Gap solitons in diatomic lattices

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We consider a nonlinear diatomic lattice of the Klein-Gordon type composed of particles with two different masses. The linear spectrum of this model exhibits a gap, which is proportional to the mass difference, in addition to the natural gap stipulated by a nonlinear substrate potential. We analyze the coupled nonlinear excitations of such a diatomic chain which have a similar origin as the well-known gap solitons appearing in nonlinear (e.g., optical) systems with a spatial periodicity. We also describe dark-profile localized structures with a frequency lying below the gap. In the limit when the gap disappears, i.e., for the case of a monoatomic chain, the gap solitons do not exist but instead there exist localized structures of a distinct type created by the nonlinearity-induced symmetry breaking between two equivalent eigenmodes of the lattice, the so-called self-supporting gap solitons.

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I. INTRODUCTION

In recent years nonlinear wave propagation through inhomogeneous and disordered media has attracted increasing attention (see, e.g., Refs. [1, 2]). One of the simplest and physically relevant examples of an inhomogeneous medium is that with a periodic change of its parameters. Adding spatial periodicity to integrable nonlinear dynamics leads to a variety of effects. Competition of the length scales introduced by the periodicity and by nonlinearity is one of the important examples of these effects: If these length scales are very different from each other, the perturbed system can support solitonlike or breatherlike excitations, and their motion can be described by a collective-coordinate approach [3, 4]; but if the length scales are comparable, localized excitations of a standard form break up or dissipate into radiation even for relatively small perturbations [3]. However, in the later case the perturbed system may support nonlinear excitations of *a distinct type* (not existing without periodicity), the so-called *gap solitons*, discovered in 1987 by Chen and Mills [5]. The gap solitons may appear in a nonlinear (continuous) periodic medium as localized excitations when the nonlinear frequency is shifted into the linear-spectrum gap induced by periodicity of the system parameters, e.g., by a periodic change of the linear refractive index (see, e.g., Refs. [6, 7] and references therein).

On the other hand, 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 of the system. For these systems, an accurate microscopic description involves a set of coupled ordinary differential equations and discreteness effects may drastically modify the nonlinear dynamics showing properties of modulational instability [8] as well as a rich set of localized structures; some of them have been recently observed experimentally [9] and described analytically [10].

From the viewpoint of these two physically important phenomena, a nonlinear *diatomic* chain is an excellent example of a nonlinear system where localized structures may appear as a result of interplay between *spatial periodicity* and *discreteness.* Moreover, diatomic lattices may be considered as a step to understanding transport properties of nonlinear disordered systems by comparing them with quasi-periodic (e.g., Fibbonachi-like) lattices, and some studies in this direction have been already started [11].

The study of nonlinear diatomic lattices has been mostly directed towards understanding the dynamics of solitonlike excitations of acoustic and optical branches (see, e.g., Refs. [12–21]) as well as their thermal conductivity properties [11], [22], and [23]. However, in most of these studies, soliton excitations were considered for acoustic and optical modes separately, e.g., for the diatomic lattice with a nonlinear interatomic interaction, there are Korteweg–de Vries (KdV)–type solitons for the acoustic region of the spectrum. Modulated waves described by a nonlinear Schrödinger (NLS) equation, i.e., envelope solitons, exist in the acoustic and optical regions of the linear wave spectrum (see, e.g., Refs. [13, 17]). A convenient way of studying the coupled long-wave nonlinear excitations in diatomic lattices with a nonlinear interparticle interaction was proposed by Yajima and Satsuma [12], who discussed the soliton solutions in terms of normal mode coordinates.

In the present paper we consider nonlinear coupled modes in diatomic Klein-Gordon-type lattices analyzing soliton solutions in the vicinity of the gap of the linear spectrum. We find a set of new soliton excitations of diatomic lattices, which have the similar origin as the gap solitons in nonlinear optical media with a periodic change of the refractive index. We point out that the main types of nonlinear coupled modes analyzed in the present paper are not a specific property of the simplified model considered here, but they may be naturally expected in other diatomic lattices, e.g., in a diatomic lattice with a nonlinear interparticle interaction [21].

