PHYSICAL REVIEW
LETTERS

VOLUME 72 | 31 JANUARY 1994 | NUMBER 5

Localized States in Discrete Nonlinear Schrödinger Equations

David Cai, A. R. Bishop, and Niels Grønbech-Jensen
Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545
(Received 27 April 1993)

A new 1D discrete nonlinear Schrödinger (NLS) Hamiltonian is introduced which includes the integrable Ablowitz-Ladik system as a limit. The symmetry properties of the system are studied. The relationship between intrinsic localized states and the soliton of the Ablowitz-Ladik NLS is discussed, including the role of discretization as a mechanism controlling collapse. It is pointed out that a staggered localized state can be viewed as a particle of a *negative* effective mass. It is shown that staggered localized states can exist in the discrete dark NLS. The motion of localized states and Peierls-Nabarro pinning are also studied.

PACS numbers: 03.40.Kf, 52.35.Mw, 63.20.Pw

Intrinsic collapse to self-localized states in nonlinear systems is increasingly studied because of its wide physical significance in plasmas, fluids, optics, solid state, and so on [1] and the delicate mathematical details controlling existence and stability [2–5]. Pure (1+1)-dimensional integrable systems provide rigorous examples of self-localized states in the form of solitons and are by now well understood [6]. However, physical considerations which destroy complete integrability may *not* destroy collapse to stable localized states, with important consequences for mesoscopic self-organization controlling macroscopic responses. Such physical "perturbations" include integrability-breaking terms in partial differential equations, dimensionality, lattice discreteness, disorder, fluctuations (quantum, thermal), etc. [1, 5]. The properties of the intrinsic localized oscillatory states have been studied by numerical simulation [7–9] for simple monatomic lattices of particles with a nearest-neighbor harmonic and quartic anharmonic interaction in 1D and 2D. The localized states were found to have amplitude-dependent frequencies lying above the upper harmonic phonon band edge, with their particles oscillating out of phase with their neighbors. It has also been suggested that localized states can exist in the D-dimensional discrete nonlinear Schrödinger (NLS) lattice [10]. The work of Ref. [10] has established that, in a 1D NLS, a localized state lying *below* the linear phonon band reduces to a one-soliton solution in the *continuum* NLS limit.

In this paper, we propose a discrete NLS equation with "tunable" properties. The equation makes natural contact with the integrable NLS, and illuminates the role of lattice discreteness as a mechanism controlling collapse. We discuss the general properties of the localized states with an emphasis on the interplay of integrability and nonintegrability [11], discreteness, and the continuum limit. We study in detail a particular set of localized solutions that have a staggered form, i.e., the neighboring sites oscillate out of phase. Unlike the unstaggered localized states, which have the oscillation frequencies below the linear phonon band and reduce to one-soliton solutions in the continuum limit, these staggered states have oscillation frequencies above the phonon band and have no continuum counterpart. We will show that they can exist even in a discretized NLS for the dark NLS and that, in particular, they can be treated as particles of *negative* effective mass. These states, staggered or otherwise, are also reminiscent of "gap solitons" which, e.g., give rise to self-induced transparency in electromagnetic wave transmission through a superlattice whose dielectric constant is periodic in space [12, 13]. In our case, the underlying periodicity arises from the intrinsic discreteness of the system. Finally, we will analyze the modulational stability of the system to gain insight into the formation and destruction of these localized states. For a complete picture of our system, we also present results from numerical simulations.

0031-9007/94/72(5)/591(5)$06.00

The discrete 1D NLS equation we study is

$$i\dot{\phi}_n = -(\phi_{n+1} + \phi_{n-1}) - [\mu(\phi_{n+1} + \phi_{n-1}) + 2\nu\phi_n]|\phi_n|^2, \quad (1)$$

where the overdot stands for the derivative with respect to time t, n is a site index, and $\mu \geq 0$. This can be derived from the Hamiltonian

$$H = -\sum_n \phi_n\phi_{n+1}^* + \phi_n^*\phi_{n+1} - \frac{2\nu}{\mu}\sum_n |\phi_n|^2 + \frac{2\nu}{\mu^2}\sum_n \ln(1+\mu|\phi_n|^2)$$

with the deformed Poisson brackets

$$\{\phi_n, \phi_m^*\} = i(1+\mu|\phi_n|^2)\delta_{nm}\,,$$
$$\{\phi_n, \phi_m\} = \{\phi_n^*, \phi_m^*\} = 0\,,$$

and the equation of motion $\dot{\phi}_n = \{H, \phi_n\}$. We will refer to this system as IN-DNLS. The system has an energy conservation law. The quantity $\mathcal{N} = \mu^{-1}\sum_n \ln(1+\mu|\phi_n|^2)$ is also conserved and serves as a norm. Notice that the limits of $H, \mathcal{N}$ exist, as $\mu \to 0$.

