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Class of localized structures in nonlinear lattices

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The existence of a new class of localized structures in nonlinear lattices is proved analytically and it is pointed out that such excitations have been recently observed experimentally [B. Denardo *et al.*, Phys. Rev. Lett. **68**, 1730 (1992)] in the form of the so-called "noncutoff kinks." These localized structures appear to be due to nonlinearity-induced breaking of symmetry between two equivalent eigenmodes of the lattice, and they probably exist in a large variety of nonlinear *discrete* systems.

One of the well-known effects of nonlinearity is to support stable propagation of localized structures in the frequency and velocity domains where propagation of linear waves is impossible. These localized structures may appear as a result of interplay between dispersion and nonlinearity. Many problems of nonlinear dynamics of spatially extended systems involve continuous, so that nonlinear localized excitations are naturally described as soliton solutions of different kinds of partial differential equations. However, models describing microscopic phenomena in solid-state physics are inherently discrete, with the lattice spacing between the atomic (or molecular) sites being a fundamental physical parameter for the systems. For these systems, an accurate microscopic description involves a set of coupled ordinary differential equations and nonlinear dynamics of such discrete systems is not well understood yet. As has been shown, in the case of a strong anharmonicity localized structure in chains with a nonlinear interatomic interaction may exist as intrinsic localized modes involving only a few particles.[1] However, these localized modes may be also treated as a discrete version of the (bright) envelope solitons, and they possess many properties of the proper soliton solutions of the nonlinear Schrödinger (NLS) equation derived for a wave envelope.[2,3] Another example is kinks in the upper cutoff mode of a nonlinear chain (in which each particle oscillates with the opposite phase with its immediate neighbors), which are approximately described by an NLS equation (see, e.g., Ref. 4) and correspond to excitations of a dark-soliton type. Nevertheless, due to specific properties of discrete systems, one may expect existence of other types of localized structures which have no direct analog in continuum models. In the present paper, taking the discrete Klein-Gordon model as a particular but rather general example, I show analytically that a new type of localized structure in nonlinear lattices may exist as a result of nonlinearity-induced symmetry breaking between two equivalent linear eigenmodes of the chain. These localized structures may exist independently on the type of nonlinearity (self- or defocusing) and they are likely fundamental nonlinear excitations of discrete systems. I point out that in the recent paper by Denardo *et al.*[5] the nonlinear structures described here have been already observed experimentally in a damped and parametrically driven lattice of coupled pendulums as the so-called "noncutoff kinks" and the results have been confirmed by a simplified numerical model.

The physical idea and the properties of the solutions obtained do not depend drastically on the type of a nonlinear chain, but, for definiteness, I consider the discrete Klein-Gordon model as a particular but rather general example, i.e., a one-dimensional chain made of particles (atoms) with unit mass, harmonically coupled with their nearest neighbors, and subjected to a nonlinear symmetric on-site potential. The same model has been analyzed recently to modulational instability[6] and it was used in numerical simulations to show different localized structures in a damped and parametrically driven chain of pendulums.[5] Denoting by $u_n(t)$ the displacement of atom n, its equation of motion may be written in the form

$$\ddot{u}_n + K(2u_n - u_{n+1} - u_{n-1}) + \omega_0^2 u_n - \beta u_n^3 = 0, \tag{1}$$

where K is the coupling constant, ω_0 is the frequency of small-amplitude on-site vibrations in the substrate potential, and β is the anharmonicity parameter of the potential. The model given by Eq. (1) may be also considered as a small-amplitude expansion of the well-known sine-Gordon model, and numerous physical applications of both these models have been widely discussed in the literature (see, e.g., Ref. 7 and references therein).

Linear oscillations of the chain (1) of the frequency ω and wave number q are described by the dispersion law

$$\omega^2 = \omega_0^2 + 4K \sin^2\left(\frac{qa}{2}\right), \tag{2}$$

a being the lattice spacing. As it follows from Eq. (2), the linear spectrum has a ("natural") gap ω_0, and it is limited by the cut-off frequency $\omega_{\max}^2 = \omega_0^2 + 4K$ due to discreteness. The most interesting point of the discrete model spectrum is the point $q = \pi/2a$, which corresponds to the wavelength-four linear mode. In *any discrete lattice* there are two equivalent modes of such a type: at $q = \pi/2a$ all even particles are at rest and the odd ones oscillate with the opposite phases at the frequency $\omega_1^2 = \omega_0^2 + 2K$, or, vice versa, all odd particles are at rest but the even ones oscillate with the opposite phases at the same frequency. However, in a *diatomic* linear chain these modes exhibit a ("internal") gap in the linear spectrum and this gap is naturally proportional to the mass difference (see, e.g., Ref. 8 and references therein). The physical problem I would like to study here is: Can nonlinearity itself induce a gap in the cw spectrum of a nonlinear chain and what is a physical consequence of this effect?