The paper is organized as follows. In Sec. II we present our model which is, in fact, a diatomic Klein-Gordon chain. In Sec. III we discuss nonlinear coupled modes in the diatomic chain existing with the frequencies lying in the vicinity of the gap of the linear spectrum, and we describe new soliton solutions. An interesting limit of a monoatomic chain is discussed in Sec. IV where the gap solitons transform into kink-profile localized structures. Section V concludes the paper.

II. MODEL

The physical model we consider in the present paper is the discrete Klein-Gordon-type diatomic chain, i.e., a one-dimensional chain made of particles (atoms) with two different masses, m and M ($m < M$), harmonically coupled with their nearest neighbors, and subjected into a nonlinear symmetric on-site potential. The similar model, but for a piecewise quadratic substrate, has been analyzed in Ref. [15]. However, as it follows from the subsequent analysis, the main properties of the soliton solutions obtained are mostly related to the specific structure of the linear spectrum of the diatomic lattice, and the choice of the nonlinear model (which was made to simplify the final results) is not a principal point of our analysis.

Denoting by $u_n(t)$ the displacement of atom n, its equation of motion may be written in the form

$$m_n \frac{d^2 u_n}{dt^2} + K(2u_n - u_{n+1} - u_{n-1}) + \alpha u_n - \beta u_n^3 = 0, \tag{1}$$

where K is the coupling constant, and α and β are parameters of linear and nonlinear terms. We assume the chain consists of atoms of two masses, so that $m_n = m$ for $n = 2j$ and $m_n = M$ ($M > m$) for $n = 2j + 1$. To simplify Eq. (1), it is convenient to write the equations of motion for atoms with odd and even numbers separately, introducing two wave fields,

$$u_n = v_n \quad \text{for } n = 2j, \qquad u_n = w_n \quad \text{for } n = 2j+1, \tag{2}$$

and to write the equations as

$$m \frac{d^2 v_n}{dt^2} + K(2v_n - w_{n+1} - w_{n-1}) + \alpha v_n - \beta v_n^3 = 0, \tag{3}$$

$$M \frac{d^2 w_n}{dt^2} + K(2w_n - v_{n-1} - v_{n+1}) + \alpha w_n - \beta w_n^3 = 0. \tag{4}$$

The linear properties of such a diatomic chain are well known. For the model (1) the dispersion relation for linear waves has two different branches,

$$\omega_{1,2}^2 = \frac{1}{2mM}\left[(\alpha + 2K)(m + M) \pm \sqrt{(\alpha + 2K)^2(m - M)^2 + 16K^2 mM \cos^2(qa)}\right], \tag{5}$$

where ω and q are the wave frequency and wave number of linear waves, the minus corresponds to the low-frequency ("acoustic") mode, and the plus corresponds to the high-frequency ("optical") mode. These modes are separated by the gap $\Delta\omega = \omega_2 - \omega_1 > 0$, where

$$\omega_1^2 = \frac{\alpha + 2K}{M}, \quad \omega_2^2 = \frac{\alpha + 2K}{m}. \tag{6}$$

In principle, both these modes are optical ones, because in the linear spectrum there is also a natural gap ω_0 so that for small wave numbers these two modes are characterized by the two (optical) frequencies, ω_0 and ω_m, which in the limit $(M - m) \ll (M + m)$ may be presented in the form,

$$\omega_0^2 \approx \frac{\alpha}{m_c}\left(1 - \frac{\alpha \epsilon^2}{16K}\right), \qquad \omega_m^2 \approx \left(\frac{\alpha + 4K}{m_c}\right)\left[1 + \frac{\epsilon^2(\alpha + 4K)}{16K}\right], \tag{7}$$

where

$$m_c = \tfrac{1}{2}(m + M), \quad \epsilon = \frac{(m - M)}{m_c} \ll 1. \tag{8}$$

However, we will use the notation "acoustic" for the lower branch assuming, for example, the possible limit case $\alpha = 0$, when the lower branch is indeed acoustic.