If $\mu = 0$, Eq. (1) reduces to a familiar discrete NLS equation (referred to as N-DNLS below) which is nonintegrable. If $\nu = 0$, Eq. (1) is the Ablowitz-Ladik NLS (referred to as I-DNLS), which is integrable and possesses an infinite number of conservation laws [6]. Because of the scaling property between the nonlinear coefficient and the amplitude, both N-DNLS and I-DNLS have a single measure for the strength of the nonlinearity, respectively, $\nu|\phi|^2$ and $\mu|\phi|^2$, while IN-DNLS has two, $\mu|\phi|^2$ and ν/μ. All these DNLS equations are discretizations, up to a trivial gauge transformation, of the integrable continuum NLS equation, $i\dot{\phi} = -\phi_{xx} - 2\kappa|\phi|^2\phi$, which possesses bright and dark soliton solutions for $\kappa > 0$ and $\kappa < 0$, respectively. However, the discreteness of the systems gives rise to several interesting features which are not present in the continuum limit.

We seek an oscillating solution of IN-DNLS in the form

$$\phi_n = \psi_n e^{-i(\omega t - \alpha n + \sigma_0)},$$

where ψ_n is real and σ_0 is a constant phase. From the real and the imaginary parts of Eq. (1), we have

$$(\hat{\Omega}\hat{\psi})_n \equiv \omega\psi_n + \cos\alpha(\psi_{n+1} + \psi_{n-1}) + [\mu\cos\alpha(\psi_{n+1} + \psi_{n-1}) + 2\nu\psi_n]\psi_n^2 = 0, \quad (2)$$

$$\dot{\psi}_n = -(\psi_{n+1} - \psi_{n-1})(1+\mu\psi_n^2)\sin\alpha, \quad (3)$$

where $\hat{\psi}$ is the column vector, $\{\psi_1, \psi_2, ..., \psi_n ...\}$, and $\hat{\Omega}$ is the matrix defined by the left hand side of Eq. (2). Equation (2) with vanishing boundary condition constitutes a nonlinear algebraic eigenvalue problem for localized states. Equation (3) determines the time evolution of the localized states. [Note that the above ansatz and results (2) and (3) are readily generalized to $D > 1$.] When $\alpha = 0$ or π, ϕ_n is stationary. We shall call a localized state staggered if $\alpha = \pi$, and unstaggered if $\alpha = 0$. From Eq. (2), we have

$$\omega = -2\cos\alpha - \mu\cos\alpha\frac{\sum_n(\psi_{n+1} + \psi_{n-1})\psi_n^2}{\sum_n \psi_n} - 2\nu\frac{\sum_n \psi_n^3}{\sum_n \psi_n}.$$

Clearly, if $\psi_n > 0$ and $|\nu|$ is not too large, the staggered state lies above the phonon band, while the unstaggered state lies below. Particularly, if $\mu = 0$, there is no such localized state, staggered or unstaggered, below the phonon band for $\nu < 0$, or above the phonon band for $\nu > 0$. In the following discussion, we focus mainly on those staggered states whose frequencies lie outside the phonon band.

One can easily show that IN-DNLS possesses the following reflectional symmetry: If an unstaggered state, $\psi_n \exp(-i\omega t)$, is a solution of the eigenvalue problem (2), then the staggered state, $(-1)^n\psi_n \exp(i\omega t)$, is a solution of the dual eigenvalue problem, i.e., Eq. (2) with $\nu \to -\nu$. From this symmetry, for N-DNLS, it follows that there exists a staggered localized state whose frequency is above the phonon band for $\nu < 0$ *if* there is an unstaggered localized state below the phonon band for $\nu > 0$. Later we will return to the stability issue of the staggered localized states in the dark N-DNLS (i.e., $\mu = 0$, $\nu < 0$).

