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Stability of Discrete Solitons and Quasicollapse to Intrinsically Localized Modes

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An analytical stability criterion for discrete solitons is presented. Its evaluation proves that discreteness reduces (in comparison with the continuum results) the critical nonlinearity parameter (which separates stable and unstable regimes). Unstable discrete solitons may "collapse" into the more stable intrinsically localized states. The theory applies to a discrete nonlinear Schrödinger equation, but can be generalized to other systems.

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Systems with competition between nonlinearity and dispersion are rather well studied, especially in the continuum limit. As a result of a balance between nonlinear and dispersive effects, specific nonlinear objects, namely *solitary waves*, may appear [1,2]. They can be stable (corresponding, e.g., to the stable solitons) or unstable. The latter means that dispersion balances nonlinear steepening only in the stationary case. Small perturbations around the solitary wave may break this balance leading to instability and perhaps collapse. The stability of solitary waves has been studied in many physically different and important nonlinear problems. For continuous systems a rather well-developed formalism exists (see, e.g., [3,4]). The situation is different for discrete systems. Here, in principle, not so many results were obtained analytically. For example, in the often used Schrödinger limit, we only know the case discussed in the pioneering work of Ablowitz and Ladik [5] where analytical predictions can be made. However, this integrable form of discretization does not occur in most physically motivated models, such as coupled nonlinear atomic strings with onsite or intersite anharmonic potentials, arrays of coupled optical waveguides, proton dynamics in hydrogen-bonded chains, the Davydov and Holstein models for transport of excitation energy in biophysical systems, and so on.

Localized modes in discrete nonlinear systems have been a subject of intensive but mainly numerical investigations during the past years (see, e.g., [5–16]). Different types of localized states were found, and very elegant and efficient schemes have been developed [15] for calculating whole families of solitary wave solutions. Of course, a broad discrete solution may be described with the help of the continuum approximation. However, there exist other types of discrete modes that definitely will not obey the continuum limit [6,9]. Some of these solutions show stable behavior in numerical experiments. It should be noticed, however, that numerical simulations cannot prove stability in the strict sense. Thus, analytical criteria are urgently called for, and it is the primary motivation of this Letter to develop analytical stability criteria for discrete solitary waves. For demonstration, we have to choose a specific model. We consider the spatially one-dimensional nonintegrable discrete nonlinear Schrödinger equation with arbitrary power nonlinearity. It is known that such a system can be used to model, for instance, the main features of multidimensional equations [17,18]. However, the procedure outlined in this Letter is applicable to more general types of nonlinear equations, e.g., discrete Schrödinger equations with quite arbitrary nonlinear potentials V (not necessary power nonlinearities).

Besides being of fundamental interest, stability investigations [14] have important consequences for the dynamical features of nonlinear systems. Recently, the nonintegrable dynamics of a discrete system was discussed by introducing a "tunable" nonlinearity [16] into the integrable nonlinear Schrödinger equation. There has also been much interest in the formation of very localized self-trapped states, motivated by an important role that they may play in the nonlinear DNA dynamics [12]. One possible mechanism to obtain narrow large amplitude standing states is modulational instability and subsequent energy localization [16]. Energy, initially broadly dis-

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tributed in a nonlinear lattice, will be localized into large amplitude excitations by inelastic interactions of the small amplitude solitons [13]. This mechanism evidently depends on the stability properties of steady state solutions. Wave collapse may also provide an explanation for the appearance of very localized self-trapped states [16–19] from an initially wide field distribution. The link between a wave collapse (blowup) in a nonlinear system with the instability of stationary states is well known for continuous models [17]. We shall demonstrate that instability of the stationary states in the discrete system corresponds to the well-known continuum wave collapse in a modified form: we call it the quasicollapse to intrinsically localized modes. Of interest is the final state of an unstable discrete mode, i.e., whether it is an extremely spiky stationary mode plus "radiation," or an oscillating localized mode, or something else. We shall answer this question by numerical simulations.