The most interesting region of the linear spectrum is the vicinity of the maximum value of the wave number q, i.e., the region $|q - \pi/2a| \ll 1$, where two branches with the opposite signs of the dispersion are separated by the gap. The lower branch ends at the point ω_1 (see Fig. 1) defined in Eq. (6), and in the vicinity of this point the heavy particles oscillate with the higher amplitudes than the light ones, and at $q = \pi/2a$ the light particles are at rest and the heavy ones oscillate with the opposite phases. The upper branch ends at the point ω_2 [see Fig. 1 and Eq. (6)] and in this case the heavy particles practically do not oscillate while the light particles oscillate with the opposite phases. In the limit $M = m$ the

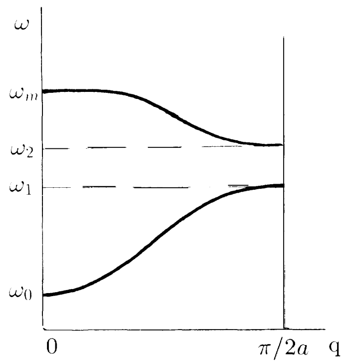

FIG. 1. Dispersion curves of a linear diatomic chain. "Acoustic" (the lower curve) and "optical" (the upper curve) branches are separated by the gap $\Delta\omega = \omega_2 - \omega_1$, $\omega_{1,2}$ being defined in Eq.(6).

frequencies ω_1 and ω_2 coincide, and the gap in the linear spectrum disappears.

III. COUPLED MODES IN A DIATOMIC LATTICE

The existence of the gap in the linear spectrum of the model (1) suggests making a comparison with the so-called gap solitons which may exist in a nonlinear system with a periodic modulation of its parameters. The theory of gap solitons describes the interaction of two linear branches (e.g., lower and upper ones) which, due to nonlinear coupling between the modes, allow localized structures with the frequencies lying in the gap (see, e.g., Refs. [6, 7]). Similar to that case, we will analyze soliton excitations in the vicinity of the gap of the linear spectrum, i.e., for the wave numbers close to the limit value $q = \pi/2a$. In the linear limit, the motion of the odd and even atoms is exactly decoupled at $q = \pi/2a$. The nonlinearity breaks the symmetry and one can look at the problem as that of the coupling of two spatially distinct modes. As will be seen below, the final coupled excitation, however, does not have a simple limit for vanishing nonlinearity term. There is an analogy, however, with localized or resonance modes in a harmonic chain with an impurity. The gap is proportional to the mass difference $(M - m)$ [see Eqs. (5) and (6)], so that the soliton properties (and existence of solitons themselves) strongly depend on this parameter.

As has been mentioned in Sec. II, the lower and upper branches of the linear spectrum end at the frequencies ω_1 and ω_2, respectively. The frequency ω_1 corresponds to such oscillations of the diatomic chain when the light particles are at rest, and the heavy particles oscillate with the opposite phases, while the frequency ω_2 corresponds to the opposite case: the heavy particles are at rest, and the light ones oscillate with the opposite phases. This structure of the upper and lower branches suggests looking for solutions in the vicinity of the point $q = \pi/2a$, making the following ansatz:

$$v_{2k} = (-1)^k[v(2k,t)e^{i\omega_1 t} + v^*(2k,t)e^{-i\omega_1 t}], \tag{9}$$

$$w_{2k+1} = (-1)^k[w(2k+1,t)e^{i\omega_1 t} + w^*(2k+1,t)e^{-i\omega_1 t}], \tag{10}$$

where $\omega_1^2 = (\alpha + 2K)/M$ is the largest frequency of the lower branch (the lower frequency of the gap). Assuming that the functions $v(2k,t)$ and $w(2k+1,t)$ are slowly varying in space and time, and making the so-called "rotating-wave" approximation, i.e., keeping only the terms proportional to the first harmonic, we may find from Eqs. (3) and (4) the system of two-coupled equations,