For I-DNLS, we can exactly solve the nonlinear eigenvalue problem. The localized solutions are of the form

$$\phi_n = \frac{\sinh\beta}{\sqrt{\mu}}\text{sech}[\beta(n - ut - x_0)]e^{-i(\omega t - \alpha n + \sigma_0)}\,, \quad (4)$$

$$\omega = -2\cos\alpha\cosh\beta\,, \quad (5)$$

$$u = 2\beta^{-1}\sin\alpha\sinh\beta\,, \quad (6)$$

and have the energy $E = H$:

$$E = -4\mu^{-1}\cos\alpha\sinh\beta. \quad (7)$$

These localized states are precisely the exact one-soliton solutions obtained via, e.g., the inverse spectral transform [6]. One can readily show that the solutions in Eq. (4), under the above reflectional transformation, transform to a set of solutions identical to the original set in Eq. (4) but with a different parametrization. It follows that these one-soliton solutions possess this exact self-dual reflectional symmetry.

Another striking property related to these localized states in I-DNLS is that they have *continuous* translational symmetry and for each β there exists a band of velocities at which a localized state can travel [see Eq. (6)] without experiencing any Peierls-Nabarro (PN) pinning from the lattice discreteness [see Eq. (7)] [14]. This is in contrast to the case of N-DNLS in which a moving localized state experiences dispersion and eventually decays [10]. We note in passing that, contrary to the general discrete case, a soliton of some fixed amplitude in the continuum NLS can always be Galileo boosted to

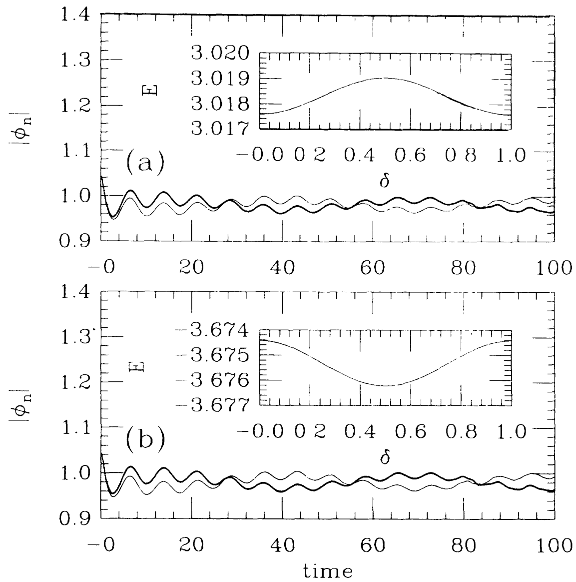

FIG. 1. Time evolution of the amplitudes $|\phi_n|$ at n = 100 (thin line) and 101 (thick line) are shown here for (a) a trapped staggered localized state that oscillates around δ = 0.5 at the top of the Peierls-Nabarro (PN) potential for ν = 0.1 with the initial parameters $\alpha = 0.314 \times 10^1$, $\beta = 1$, x_0 = 100.5; (b) an unstaggered localized state at the bottom of the PN potential for $\nu = -0.1$ with the initial parameters $\alpha = 0.2 \times 10^{-3}$, $\beta = 1$, $x_0 = 100.5$. The insets show their corresponding PN potentials ($\mu = 1$) (see text).

any velocity.

With the nonlinear μ term, we expect that the localized states in IN-DNLS are more robust against dispersion while translating, since the PN barrier is reduced by the presence of the nonlinear nearest-neighbor interaction. We demonstrate this by using an ansatz for a localized state to calculate the total energy E of the state as a function of δ, the position of the center of the localized state between two neighboring lattice sites. The ansatz is

$$\phi_n = (\lambda)^n \frac{\beta}{\sqrt{\mu + \lambda\nu}} \mathrm{sech}[\beta(n+\delta)],$$

where $\lambda = 1, -1$ for the unstaggered, staggered state, respectively. This ansatz is a good representation of a localized state from our analytical study [see Eq. (9) below] and numerical simulation for small $|\nu|/\mu$ and small β. Notice that, in the terminology of [4, 9], such a staggered state with $\delta = 0.5$ is an even-parity mode and $\delta = 0$ is an odd-parity mode. This classification loses its usefulness for the solitons in the I-DNLS which have continuously translational symmetry. The function $E(\delta)$ shows that, for $\nu < 0$, a localized state whose center is located at the midpoint between two lattice sites has a lower total energy than one located precisely at a lattice site, regardless of the state being staggered or unstaggered, and for $\nu > 0$, the situation is reversed (see Fig. 1). The energy difference between $\delta = 0$ and $\delta = 0.5$ becomes more and more pronounced with the increase of $|\nu|/\mu$ or with the increase of the amplitude of a localized state. This energy difference will act as a barrier to the translation of a localized state. In our simulation, we found that a very localized state (i.e., with large amplitude) is pinned and cannot move. By reducing the amplitude or ν, a state which is very localized can travel at the *group velocity*, $V_g \approx 2\sin\alpha$, which is derived from the linear dispersion relation of the NLS; this traveling state continuously emits a small and long phonon tail and gradually slows down. We also observed that some of the states of this kind will slow down to a threshold velocity, at which the state is abruptly pinned. In this context, we introduce an important concept, namely, that a staggered localized state can be viewed as a particle with a *negative* effective mass. From Eq. (7), for $\alpha = \alpha_s$ or $\pi + \alpha_s$, $|\alpha_s| \ll 1$, the energy can be expressed as

