replacement (4.5) converts (2.2) to

$$C_0(t)=J_0(2Vt)+i\Delta\int_0^t dt' C_0(t')J_0[2V(t-t')] + i(\chi-\Delta)\int_0^t dt' f(t')C_0(t')J_0[2V(t-t')] . \tag{4.6}$$

Let us first consider the extreme case when the function $f(t)$ decays to 0 *immediately*. This is the case when, in terms of the exponential approximation, $\alpha$ tends to infinity. Equation (4.6) reduces to the simple linear defect case (4.1). The quantity $\tilde{G}(s)$ in (4.3) has one simple pole at $s=i\sqrt{\Delta^2+4V^2}$. The long-time behavior of the amplitude $C_0(t)$ is thus given by

$$C_0(t)\sim\frac{\Delta}{\sqrt{\Delta^2+4V^2}}e^{it\sqrt{\Delta^2+4V^2}} . \tag{4.7}$$

The long-time limit of the trap site probability is obtained by taking the square of the absolute value of (4.7) and the energy lowering is obtained by multiplying the result by the nonlinearity $\chi$. Self-consistency of the procedure requires, however, that this energy lowering be equal to $\Delta$:

$$\Delta=\frac{\chi\Delta^2}{\Delta^2+4V^2} . \tag{4.8}$$

Equation (4.8) is solved as

$$\Delta=\frac{\chi\pm\sqrt{\chi^2-16V^2}}{2} \quad \text{or } \Delta=0 . \tag{4.9}$$

Since it is clear from (4.9) that a nonzero solution for $\Delta$ exists only if $\chi$ is greater than $4V$, we have demonstrated the existence of the trapping-detrapping transition for the extreme case considered.

Let us next consider the exponential representation of $f(t)$ with arbitrary $\alpha$. Using the shift theorem of Laplace transforms, we can write (4.6) as

$$\tilde{C}_0(s)=\tilde{G}(s)+i(\chi-\Delta)\tilde{G}(s)\tilde{C}_0(s+\alpha) \tag{4.10}$$

and carry out an iteration to obtain an explicit expression for $\tilde{C}_0(s)$:

$$\tilde{C}_0(s)=\tilde{G}(s)\left[1+\sum_{n=1}^{\infty}e^{in\pi/2}(\chi-\Delta)^n\prod_{m=1}^{n}\tilde{G}(s+m\alpha)\right] . \tag{4.11}$$

There is one simple pole on the right-hand side of (4.11) which gives a nondecaying amplitude at long times. As before, the pole is at $s=-i\sqrt{\Delta^2+4V^2}$. Evaluation of the residue of the pole yields an expression for the trap site amplitude at long times. Proceeding exactly as in the case for $\alpha\to\infty$ discussed above, we obtain the energy lowering. Once again, the requirement of self-consistency dictates that we equate the energy lowering to $\Delta$ and obtain thereby a condition for the transition:

$$\Delta=\left[\frac{\chi\Delta^2}{\Delta^2+4V^2}\right]\left[1+\sum_{n=1}^{\infty}e^{in\pi/2}(\chi-\Delta)^n\prod_{m=1}^{n}\tilde{G}(i\sqrt{\Delta^2+4V^2}+m\alpha)\right]^2 . \tag{4.12}$$

Equation (4.12) is the counterpart of (4.8) for this case of arbitrary $\alpha$. The quantity $\tilde{G}(s)$ has already been defined earlier in (4.3). The existence of the trapping-detrapping transition is again established clearly as in the simpler case above. The specific transition value of $\chi/V$ depends on the value of $\alpha$. We solved (4.12) numerically for a selected value of $\alpha$, viz., $\alpha=1.9V$. The results are displayed graphically in Fig. 3. The difference between the right-hand side of (4.12) and $\Delta$ has been called the function $F(\Delta)$ in Fig. 3 and we have plotted it vs $\Delta$ for various values of the ratio of the nonlinearity to the transfer interaction. For $\chi/V=3.0$, there is only one root and it lies at the origin. This indicates a complete decay of the trap site probability at long times and signifies *free* behavior. The appearance of a root at the nonzero value of $\Delta$ which we see for $\chi/V=3.4$ shows, on the other hand, that we have self-trapping. A trapping-detrapping transition takes place at $\chi/V=3.2$ when the $F(\Delta)$ curve just touches the $\Delta$ axis.