$$im\omega_1\frac{\partial v}{\partial t} + \tfrac{1}{2}m\Delta\omega^2 v - aK\frac{\partial w}{\partial x} - \tfrac{3}{2}\beta|v|^2 v = 0, \tag{11}$$

$$iM\omega_1\frac{\partial w}{\partial t} + aK\frac{\partial v}{\partial x} - \tfrac{3}{2}\beta|w|^2 w = 0, \tag{12}$$

where $\Delta\omega^2 \equiv \omega_2^2 - \omega_1^2$, and the variable $x = 2ak$ is treated as continuous one.

The system (11) and (12) describes gap solitons in the diatomic lattice and in some sense it is similar to the system of coupled NLS equations arising in the theory of gap solitons in nonlinear (continuous) media with spatially periodic parameters. However, there are a few important differences, e.g., the coupling between the two modes in Eqs. (11) and (12) is due to the derivative terms but not due to the cross-phase modulation and linear terms as it is in optical models. It makes the final localized structures different, too.

Analyzing localized structures in the framework of the system (11) and (12), we look for stationary solutions in the form

$$(v,w) \propto (f_1, f_2)e^{-i\Omega t}, \tag{13}$$

so that the stationary solutions are described by the system of two ordinary differential equations of the first order,

$$\frac{df_1}{dz} = -\Delta_2 f_2 + \lambda f_2^3, \tag{14}$$

$$\frac{df_2}{dz} = \Delta_1 f_1 - \lambda f_1^3, \tag{15}$$

where

$$\Delta_1 \equiv m(\omega_1\Omega + \tfrac{1}{2}\Delta\omega^2), \quad \Delta_2 \equiv M\omega_1\Omega, \tag{16}$$

with the normalizations $z = x/aK$ and $\lambda = 3\beta/2$. Equations (14) and (15) describe the dynamics of a Hamiltonian system with one degree of freedom and the conserved energy,

$$E = -\tfrac{1}{2}(\Delta_1 f_1^2 + \Delta_2 f_2^2) + \tfrac{1}{4}\lambda(f_1^4 + f_2^4), \tag{17}$$

and the functions f_1 and f_2 may be considered as the generalized coordinate and momentum, respectively. Equations (14) and (15) may be easily integrated with the help of the auxiliary function $g = (f_1/f_2)$ for which the following equation is valid:

$$\left(\frac{dg}{dz}\right)^2 = (\Delta_2 + \Delta_1 g^2)^2 + 4\lambda E(1+g^4). \quad (18)$$

Then the solutions for f_1 and f_2 may be found with the help of the following relations:

$$f_2^2 = \frac{1}{\lambda(1+g^4)}\left[(\Delta_2+\Delta_1 g^2)^2 \pm\sqrt{(\Delta_2+\Delta_1 g^2)^2 + 4\lambda E(1+g^4)}\right], \quad (19)$$

$$f_1 = g f_2. \quad (20)$$

Different kinds of solutions, including localized ones, are characterized by different values of the energy E, as well as by the parameters Δ_1 and Δ_2. It is convenient to analyze the solution structures on the phase plane (f_1, f_2), where localized (soliton) solutions correspond to separatrix curves. Let us fix the sign of the nonlinearity parameter, say $\lambda > 0$. Then, the existence of localized solutions depends on the values of the frequency Ω. Analyzing the critical points on the phase plane (f_1, f_2), we naturally distinguish a few important cases.