$$E = -\frac{4\lambda\sinh\beta}{\mu}\cos\alpha_s = -\frac{4\lambda\sinh\beta}{\mu} + \frac{\lambda\beta^2}{2\mu\sinh\beta}u^2,$$

which exhibits a *negative* (positive) effective mass for staggered (unstaggered) state. Obviously, a localized state of a negative effective mass is mechanically unstable (stable) at a minimum (maximum) of the PN potential and it tends to run away from the minimum. This is confirmed by our simulation. In Fig. 1, we present cases in which a trapped staggered (unstaggered) localized state is oscillating at the top (bottom) of the PN potential for $\nu > 0$ ($\nu < 0$).

Now we turn to discussing localized states in the low amplitude limit. As pointed out in [2], lattice Green's function methods can be utilized to study the existence of nonlinear localized states. From the linear part of Eq. (2) we derive the lattice Green's function

$$G_\alpha(n,m) = \frac{1}{N}\sum_q \frac{e^{iq(n-m)}}{\omega_\alpha(q) - \omega} \longrightarrow -\frac{(\mathrm{sgn}\omega)^{|n-m|+1}}{\sqrt{\omega^2 - 4\cos^2\alpha}}\left(\frac{\sqrt{\omega^2 - 4\cos^2\alpha} - |\omega|}{2\cos\alpha}\right)^{|n-m|},$$

as $N \to \infty$, for $|\omega/(2\cos\alpha)| > 1$, where $\omega_\alpha(q) = -2\cos\alpha\cos q$ is the eigenvalue for the linear part of Eq. (2). It can be shown that the localized states satisfy the following equation:

$$\psi_n = \sum_m G_\alpha(n,m)[\mu\cos\alpha(\psi_{m+1} + \psi_{m-1}) + 2\nu\psi_m]\psi_m^2. \quad (8)$$

For a stationary state whose frequency is very close to the band edge, i.e., $\omega = -\lambda(2 + \Delta^2)$, $0 < \Delta \ll 1$, we see that the Green's function has the asymptotic form

$$G_\alpha(n,m) \longrightarrow \frac{\lambda}{2\Delta}e^{-\Delta|n-m|}, \quad \text{as } \Delta \to 0.$$

Then Eq. (8) can be solved to obtain an asymptotic localized solution

$$\phi_n = (\lambda)^n \frac{\Delta}{\sqrt{\mu + \lambda\nu}} \operatorname{sech}(\Delta n) e^{i[\lambda(2+\Delta^2)t]}, \tag{9}$$

which is a localized state with a large width and a small amplitude. It can clearly be seen that a low amplitude staggered state has lower (higher) frequency, ω_{IN}, than ω_I of a localized I-DNLS state if they have the same amplitude and $\nu > 0$ ($\nu < 0$). They are related by

$$\omega_{IN} = \frac{(\mu - \nu)\omega_I + 2\nu}{\mu}. \tag{10}$$

From our numerical simulation, we found that this relationship holds rather well even for very localized staggered states (see Fig. 2).

Next we analyze spatially uniform, i.e., n-independent, solutions and their stability. The modulational instability of these spatially uniform states is indicative of the numerical stability of a localized state. As is well known, in the continuum limit, phonons in bright NLS are linearly unstable and they will focus to form a soliton, whereas the phonons in dark NLS are stable and there is no localized solution for vanishing boundary condition. From Eq. (2), we have the nonlinear dispersion relation, $\omega = -2\cos\alpha - 2(\mu\cos\alpha + \nu)\psi^2$, for the state $\psi_n = \psi$, independent of n. To study the linear stability of these states with periodic boundary conditions, $\phi_n = \phi_{n+N}$, we seek a solution in the completely general form [15]: $\phi_n = [\psi_n + u_n(t)]\exp[-i(\omega t - \alpha n)]$, where u_n is a small perturbation. Defining $\hat{u} = \hat{u}_1 + i\hat{u}_2$, the linearized equation can be written as