Under the replacement (4.5), we have shown unequivocally that a transition from free to self-trapped behavior does occur in our system when we represent the function $f(t)$ as an exponential. The transition value of $\chi/V$ depends on the value of the exponent $\alpha$ chosen. We have seen that the numerically observed critical value of $\chi/V=3.2$ is obtained for $\alpha=1.9V$. This value of the exponent is close to $2V$, the reciprocal of a natural time constant for the quasiparticle in the chain considered. We have also seen analytically that $\chi/V=4.0$ when the exponent is infinitely large. It can be shown with the help of (4.12) that the critical value is $\chi/V=2.54$ in the opposite limit of a vanishing exponent. It is comforting to notice that, although we have to take the value of the exponent in an *ad hoc* manner, the transition is assured for *any* such value, and that the extremes $\alpha\to\infty$ and $\alpha\to0$ bracket the transition value of $\chi/V$ between 4.0 and 2.54.

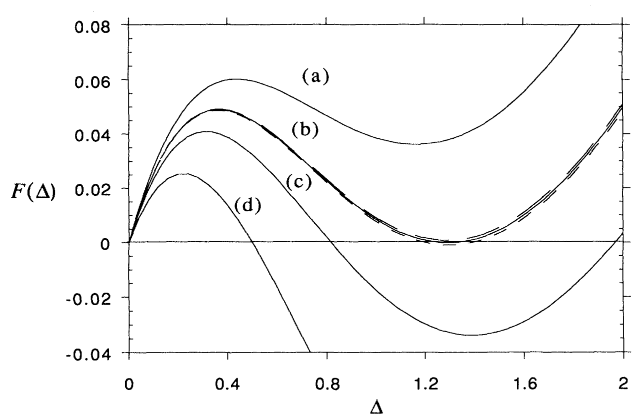


FIG. 3. The function $F(\Delta)$ plotted vs $\Delta$ in units of $V$. The roots of $F(\Delta)$ are solutions representing self-trapped states for $\Delta\neq0$. The curves are for several values of $\chi$, as follows: (a) $\chi=3.00V$; (b) $\chi=3.21V$, $\chi=3.205V$, and $\chi=3.20V$; (c) $\chi=3.40V$; (d) $\chi=4.00V$. The three curves labeled by (b) are in the neighborhood of the transition. For $\chi<3.205V$, the only root is at $\Delta=0$, indicating the absence of self-trapping. For $\chi\geq3.205V$, there are two roots besides the root at zero; self-trapping is a possibility. The value of $\alpha$ was chosen to be $1.875V$ so that the transition indicated by this figure would occur in the neighborhood of $\chi=3.20V$, in agreement with the numerical calculations.

All possible transition values in our approximation thus lie quite close to the numerically observed value 3.205.

## V. EXTENSION TO HIGHER DIMENSIONS

Our analysis can be easily extended to higher dimensions. We consider a simple square and a simple cubic lattice. The counterpart of (2.2) for a two-dimensional lattice with nearest-neighbor interactions $V$ is

$$C_0(t)=J_0^2(2Vt)+i\chi\int_0^t dt'|C_0(t')|^2C_0(t')J_0^2[2V(t-t')] , \tag{5.1}$$

whereas for the corresponding three-dimensional lattice it is

$$C_0(t)=J_0^3(2Vt)+i\chi\int_0^t dt'|C_0(t')|^2C_0(t')J_0^3[2V(t-t')] . \tag{5.2}$$

The only change relative to (2.2) is the appearance of the square and the cube of the Bessel function propagator, respectively.