When $\Omega < -\Delta\omega^2/2\omega_1$, the parameters Δ_1 and Δ_2 are negative and the only critical point on the phase plane is the point $f_1 = f_2 = 0$: Separatrix curves and nontrivial localized solutions are absent. However, if

$$-(\Delta\omega^2/2\omega_1) < \Omega < 0, \quad (21)$$

the parameter Δ_1 is positive, and the dynamical system (14) and (15) has three critical points: a saddle point at $f_1 = f_2 = 0$, and two centers at the points $f_2 = 0$, $f_1 = \pm f_{01}$, where $f_{01}^2 = \Delta_1/\lambda$ (see Fig. 2). The separatrix curve for this case is shown in Fig. 2 and the corresponding shapes of the envelope functions f_1 and f_2 are depicted in Fig. 3. The condition (21) has the simple physical sense. Indeed, let us introduce the frequency of the localized solution, $\omega' = \omega_1 - \Omega$, according to Eqs. (9), (10), and (13). Then, assuming the frequency Ω small (the approximation of slowly varying envelopes), the condition (21) may be rewritten in the form

$$\omega_1^2 < \omega'^2 < \omega_2^2, \quad (22)$$

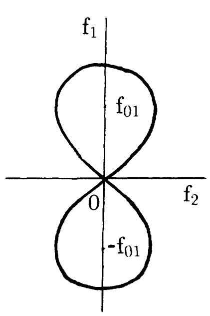

FIG. 2. The separatrix curve of the dynamical system (14) and (15) for $\Delta_1 > 0$ and $\Delta_2 < 0$.

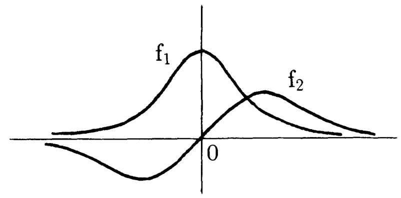

FIG. 3. The structure of the soliton excitations corresponding to the upper separatrix curve in Fig. 2.

where we have used the approximate relation $\omega'^2 \approx \omega_1^2 - 2\omega_1\Omega$. So, the localized structures found in this case may be called *gap solitons* and they naturally appear when the nonlinear frequency lies within the gap of the linear spectrum $\Delta\omega = \omega_2 - \omega_1$. In this case, the envelope of the light atom vibrations has the standard soliton shape. This result is natural because this type of nonlinearity (for $\beta > 0$) leads to a wave localization for the positive dispersion, i.e., provided $d^2\omega/dq^2 > 0$, but for $q \approx \pi/2a$ this condition is valid only for the light-atom vibrations. In the same time, the heavy-atom oscillations cannot be localized themselves, but, as we have shown, they may be localized due to *interaction* with the upper branch, and as a consequence, the shape of these oscillations differs from the standard soliton form.

To find exact solutions corresponding to the gap solitons we note that the separatrix curves on the phase plane (Fig. 2) correspond to $E = 0$, and Eq. (18) may be easily integrated to give

$$g = \mp\sqrt{\frac{|\Delta_2|}{\Delta_1}}\coth y, \qquad y \equiv z\sqrt{\Delta_1|\Delta_2|}, \quad (23)$$

which yields the soliton solutions for the f_1 and f_2 envelopes,

$$f_2^2 = \frac{2(\Delta_2+\Delta_1 g^2)}{\lambda(1+g^4)} = \frac{2|\Delta_2|\Delta_1^2\sinh^2 y}{\lambda(\Delta_1^2\sinh^4 y + \Delta_2^2\cosh^4 y)}, \quad (24)$$

$$f_1^2 = g^2 f_2^2 = \frac{2\Delta_2^2\Delta_1\cosh^2 y}{\lambda(\Delta_1^2\sinh^4 y + \Delta_2^2\cosh^4 y)}. \quad (25)$$

As follows from Eqs. (24) and (25) that the function $f_1(y)$ is symmetric and its maximum value is $(f_1)_{\max} = \sqrt{2\Delta_1/\lambda}$, but the function $f_2(y)$ is asymmetric, with the maximum value $(f_2)_{\max}$,

$$(f_2)^2_{\max} = \frac{1}{\lambda}\left(\sqrt{\Delta_1^2+\Delta_2^2} - |\Delta_2|\right).$$