$$\begin{pmatrix} \dot{\hat{u}}_1 \\ \dot{\hat{u}}_2 \end{pmatrix} = \begin{pmatrix} 0 & \hat{\Omega} \\ \hat{J} & 0 \end{pmatrix} \begin{pmatrix} \hat{u}_1 \\ \hat{u}_2 \end{pmatrix},$$

where $\hat{\Omega}$ is the matrix defined in Eq. (2), and $\hat{J}$ is the associated Jacobian matrix. The solutions are linearly stable if and only if the eigenvalue problem, $\det(\hat{J}\hat{\Omega} - \lambda^2\hat{I}) = 0$, has only real and nonpositive solutions for λ. There exists at least one zero eigenvalue as a consequence of $\hat{\Omega}\hat{\psi} = 0$. It is straightforward to show that, for $\mu \geq 0$, the unstaggered spatially uniform solutions are stable if $\nu > -\mu\cos^2(\pi/N)$ and their amplitude $\psi^2 \leq \sin^2(\pi/N)/[\nu + \mu\cos^2(\pi/N)]$, and they are always stable if $\nu \leq -\mu\cos^2(\pi/N)$. The staggered spatially uniform solutions are stable if $\nu < \mu\cos^2(\pi/N)$ and their amplitude $\psi^2 \leq \sin^2(\pi/N)/[\mu\cos^2(\pi/N) - \nu]$, and are always stable if $\nu \geq \mu\cos^2(\pi/N)$. From the stability of these solutions we expect that, for $\nu < \mu$, the staggered localized states are stable since the staggered phonons are generally unstable as $N \to \infty$, and, in particular, the dark N-DNLS has stable staggered localized states and the unstaggered localized states decay to stable unstaggered phonons. These phenomena were indeed observed in our simulation. For example, an initially staggered localized state readjusts its shape to become a stable localized state, while an initially unstaggered localized state always decays to a spatially extended, unstaggered small amplitude state for the dark N-DNLS.

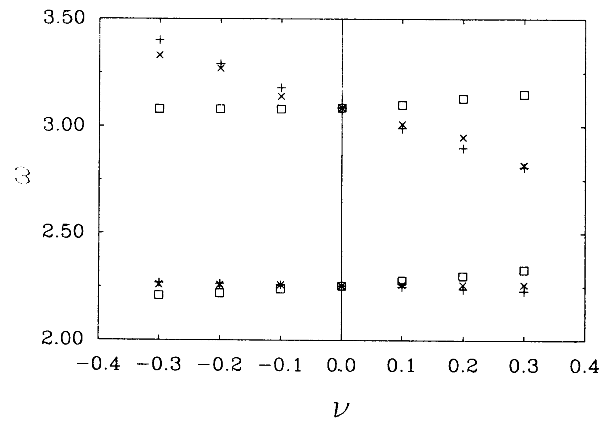

FIG. 2. "×" shows frequency, ω_{IN}, obtained by Fourier transform, of a staggered localized state in IN-DNLS ($\mu = 1$); as reference, "□" shows the frequency, ω_I, of the localized state of the same amplitude in I-DNLS ($\mu = 1$). "+" shows ω_{IN} predicted by Eq. (10). The higher branch is for states with $\beta \approx 1$ and the lower one is for less localized states with $\beta \approx 0.5$ (see text).

In conclusion, the new discrete NLS we proposed here has enabled us to demonstrate clearly how the reflection symmetry and translational symmetry of the integrable DNLS are broken by on-site nonlinearity. We have pointed out that the localized states in I-DNLS in the sense of [2–4] are the Ablowitz-Ladik solitons. We have demonstrated that the motion of a staggered state can be understood as a particle of negative effective mass. We have also shown that staggered localized states exist and are stable in the dark N-DNLS. Furthermore, the analysis of the modulational instability of spatially uniform states has deepened our understanding of the creation and decay processes of a localized state. We have also discussed the properties of Peierls-Nabarro potential which is intimately related to the nonintegrability of the Hamiltonian and which can be continuously tuned in our model. This controlling mechanism can be utilized in the study of the transport properties of the localized states, especially in the study of the *dynamical* competition of the localizations induced by nonlinearity and by randomness in the Anderson sense.

We thank F. Bronold for interesting discussions and acknowledge support for this work by the U.S. DOE.

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