To answer this question I will introduce the new variables for the displacements of the atoms at different sites, i.e., $u_n = v_n$, for $n = 2k$, and $u_n = w_n$, for $n = 2k+1$, to present Eq. (1) for odd and even numbers separately,

$$\ddot{v}_n + K(2v_n - w_{n+1} - w_{n-1}) + \omega_0^2 v_n - \beta v_n^3 = 0, \tag{3}$$

$$\ddot{w}_n + K(2w_n - v_{n+1} - v_{n-1}) + \omega_0^2 w_n - \beta w_n^3 = 0. \tag{4}$$

Looking now for solutions in the vicinity of the point $q = \pi/2a$, I use the following ansatz:

$$v_{2k} = (-1)^k [V(2k,t)e^{i\omega_1 t} + V^*(2k,t)e^{-i\omega_1 t}], \tag{5}$$

$$w_{2k+1} = (-1)^k [W(2k+1,t)e^{i\omega_1 t} + W^*(2k+1,t)e^{-i\omega_1 t}], \tag{6}$$

where $\omega_1^2 = \omega_0^2 + 2K$ is the frequency of the wavelength-four linear mode, assuming that the functions $V(2k,t)$ and $W(2k+1,t)$ are slowly varying in space and time. Substituting Eqs. (5) and (6) into Eq. (1) and making the so-called "rotating-wave" approximation, i.e., keeping only the terms proportional to the first harmonic, I finally get the system of two coupled equations,

$$i\omega_1 \frac{\partial V}{\partial t} - aK\frac{\partial W}{\partial x} - \frac{3}{2}\beta |V|^2 V = 0, \tag{7}$$

$$i\omega_1 \frac{\partial W}{\partial t} + aK\frac{\partial V}{\partial x} - \frac{3}{2}\beta |W|^2 W = 0, \tag{8}$$

where the variable $x = 2ak$ is treated as a continuous one. The coupled nonlinear equations (7) and (8) are derived under the assumption of the following scale properties: The displacements V and W are of the order of ϵ, ϵ being a small parameter, the variables t and x are slow ones, i.e., $x \to \epsilon^2 t$, and $x \to \epsilon^2 x$. In fact, Eqs. (7) and (8) represent the first nontrivial step in rigorously applying an asymptotic expansion to Eqs. (3) and (4).

Looking for the continuous-wave (cw) spectrum of this nonlinear system, I find the result

$$(\omega_1\omega' - \tfrac{3}{2}\beta V_0^2)(\omega_1\omega' - \tfrac{3}{2}\beta W_0^2) = a^2K^2q'^2, \tag{9}$$

where ω' and q' are the frequency and wave number of the odd and even cw solutions with the amplitudes W_0 and V_0, respectively. The dispersion relation (9) exhibits *a nonlinearity-induced gap* in the cw spectrum and this gap is proportional to the difference in the amplitudes of odd and even particles oscillations,

$$\Delta\omega' = \frac{3\beta}{2\omega_1}|V_0^2 - W_0^2|. \tag{10}$$

Appearence of the gap in the cw spectrum may be a factor of the wave localization at the frequency ω_1 provided the nonlinearity will be large enough. However, this kind of localized structure has to differ drastically from the standard localized excitations of nonlinear (continuous or discrete) models. Indeed, both of the wavefield components, the odd and even ones, cannot be vanishing in the same direction because there is no gap in the linear spectrum and small-amplitude oscillations at that frequency will be delocalized.

Analyzing this kind of localized structure, I look for stationary solutions of Eqs. (7) and (8) in the form

$$(V,W) \propto (f_1, f_2)e^{-i\Omega t}, \tag{11}$$

assuming, for simplicity, the function f_1 and f_2 to be real. As a matter of fact, the system (7) and (8) may have more complicated solutions, e.g., those with a spatially dependent phase. Then, the stationary solutions of Eqs. (7) and (8) are described by the system of two ordinary differential equations of the first order,

$$\frac{df_1}{dz} = -\omega_1\Omega f_2 + \lambda f_2^3, \tag{12}$$

$$\frac{df_2}{dz} = \omega_1\Omega f_1 - \lambda f_1^3, \tag{13}$$

where $z = x/aK$ and $\lambda = 3\beta/2$. Equations (12) and (13) describe the dynamics of a Hamiltonian system with one degree of freedom and the conserved energy

$$E = -\frac{1}{2}\omega_1\Omega(f_1^2 + f_2^2) + \frac{1}{4}\lambda(f_1^4 + f_2^4), \tag{14}$$

and they may be easily integrated with the help of the auxiliary function $g = (f_1/f_2)$, for which the following equation is valid:

$$\left(\frac{dg}{dz}\right)^2 = \omega_1^2\Omega^2(1+g^2)^2 + 4\lambda E(1+g^4). \tag{15}$$