Localized soliton solutions exist also in the case $\Omega > 0$, when both coefficients in Eqs. (14) and (15), i.e., Δ_1 and Δ_2, are positive. For this case the wave frequency $\omega' = \omega_1 - \Omega$ lies *below* the gap of the linear spectrum, and completely localized solutions for both these modes are naturally impossible to exist. In this case, each critical

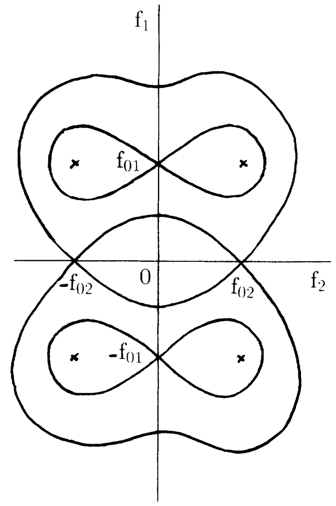

FIG. 4. The separatrix curves of the dynamical system (14) and (15) for $\Delta_1, \Delta_2 > 0$.

point in Fig. 2 splits into three points making the phase plane (f_1, f_2) more complicated (see Fig. 4). In particular, there are separatrix curves of two different types. One of them is similar to the case considered above, but the oscillations of the light atoms do not vanish at the infinities because f_1 tends to $\pm f_{01}$, where $f_{01}^2 = \Delta_1/\lambda$. The other type of the separatrix curves corresponds to a kink-type solution for the heavy particles and a localized excitation of the light ones (see Fig. 5). For all these cases the shapes of the soliton excitations may be found explicitly in the way presented above. For example, for the kink-type solitons the energy E may be calculated using the asymptotics: $f_1 \to 0$, $f_2 \to \pm f_{02}$, $f_{02}^2 = \Delta_2/\lambda$, which yields $E = -\Delta_2^2/4\lambda$, and the solution of Eq. (18) takes the form

$$g = \frac{\sqrt{2\Delta_1\Delta_2}}{\sqrt{\Delta_1^2 - \Delta_2^2}\sinh(\sqrt{2\Delta_1\Delta_2}z)}. \tag{26}$$

The soliton profiles may be found with the help of the relations,

$$f_2^2 = \frac{1}{\lambda(1+g^4)}\left[(\Delta_2 + \Delta_1 g^2) - g\sqrt{2\Delta_1\Delta_2 + (\Delta_1^2 - \Delta_2^2)g^2}\right], \tag{27}$$

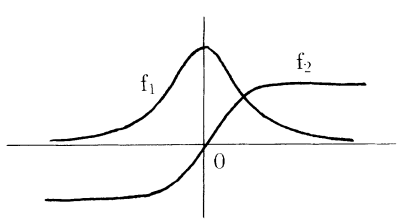

FIG. 5. Dark-profile excitations in the diatomic chain, corresponding to the upper separatrix between the saddle points $(-f_0, f_0)$ in Fig. 4.

$$f_1^2 = g^2 f_2^2. \tag{28}$$

As follows from Eq.(28), the function f_2 has a kink-type shape, but the function f_1 is indeed localized with the maximum value $(f_1)_{\max}$,

$$(f_1)^2_{\max} = \frac{1}{\lambda}(\Delta_1 - \sqrt{\Delta_1^2 - \Delta_2^2}).$$

The existence of the described kink-type solitons in a diatomic lattice is not a surprising result. Indeed, for the selected sign of the nonlinearity parameter, $\beta > 0$, the upper part of the acoustic branch (for the heavy particles) has the negative dispersion, $d^2\omega/dq^2 < 0$, so that wave localization is not possible for this mode and instead dark solitons of the kink-type shape appear. The dark solitons of the lower branch are accompanied by a localized structure of the light particles for which the dispersion is positive and localization is naturally expected.