As in the case of (2.2), we have solved (5.1) and (5.2) numerically. We have found, as expected, that the trapping-detrapping transition persists in higher dimensions. In fact, it is even more abrupt. For the square lattice, the critical value of the ratio of the nonlinearity to the intersite transfer interaction is given by

$$\frac{\chi}{V}=6.72, \quad \text{in a 2D system} . \tag{5.3}$$

The critical value in a cubic lattice is given by

$$\frac{\chi}{V}=9.24, \quad \text{in a 3D system} . \tag{5.4}$$

In all three cases considered, the population which remains localized as $t$ tends to infinity approaches zero abruptly as a function of $\chi/V$, as $\chi/V$ takes on the critical value. While this is not obvious in the one-dimensional case, the behavior is quite apparent in the 2D and 3D cases. The time-dependent behavior of the probability to remain on the initially occupied site for the three-dimensional case is shown in Fig. 4.

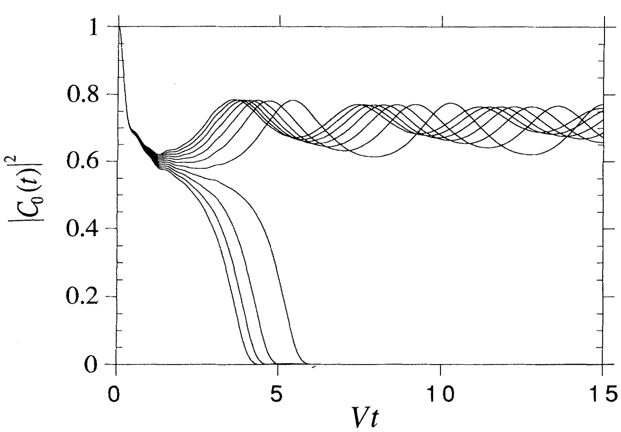


FIG. 4. The probability to remain at the initially occupied site $|C_0(t)|^2$ plotted as a function of dimensionless time $Vt$ when the nonlinear defect is in a three-dimensional (simple cubic) lattice. The curves have been calculated from the numerical solution of (5.2) for values of $\chi/V$ between 9.20 and 9.30. The three curves indicating a complete decay of the probability at the initial site are for $\chi/V$=9.20, 9.21, and 9.23, respectively. The seven curves which show no decay are for $\chi/V$=9.24, 9.25, 9.26, 9.27, 9.28, 9.29, and 9.30, respectively.

## VI. SUMMARY AND DISCUSSION

The system we study in this paper is a quantum-mechanical quasiparticle which moves on a lattice and is trapped by a special site in the lattice. The special feature of the trapping site is that it introduces a nonlinearity typical of the nonlinear Schrödinger equation which has come under intense investigation in recent times.[4–10] Specifically, the site energy of the quasiparticle at the trapping site is lowered whenever the trapping site is occupied. The amount of energy lowering is proportional to the probability of occupation of the trap site.

Our primary tool of investigation has been numerical calculations aided by analytical procedures. Through numerical calculations we have observed what appears to be a trapping-detrapping transition whenever the trap site is occupied initially. Figures 1 and 2 show the transition behavior. The peculiar change in the time dependence of the trap site probability which occurs as one crosses the critical value of the ratio of the nonlinearity to the transfer interaction is shown in Fig. 1. A characteristic dependence of the period of recurrences on the difference of this ratio from the critical value is shown in Fig. 2. The critical value of this ratio $\chi/V$ we find through our numerical calculations is 3.205.