For demonstration of the method, let us consider

$$i\dot{U}_n + U_{n+1} - 2U_n + U_{n-1} + (\sigma + 1)|U_n|^{2\sigma}U_n = 0. \tag{1}$$

This equation, with nonlinear potential $V(|U_n|^2) = (\sigma + 1)|U_n|^{2\sigma}$, is of Hamiltonian form and may be written as $i\dot{U}_n = \partial H/\partial U_n^*$, with Hamiltonian $H = \sum_n |U_n - U_{n-1}|^2 - \sum_n |U_n|^{2\sigma+2} = \text{const}$. Here $\sigma > 0$ is a free parameter, being introduced to cover different applications. Also $P = \sum_n |U_n|^2$ is a conserved quantity.

First, we focus on the case of a finite number of coupled equations with periodic boundary conditions ($U_{-N} = U_N$, where $2N + 1$ is the total number of oscillators). The infinite chain will be treated afterwards. Stationary standing solutions of Eq. (1) have a nonlinear frequency shift λ, which is introduced via $U_n = G_n \exp(i\lambda t)$. The shape of G_n is determined by

$$G_{n+1} - 2G_n + G_{n-1} - \lambda G_n + (\sigma + 1)|G_n|^{2\sigma}G_n = 0. \tag{2}$$

One may be tempted to believe that the following procedure is the most promising one: Consider (2) as a nonlinear, algebraic eigenvalue problem for λ. Prove the existence of solutions of Eq. (2) by minimizing H under the constraint of fixed P. Obvious advantage of this approach would be a simultaneous proof of stability. Note that, for fixed P, H is bounded from below because of $H \geq -\max|U_n|^{2\sigma}P \geq -P^{\sigma+1}$. In the case of finite N the minimum will be attained on some state being evidently stable (with respect to perturbations with the same value of P). It should be noted, however, that in this way one cannot prove that solutions exist for arbitrary (continuous) λ, since λ is a Lagrange multiplier to be determined from the constraint $P = \text{const}$. This difficulty is a consequence of the absence of scaling invariance here, which, on the other hand, takes place in the continuum approximation. A further disadvantage of this approach would be that one could not obtain unstable stationary states.

That is why we proceed differently. Let us study the problem of minimizing W with constraint $I = \text{const}$, where W and I are defined as $W = \sum_n (U_n - U_{n-1})^2 + \tilde{\lambda}\sum_n U_n^2$, $I = \sum_n U_n^{2\sigma+2}$. Here U_n is supposed to be a real function. Minimizing W for fixed I we obtain $U_{n+1} - 2U_n + U_{n-1} - \tilde{\lambda}U_n + \mu(\sigma + 1)U_n^{2\sigma+1} = 0$, where μ is the Lagrange multiplier. The existence of the minimum follows from the fact that W is bounded from below for fixed I; e.g., zero is a lower bound. Because of finiteness of N, the minimum has to be attained on some solution $U_n \equiv F_n$. By using the scaled amplitude $G_n = \mu^{\frac{1}{2\sigma}}F_n$ and $\tilde{\lambda} = \lambda$ the equation for U_n can be transformed into the original equation for G_n, i.e., Eq. (2), if $\mu > 0$. If $\mu < 0$ we use $G_n = (-1)^n|\mu|^{\frac{1}{2\sigma}}F_n$ and $\tilde{\lambda} = \lambda - 4$. It should be pointed out that the dependence on λ is smooth. For a finite chain, in principle, the parameter λ can be negative. For an infinite chain the boundary condition is $G_n \to 0$ as $|n| \to \infty$. The main difference to the case of finite N is that one has to prove that the minimum of W will be attained by some solution of Eq. (2). This follows, however, in the strict mathematical sense from a compactness lemma which ensures the survival of the constraint $I = \text{const}$. For compactness, it is sufficient to show $I_N := \sum_{n=N}^{\infty} \tilde{G}_n^{2\sigma+2} \to 0$ uniformly for $N \to \infty$, where $\tilde{G}_n$ is a test function. From the physical point of view it is obvious (and it can be proven rigorously) that the minimization of W implies $\tilde{G}_n \to 0$ monotonically for $n \to \infty$. Thus $\tilde{G}_n^2 < |\text{const}| \times P/n$, and the desired behavior of I_N follows for $\sigma > 0$. For $G_n \to 0$ as $|n| \to \infty$, the basic types of stationary solutions can be classified in the following way: (I) positive, *even* parity, with single maximum on-site; (II) positive, *even* parity, with single maximum inter-site. The next interesting solution types are (I′) *odd* parity (one node) and zero on-site, (II′) *odd* parity (one node) and zero inter-site, and so on, when the number of nodes increases. The validity of this classification has been verified by numerical calculations based on a shooting method and with the help of generating functions. In the following, for the reason of simplicity, we shall concentrate on the behaviors of types I and II; we call them ground states since they have the lowest numbers of nodes.