IV. COUPLED MODES IN A MONATOMIC LATTICE

In the previous section we have described a set of soliton excitations which may exist in the vicinity of the gap of the linear spectrum, the gap being proportional to the mass difference. When the soliton frequency lies outside the gap (e.g., below if $\beta > 0$), the localization is impossible, and the nonlinear soliton wave is just a kink-profile excitation. In the limit of a monoatomic chain the linear gap disappears and gap solitons do not exist. However, interesting localized structures are also possible in this case and they may be considered as an unusual limit of the localized modes existing for the diatomic lattice.

Let us consider a monoatomic Klein-Gordon chain, i.e., just the model (1) at $m_n = m$ for all n. The linear spectrum of this chain,

$$\omega^2 = \omega_0^2 + \frac{4K}{m}\sin^2\left(\frac{qa}{2}\right), \quad \omega_0^2 = \frac{\alpha}{m}, \tag{29}$$

has no gap and it is limited by the cutoff frequency $\omega_{\max}^2 = \omega_0^2 + 4K/m$ due to discreteness. In spite of the point that $q = \pi/2a$ is not the end point of the spectrum, it is still the most interesting one. In any discrete lattice there are two equivalent modes of such a type: all even particles are at rest and the odd ones oscillate with the opposite phases at the frequency $\omega_1^2 = (\alpha + 2K)/m$, or, vice versa, all odd particles are at rest but the even ones oscillate with the opposite phases at the same frequency. Then, the interesting problem is: Can nonlinearity itself induce a gap in the cw spectrum and what is the physical consequence of this effect?

To answer this question, we will introduce again the variables v_n and w_n for the displacements of atoms at different sites, to write the equations of motion for the odd and even numbers separately. These equations are Eqs. (3) and (4) at $m = M$. Looking again for solutions in the form (9) and (10), we finally obtain the system of two-coupled nonlinear equations,

$$im\omega_1\frac{\partial v}{\partial t} - aK\frac{\partial w}{\partial x} - \tfrac{3}{2}\beta|v|^2 v = 0, \tag{30}$$

$$im\omega_1\frac{\partial w}{\partial t}+aK\frac{\partial v}{\partial x}-\tfrac{3}{2}\beta|w|^2w=0, \quad (31)$$

which are Eqs. (11) and (12) at $m = M$. Making the same procedure as before, we find for the stationary solutions (13) the following system of two ordinary differential equations [cf. Eqs. (14) and (15)]:

$$\frac{df_1}{dz}=-\Delta f_2+\lambda f_2^3, \quad (32)$$

$$\frac{df_2}{dz}=\Delta f_1-\lambda f_1^3, \quad (33)$$

where $\Delta = m\omega_1\Omega$ and $\omega_1^2 = \omega_2^2 = (\alpha + 2K)/m$. In spite of the fact that the dynamical system (32) and (33) is similar to Eqs. (14) and (15), the structure of the separatrix curves on the phase plane (f_1, f_2) drastically differs from the cases considered above (see Fig. 6). 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 $f_0^2 = \Delta/\lambda$. Calculating the value of E (at $\Delta_1 = \Delta_2 = \Delta$) for these separatrix solutions, $E = -\Delta^2/4\lambda$, we easily integrate Eq. (18) at $\Delta_1 = \Delta_2 = \Delta$ and find the soliton solutions,

$$g(z)=\exp(\pm\sqrt{2}\Delta z), \quad (34)$$

$$f_2^2=\frac{\Delta e^{\mp\sqrt{2}\Delta z}[2\cosh(\sqrt{2}\Delta z)\pm\sqrt{2}]}{2\lambda\cosh(2\sqrt{2}\Delta z)}, \qquad f_1=gf_2. \quad (35)$$

The solutions (34) and (35), but for negative Δ, exist also for defocusing nonlinearity when $\lambda < 0$.