In order to support the numerical findings, we have considered an approximate but representative evolution of the system by replacing the trap site probability in the integral equation (2.2) by a simple function which possesses the numerically suggested features that it begins at the value 1, and decays over a characteristic time to some value $\Delta$. We carry out a self-consistency procedure to determine the value of $\Delta$, the idea being that a zero value marks free behavior while a nonzero value signifies self-trapping. We indeed find the existence of the transition we seek, the critical value of $\chi/V$ being dependent on the characteristic time of the decay of the function chosen to represent the trap site probability in the integrand of (2.2). The critical value at which the transition value occurs lies between 2.54 and 4.0. These extremes bracket, and are quite close to, the numerically observed value 3.205 for the original problem treated without approximation.

We have found that the transition persists in higher dimensions and that its abruptness increases with dimension. The transition values of $\chi/V$ are 6.72 and 9.24, respectively, in two and three dimensions.

Have we given an unequivocal proof of the existence of the transition that we appear to have observed numerically? Unfortunately we cannot answer in the affirmative, in spite of the fact that extremely suggestive analytical arguments and results are available. We believe we can safely assert that under the single assumption that the probability of the initially occupied trap site tends to a *constant* at long times, we can be assured of the existence of the transition. It might be helpful to examine in this regard the relation between our problem and that of the *stationary* aspects of the linear defect problem. It is well known that a linear chain with a static impurity has exactly one exponentially localized eigenstate, centered about the impurity. All the other states are extended. Thus when we see self-trapping, and also see that $|C_0(t)|^2 \sim$constant, it means that at $t=\infty$ there is necessarily a nonzero population in the localized eigenstate of the linear chain. Thus the process of self-trapping is ultimately the process of populating the localized eigenstate. Useful insights may be gleaned from an examination of the shape and extent of the localized eigenstate formed by a static defect. Such an examination has been presented in the Appendix.

## ACKNOWLEDGMENT

We thank Marek Kuś for many useful conversations which showed us, in at least one case, the error of our ways.

## APPENDIX

In this appendix we discuss the relation between the observed trapping-detrapping transition and the properties of the stationary states of the corresponding linear problem. The relevance of this relation stems from the observation that, at long times $|C_0(t)|^2 \sim$constant, and the system might be analyzed in terms of the superposition of eigenfunctions.

For a static defect, the extent of the localized state depends on the strength of the impurity. The larger the impurity, the more strongly localized is the state, and the weaker the impurity, the less strongly localized is the state. In our paper, we always ask for the probability remaining at the impurity site. This can be found by projecting onto the localized eigenstate. At long times, the system is stationary, and the wave function $|\Psi(t)\rangle$ may be written as a sum over the eigenstates of the system, $|\phi_j\rangle$,

$$|\Psi(t)\rangle = c_l e^{-iE_l}|\phi_l\rangle + \sum_j c_j e^{-iE_j t}|\phi_j\rangle \ . \tag{A1}$$

The sum is over the extended states, and we have explicitly pulled the localized state $|\phi_l\rangle$ out of the sum. The amplitude to be at site zero at long times is given by

$$\langle 0|\Psi(t)\rangle = c_l e^{-iE_l t}\langle 0|\phi_l\rangle + \sum_j c_j e^{-iE_j t}\langle 0|\phi_j\rangle \ , \tag{A2}$$

where $\langle 0|$ is the adjoint of the state at site zero. The sum in (A2) decays in time, leaving only the first term corresponding to the localized state. Therefore, the probability $P$ to be at site zero at long times is given by

$$P = |C_0(\infty)|^2 = |\langle 0|\phi_l\rangle|^2 |c_l|^2 \ . \tag{A3}$$

In (A3) the probability is given by the product of two terms. The first is the square of the overlap of the site state $|0\rangle$ with the localized state, and the second, $|c_l|^2$, is the probability to be in the localized state. If the strength of the impurity at long times is $\Delta$, then the overlap is easily calculated, and found to be $\Delta/\sqrt{\Delta^2+4V^2}$. Substituting this result into (A3) gives