Linearizing Eq. (1) in the form $U_n = (G_n + f_n + ig_n)\exp(i\lambda t)$, we get, by decomposing into real and imaginary parts, the following dynamical system for the real perturbations f_n and g_n: $\dot{f}_n = H_+ g_n$, $\dot{g}_n = -H_- f_n$. These equations can be combined to the second-order equation

$$\ddot{f}_n = -H_+ H_- f_n, \tag{3}$$

where the matrices H_+ and H_- are defined by $H_+ f_n = -f_{n+1} + 2f_n - f_{n-1} + \lambda f_n - (\sigma + 1)G_n^{2\sigma}f_n$ and $H_- f_n = -f_{n+1} + 2f_n - f_{n-1} + \lambda f_n - (2\sigma + 1)(\sigma + 1)G_n^{2\sigma}f_n$, respectively. The stability of a stationary solution G_n is determined by the properties of the operators H_+ and H_-. Let us first consider only perturbations which possess the same symmetry (parity) as the stationary state G_n.

By definition, G_n realizes the minimum of W for fixed

I, and therefore, varying $W - \mu I$ near the minimum [introduce $G_n + s_n$ and define the scalar product $(s,r) := \sum_n s_n r_n$], we find $(s, H_- s) \geq 0$, under the additional constraint $(s, G^{2\sigma+1}) = 0$. Since $(s, H_- s) \leq (s, H_+ s)$, we may conclude that the matrix H_+ is non-negative. The proof is rather obvious. Assume H_+ has a negative eigenvalue. If the corresponding eigenvector is orthogonal to $G_n^{2\sigma+1}$ then we have found a contradiction immediately. If not, we may construct from this eigenvector and G_n a new vector being orthogonal to $G_n^{2\sigma+1}$ and breaking the non-negativeness of H_-. Note that $H_+ G_n = 0$. In a similar way we may prove that the matrix H_- has only one negative eigenvalue. Assume that two negative eigenvalues of H_- exist. Using linear combinations of the corresponding eigenvectors, we may construct a vector r_n satisfying the conditions $(r, G^{2\sigma+1}) = 0$ and $(r, H_- r) < 0$. However, that is impossible as we demonstrated above. Note that the existence of *one* negative eigenvalue is a consequence of $(G, H_- G) < 0$.

Since the matrix H_+ is positive semidefinite, the stability is determined by the definiteness properties of the operator H_- for vectors being orthogonal to G_n. There are two possibilities. First, consider the case of instability. Assume that $(G, H_-^{-1} G) > 0$ and construct the vector components $Q_m = -\frac{(G, H_-^{-1} G)}{(e_-, G)} e_{-m} + H_-^{-1} G_m$, where e_- is the eigenvector of H_- with negative eigenvalue ζ_-. One may check that $(Q, H_- Q) < 0$ and $(Q, G) = 0$. Thus, under the above assumptions the ground state is unstable.