The results (34) and (35), together with (13), (9) and (10), give the shapes of the localized structures in the discrete nonlinear lattice. Because all combinations of signs are possible in Eq.(35), there are *four* solutions of this type. Let us fix the sign in Eq. (34), 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, $f_0 = \sqrt{\Delta/\lambda}$. At the same time the amplitude of the odd-particle oscillations vanishes (see Fig. 7). However, when $z \to -\infty$, the function $g(z)$ tends to zero,

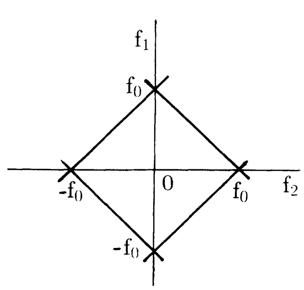

FIG. 6. The separatrix curves of the dynamical system (32) and (33) for $\Delta > 0$.

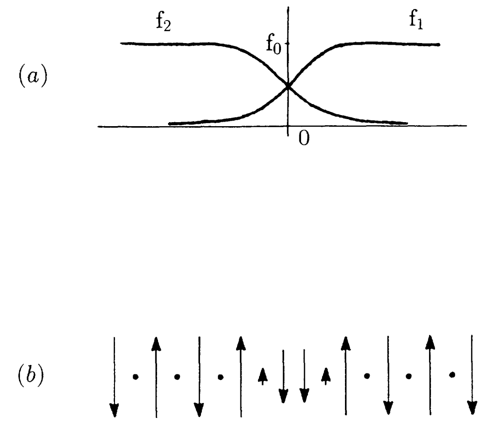

FIG. 7. The odd and even components for the soliton solutions (35) (a) and the diagrammatic representation of the whole localized structure in a monoatomic chain (b).

and the asymptotic behavior of the even and odd components is just 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 the opposite polarities, so that each of them cannot be localized in two directions. This is the direct consequence of the nonlinearity-induced gap in the cw spectrum [10], the gap disappearing in the linear limit. In some sense, these structures can be considered as an unusual limit of the soliton excitations in the diatomic nonlinear chain discussed above.

It is important to note that the localized structures described in the present section 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 [9]. The authors have observed also the standard cutoff kinks described as fundamental dark solitons by a 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 [9]. 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 modes, indicate that these structures are general phenomena which can occur in many other lattice systems.

At last, it is interesting to compare the localized structures described in this section with the gap solitons discussed above. As we have seen, the gap solitons may exist in a diatomic nonlinear lattice as completely localized excitations when the nonlinear frequency lies within the gap of the linear spectrum. 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 part of the particles (e.g., at the even sites) of the chain creates asymptotically a periodic potential for the other part of the particles (e.g., at the odd sites), and vice versa.

V. CONCLUSIONS

In the framework of a diatomic Klein-Gordon model, we have analyzed soliton solutions with the frequencies lying in the vicinity of the gap of the linear spectrum. We have shown analytically that such a diatomic chain may support the so-called gap solitons provided the soliton frequency lies within the gap. The gap solitons describe two-coupled and completely localized modes corresponding to heavy- and light-particle oscillations. If the frequency lies below the gap (e.g., for the "soft" nonlinearity considered in the present paper), at least one of the modes becomes delocalized and, in fact, it is a dark-soliton mode. We have derived a system of two NLS equations coupled through derivatives of the wave-field components, which describes the localized structures in the vicinity of the frequency gap, and this system differs from the standard system of two NLS equations (coupled through linear and cross-phase modulation terms) known in the theory of gap solitons. We have also considered the limit of a monoatomic chain when the gap in the linear spectrum disappears. However, such a monoatomic chain may support localized structures of a new type appearing as a result of the nonlinearity-induced symmetry breaking between two equivalent eigenmodes of the lattice. Because there is no gap in the linear spectrum, each mode of this nonlinear structure is localized only in one direction.

We believe that the existence of different localized structures described in the present paper does not depend drastically on either the type of the model selected or the type of nonlinearity (a self-focusing or defocusing one). Therefore, such nonlinear localized modes are not a specific property of the model and we may naturally expect to find them in other types of diatomic lattices.

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