Different kinds of solutions of Eq. (15) are characterized by different values of the energy E. On the phase plane (f_1, f_2) soliton solutions correspond to the separatrix curves connecting a pair of the neighboring saddle points $(0, f_0)$, $(0, -f_0)$, $(f_0, 0)$, or $(-f_0, 0)$, where $f_0^2 = \omega_1\Omega/\lambda$. Calculating the value of E for these separatrix solutions, $E = -\omega_1^2\Omega^2/4\lambda$, it is possible to integrate Eq. (15) in elementary functions and to find the soliton solutions

$$g(z) = \exp(\pm\sqrt{2}\omega_1\Omega z), \tag{16}$$

$$f_2^2 = \frac{\omega_1\Omega e^{\mp\sqrt{2}\omega_1\Omega z}[2\cosh(\sqrt{2}\omega_1\Omega z) \pm \sqrt{2}]}{2\lambda\cosh(2\sqrt{2}\omega_1\Omega z)},$$

$$f_1 = gf_2. \tag{17}$$

The solutions (16) and (17), but for negative Ω, exist also for defocusing nonlinearity when $\lambda < 0$.

The results (16) and (17) together with (11) and (5) and (6) give the shapes of the localized structures in the discrete nonlinear lattice. Because all combinations of the signs are possible in Eq. (17), there are *four* solutions of this type. Let us fix the sign in Eq. (16), say plus, to analyze the structures of the odd and even particle oscillations. When $z \to +\infty$, the function $g(z)$ tends to $+\infty$ and the amplitude of the even particle oscillations, f_1, goes to its limit value $f_0 = \sqrt{\omega_1 \Omega / \lambda}$. In the same time the amplitude of the odd particle oscillations vanishes [see Fig. 1(a)]. However, when $z \to -\infty$, the function $g(z)$ tends to zero, and the asymptotic behavior of the even and odd components is just the reverse: $f_1 \to 0$ and $f_2 \to f_0$. Therefore, the whole localized structure represents two kinks in the odd and even oscillating modes which are composed to have opposite polarities, so that both of them cannot be localized in one direction [Figs. 1(a) and 1(b)]. This result is the direct consequence of the nonlinearity-induced gap (10) in the cw spectrum (9), the gap disappearing in the linear limit. In some sense, these structures can be considered as an unusual limit of the soliton excitations in diatomic nonlinear chains.

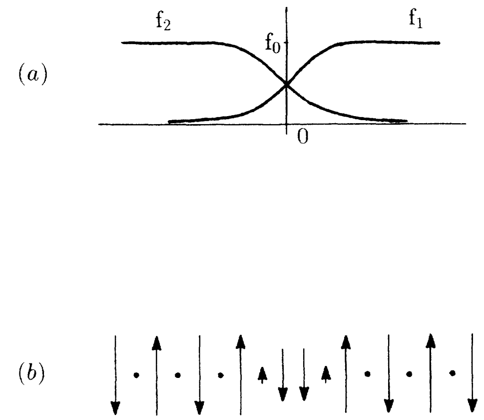

FIG. 1. (a) The odd and even components for the soliton solutions (16) and (17); and (b) diagrammatic representation of the whole localized structure of the wavelength-four mode (cf. Fig. 3 of Ref. 5).

It is important to note that the localized structures described in this paper have been recently observed experimentally as "noncutoff kinks" in a damped and parametrically driven experimental lattice of coupled pendulums and numerically in a simplified model similar to Eq. (1).[5] The authors have observed also the standard cutoff kinks described as fundamental dark solitons by an NLS equation, and domain walls which connect standing regions of different wave numbers. A parametric drive used in the study allows us to compensate the dissipation-induced decay of the structures supporting steady-state regimes which in the case of the cutoff kinks may be found analytically for a simplified perturbed model.[5] The observations of the localized structures in an actual lattice together with the analytical treatment showing a natural origin of these modes in nonlinear discrete models indicate that these structures are general phenomenon which can occur in many other lattice systems (e.g., they may be observable in a linear array of vortices[9]).

At last, it is interesting to compare the localized structures described in this paper with the so-called gap solitons discovered in 1987 by Chen and Mills.[10] As is well known, the gap solitons may exist in nonlinear (continuous) periodic media as localized excitations when the nonlinear frequency is shifted into the gap of the linear spectrum induced by *periodicity* of the system parameters, e.g., by periodical change of the linear refractive index (see, e.g., Ref. 11 and references therein). From the viewpoint of the theory of gap solitons, the nonlinear localized structures described here may be called *self-supporting gap solitons.* Indeed, the linear spectrum has no gap, but the latter may appear due to nonlinearity. Thus, one group of the particles (e.g., at the even sites) of the chain creates asymptotically *an effective periodic potential* for the other group of the particles (e.g., at the odd sites), and vice versa, forming finally two parts of the structure which is similar in parts to spatially localized gap solitons.

In conclusion, I have shown analytically that in discrete systems nonlinearity supports steady-state localized excitations of a new kind. These localized structures appear due to breaking of symmetry between two equivalent linear wavelength-four modes, i.e., due to a nonlinearity-induced gap in the cw spectrum, and existence of these localized structures does not depend on the type of nonlinearity. Due to this universality, these modes are likely fundamental excitations of discrete systems and one may naturally expect to find them in a variety of nonlinear discrete models of solid state physics.

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