Now we turn to the opposite case. Let $(G, H_-^{-1} G) < 0$. In general, any vector s can be decomposed into a component s_- parallel to e_- and a component $s_\perp$ perpendicular to e_-. We then may write $(s, H_- s) = -|\zeta_-|(s_-, s_-) + (s_\perp, H_- s_\perp)$. Abbreviating $F_n = H_-^{-1} G_n$ and making use of the requirement $(s, G) = 0$, one can derive the relation $|\zeta_-|(s_-, F_-) = (s_\perp, H_- F_\perp)$. By the Schwarz inequality we obtain $(s_\perp, H_- s_\perp) \geq |\zeta_-|^2 \frac{(s_-, F_-)^2}{(F_\perp, H_- F_\perp)}$. From the assumption $(F, H_- F) < 0$ we have $(F_\perp, H_- F_\perp) < |\zeta_-|(F_-, F_-)$. Combining all these expressions we get the desired result $(s, H_- s) \geq 0$. From here it is quite easy to exclude exponentially unstable modes (for parity-conserving perturbations); the most direct way to prove stability is to construct a Lyapunov function. One may check that the function $L = W - \mu I - W_s + \mu I_s$ (the index s denotes the stationary values) can be used. The requirements $L(G_n) = 0$, $\frac{dL}{dt} = 0$, $L(G_n + s_n) \geq 0$, for arbitrary (small but finite) s_n satisfying $(s, G) = 0$, are fulfilled.

It should be noticed that for power nonlinearities the quadratic form $\sum_n G_n H_-^{-1} G_n$ can be written as $-\frac{\partial}{\partial \lambda} \sum_n G_n^2$. Thus the necessary and sufficient stability criterion (for parity-conserving perturbations) is

$$\frac{\partial}{\partial \lambda} \sum_n G_n^2 \geq 0.$$

[For more general potentials $V(|U_n|^2)$ a sufficient instability criterion is $\sum_n G_n H_-^{-1} G_n > 0$, since we cannot assume in general a smooth λ dependence.]

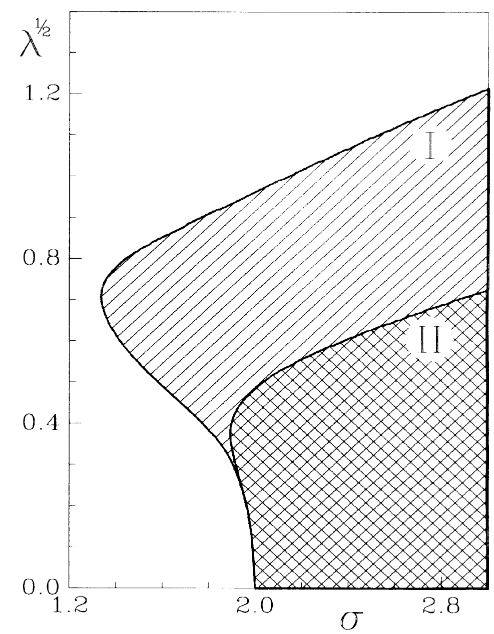

FIG. 1. Stability of solutions of types I and II with respect to parity-conserving (even) perturbations. The solitary waves of types I and II are unstable in the hatched regions to the right of the curves labeled I and II, respectively.

Quantitative conclusions require one to evaluate $P_s = \sum_n G_n^2$ as functions of λ for different parameter values of σ. The results of such a calculation are summarized in the stability diagram shown in Fig. 1.

For all points in the $(\sigma, \lambda^{1/2})$ plane, and for the solitary solutions of types I and II, we have determined the stability properties via criterion (4). We get stable and unstable regimes which are separated in Fig. 1 by the border lines named I (for type I solutions) and II (for type II solutions), respectively. The localized modes of types I or II are unstable to the rights of the curves marked I or II, respectively, i.e., in the hatched areas. One can see that the discreteness changes the critical value $(\sigma_{\rm cr})$ of σ that separates stable and unstable solitons. In the continuum limit $\sigma_{\rm cr} = 2$. From Fig. 1 one finds that discrete symmetric ground states can be unstable already for $\sigma \approx 1.4$. Our results are in qualitative agreement with [18], where the evolutions of sech-type initial distributions have been studied. There it has been demonstrated first by numerical experiments that discreteness lowers the critical value of σ, but the drastic down-shift to $\sigma_{\rm cr} \approx 1.4$ could not be predicted by these authors. This is one of the new conclusions from the general criterion (4).