$$|C_0(\infty)|^2 = \frac{\Delta}{\sqrt{\Delta^2+4V^2}}|c_l|^2 \ . \tag{A4}$$

Now, we note that (A4) is self-consistent, since what is meant by $\Delta$ is $\chi|C_0(\infty)|^2$, which is on the left-hand side of (A4). Thus we have

$$\Delta = \frac{\chi\Delta}{\sqrt{\Delta^2+4V^2}}|c_l|^2 \ . \tag{A5}$$

Equation (A5) can be solved for $\Delta$ to determine the probability remaining trapped at long times. Note that $\Delta=0$ is always a solution of (A5), which indicates no trapping. However, depending on the value of $|c_l|^2$, we may or may not find nonzero values of $\Delta$ which also satisfy (A5). If we find a nonzero solution for $\Delta$, then there is a possibility of self-trapping. Clearly, if the only solution of (A5) is $\Delta=0$, we can be sure that there can be no self-trapping for a given value of the probability $|c_l|^2$.

For a given value of the probability $|c_l|^2$, we find that a nonzero solution for $\Delta$ exists or does not exist, depending on the value of $\chi$. We believe that if the correct value of $|c_l|^2$ can be determined, then this transition will closely correspond to the transition which is observed numerically. Thus, in our minds, the process of *populating* the localized eigenstate and determining $|c_l|^2$ is what needs to be understood.

One obvious limit exists. The probability to be in the localized eigenstate at long times $|c_l|^2$ cannot be larger than 1. If we substitute this value in (A5), and solve for $\Delta$, we find that unless $\chi/V>2$, the only solution of (A5) is $\Delta=0$. We can be sure, therefore, that there will be no trapping unless $\chi/V>2$.[15]

Two other limits which can be explored in this discussion are the sudden and adiabatic limits which we explored in our time-dependent analysis. If, initially, the decaying function $\chi|C_0(t)|^2$ is suddenly replaced by its asymptotic value $\Delta$, then this corresponds to the limit $\alpha\rightarrow\infty$. In such a case, the problem is linear from the start, so that the coefficients $c_j$ and $c_l$ in (A1) are known for all time from overlaps with the initial condition. Equation (A1) becomes

$$|\Psi(t)\rangle = \langle\phi_l|0\rangle e^{-iE_l t}|\phi_l\rangle + \sum_j \langle\phi_j|0\rangle e^{-iE_j t}|\phi_j\rangle \ . \tag{A6}$$

We proceed exactly as we did before. The amplitude to be at site zero at long times is given by

$$\langle 0|\Psi(t)\rangle = \langle\phi_l|0\rangle\langle 0|\phi_l\rangle e^{-iE_l t} + \sum_j \langle\phi_j|0\rangle\langle 0|\phi_j\rangle e^{-iE_j t} \ . \tag{A7}$$

Equation (A7) corresponds to (A2). The reader will notice that in the sudden approximation, the value of $|c_l|^2$ is completely determined by the initial conditions. The probability to be in the localized state is given by the overlap of the localized state for a static defect $\Delta$ and the initial condition which is that state $|0\rangle$ is populated. Thus,

$$|c_l|^2 = \frac{\Delta}{\sqrt{\Delta^2+4V^2}} . \tag{A8}$$

The sum in (A7) decays in time, so that at long times, we find

$$|C_0(\infty)|^2 = |\langle 0|\phi_l\rangle|^2 |\langle 0|\phi_l\rangle|^2 = \frac{\Delta}{\sqrt{\Delta^2+4V^2}} \frac{\Delta}{\sqrt{\Delta^2+4V^2}} . \tag{A9}$$

The corresponding equation to (A5) is therefore

$$\Delta = \frac{\chi\Delta^2}{\Delta^2+4V^2} , \tag{A10}$$

which, as we have seen in the text, displays a transition at $\chi/V=4$.

We are not surprised that this transition point is higher than the limit $\chi/V=2$ we found above when we took $|c_l|^2$ to be 1, for the amount of probability in the localized state, as given by (A8), is considerably less than 1 when $\chi=2V$. A larger value of $\chi$ is thus required to create a defect strong enough to do the job.