In order to conclude the stability considerations, we have to comment on parity-nonconserving perturbations. It can be shown that for ground states of type I the eigenvalues of H_- are always positive, and no new instability region compared to that shown in Fig. 1 appears. On the other hand, when we consider states of type II, H_- always has negative eigenvalues, tending to zero for $\lambda \rightarrow 0$ (continuum limit). Thus the states II are *always unstable*. By a generalization of the method presented first in [4] one can derive complementary variational principles for the growth rates of the unstable states. It is then possible to quantify the time scales of the unstable growth.

We also have confirmed the analytic predictions by numerical simulations. In the following we present the nonlinear development of a linearly unstable discrete solitary wave. The numerical code is semi-implicit; the linear terms are handled by a Crank-Nicholson scheme [20], supplemented by Dirichlet or periodic boundary conditions. First, this code was used to confirm the analytic stability prediction (4) numerically. Then, in the unstable regime, it was run for long times. A typical result of the initial value problem (1) is depicted in Fig. 2. The case shown is for $N = 100$, and the initial distributions $\Re U_n = G_n - 0.01[(G,G)(H_-^{-1}G)_n - (G,H_-^{-1}G)G_n]$, $\Im U_n = \{H_+^{-1}[\Re U_n - G_n]\}_n$ for $\sigma = 1.85$, $\sqrt{\lambda} = 0.35$ have been chosen in order to start already with the most unstable perturbation.

The numerical simulation demonstrates that an unstable solution shows a collapse tendency. But in contrast to the continuum result, here the collapse will be stopped, and we can determine a nonsingular final state. We name the process quasicollapse, and the final state is a time-dependent intrinsically localized mode. It corresponds to an (oscillating) two-soliton state. Note that the case shown in Fig. 2 is typical; the time developments for other parameter values are similar. Obviously, this leads into new insight into the formation of intrinsically localized modes.

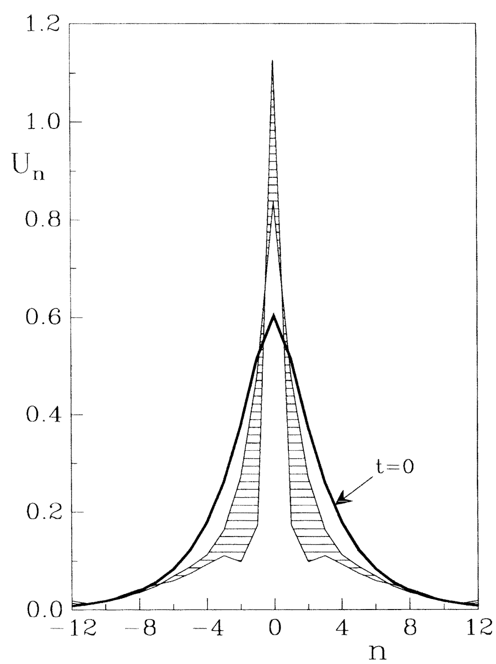

FIG. 2. Nonlinear development of an unstable ($\sigma = 1.85$, $\sqrt{\lambda} = 0.35$) discrete solitary wave (thick line) into an intrinsically localized two-soliton solution. The latter is oscillating in the hatched region.

In conclusion, we have presented an exact criterion for the stability of the ground states of the generalized discrete nonlinear Schrödinger equation. The method may be easily applied to other discrete models. By studying, for a power nonlinearity, the stability of ground states, information is gained about the quasicollapse in discrete models. Instability of some ground solutions results via an explosive-type dynamics into a fast energy localization through finite-time condensation.

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