In the adiabatic limit, we ask what happens if the decaying function $\chi|C_0(t)|^2$ is replaced by a function which decays very slowly to its asymptotic value $\Delta$. This corresponds to the limit $\alpha\rightarrow 0$. In such a case, the eigenstates of the system follow the approach to $\Delta$ *adiabatically*. Initially, the eigenstates correspond to those which would be present if the defect were of the value $\chi$. Ultimately, the eigenstates correspond to those which would be present if the defect were of the value $\Delta$. For this case (A1) can be rewritten as

$$|\Psi(t)\rangle \cong c_l e^{-itE_l(t)} |\phi_l(t)\rangle + \sum_j c_j e^{-itE_j(t)} |\phi_j(t)\rangle . \tag{A11}$$

The energies and the states have been written as explicit functions of time. To find the coefficients in (A11), we project onto the initial condition, $|\Psi(0)\rangle = |0\rangle$, as before. We find the equation analogous to (A6),

$$|\Psi(t)\rangle = \langle\phi_l(0)|0\rangle e^{-itE_l(t)} |\phi_l(t)\rangle + \sum_j \langle\phi_j(0)|0\rangle e^{-itE_j(t)} |\phi_j(t)\rangle . \tag{A12}$$

To find the amplitude remaining at site zero at long times, we close with $\langle 0|$, to obtain

$$\langle 0|\Psi(t)\rangle = \langle\phi_l(0)|0\rangle\langle 0|\phi_l(t)\rangle e^{-itE_l(t)} + \sum_j \langle\phi_j(0)|0\rangle\langle 0|\phi_j(t)\rangle e^{-itE_j(t)} . \tag{A13}$$

The sum in (A13) decays, so that at long times, the probability to be in site zero is given by

$$|C_0(\infty)|^2 = |\langle 0|\phi_l(\infty)\rangle|^2 |\langle\phi_l(0)|0\rangle|^2 . \tag{A14}$$

The first term on the right-hand side of (A14) is the square of the overlap of $|0\rangle$ and the localized state which forms when the defect is of strength $\Delta$. The second term on the right-hand side of (A14) is the square of the overlap of $|0\rangle$ and the localized state which forms when the defect is of strength $\chi$. Thus, the self-consistent equation corresponding to (A5) in the adiabatic limit is

$$\Delta = \chi \frac{\Delta}{\sqrt{\Delta^2+4V^2}} \frac{\chi}{\sqrt{\chi^2+4V^2}} , \tag{A15}$$

which has the nontrivial solution

$$\Delta = \sqrt{[\chi^4/(\chi^2+4V^2)] - 4V^2} , \tag{A16}$$

provided that $\chi/V > (2+2\sqrt{5})^{1/2} \cong 2.54$. We are not surprised that the threshold is lower than it was in the sudden approximation ($\chi/V>4$) because the amount of probability which remains in the localized state at long times is larger, making for a stronger defect for a smaller value of $\chi$.

We have now seen the importance of choosing the correct value of $|c_l|^2$. Since the actual decay of the defect is neither strictly adiabatic nor strictly sudden, it is plausible that the appropriate value of $|c_l|^2$ lies somewhere between $\Delta/\sqrt{\Delta^2+4V^2}$ and $\chi/\sqrt{\chi^2+4V^2}$. Our model of the decay of the defect by an exponential is an attempt at approximately finding the value of $|c_l|^2$. We find as a function of the decay rate $\alpha$ that $|c_l|^2$ lies somewhere between the limits provided by the sudden and adiabatic approximations, leading to a threshold value of $\chi/V$ which lies somewhere between 2.54 and 4. With satisfaction, we note that the numerical threshold occurs at $\chi/V=3.2$, and can be obtained by choosing $\alpha/V=1.9$.

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