Dynamical solitons in a one-dimensional nonlinear diatomic chain

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Solitonlike excitations with frequencies in the gap of a linear spectrum are considered for a diatomic chain with small mass difference. It is shown that these excitations represent themselves as a complicated combination of solitons of the acoustic and quasioptical branches of the spectrum. The evolution of these solutions is studied in the phase plane and analytical expressions are obtained. The situation is general for systems having two interacting fields with the same nonlinearity but with different dispersion signs.

I. INTRODUCTION

At the present time, one-dimensional anharmonic elastic chains have become a classical object with which to study nonlinear systems and, in particular, soliton dynamics.[1–3] As a rule, nonlinear waves of acoustic type in such a system are described in the framework of usual or modified Boussinesq or Korteweg–de Vries equations. The waves of quasioptical type are described by nonlinear Klein-Gordon equations with different nonlinear terms. In recent years interest in the theory of elastic soliton has shifted to the study of more realistic and complicated nonlinear elastic systems. The simplest and the most natural generalization of homogeneous elastic chain is a diatomic nonlinear chain with periodically arranged atoms of two different masses. The phonon spectrum of this system consists of two branches (acoustic and optical) and, in some sense, possesses properties of systems of both types. There are many examples of real diatomic systems. One of them is a two-component system of hydrogen-bonded dimers[4–6] (a well-known example of such a system is ice). For these systems it appeared to be possible to explain by means of a solitonic approach such properties as energy transport, dielectric polarization, and protonconductivity. Another interesting application of the nonlinear dynamics of a diatomic chain may be a one-dimensional two-component quasiperiodic lattice,[7–9] which has a singular continuum spectrum with gaps. The solution for the diatomic chain may contain some features of soliton solutions in quasiperiodic systems. (Results of Ref. 10 on soliton propagation in disordered media allow one to conclude that they may be also observed in quasiperiodic media.) From the point of view of mathematical physics, the interest in soliton dynamics in a diatomic chain is stimulated by the following fact: It is well known that the condition of existence of two-parameter solitons (which will be considered in this paper) for a fixed sign of the nonlinearity is related to the sign of a linear wave dispersion. In the case of a diatomic chain, in the gap of the phonon spectrum there exist together (when the mass difference is small) two branches of the spectrum with opposite dispersion signs corresponding to interacting acoustic and quasioptical phonons. Thus, the answer to the question concerning the character of such combined two-component solitons is not evident in this frequency region. In Ref. 11 in the framework of the nonlinear Schrödinger equation, dynaminal two-parameter solitons of the simplest kind in a one-dimensional diatomic chain were considered. Below, we will show that in the frequency region near the phonon spectrum gap, solitons may have more complicated character.

II. FORMULATION OF THE PROBLEM AND DISPERSION RELATION OF LINEAR WAVES

We consider a one-dimensional periodic diatomic chain with atoms of masses M and m ($M>m$) and anharmonic potential of nearest-neighbor interactions. For simplicity we choose the even interparticle potential

$$U(u_n-u_{n-1})=\frac{A}{2}(u_n-u_{n-1})^2+\frac{C}{4}(u_n-u_{n-1})^4 , \qquad (1)$$

where u_n is the nth-atom displacement from its equilibrium position. The corresponding equation of motion for the nth particle has the form

$$m_n\frac{d^2u_n}{dt^2}+A(2u_n-u_{n+1}-u_{n-1})+C(u_n-u_{n-1})^3 + C(u_n-u_{n+1})^3=0 . \qquad (2)$$

We take the constants A and C to be positive, the latter sign meaning that we have nonlinearity of a "hard" character and that all the frequencies of vibrations increase with increasing amplitudes.

Let us introduce the following notation for the displacements of atoms of different masses:

$$u_n = v_n\ ,\quad m_n = m \quad \text{for } n = 2s\ ,$$
$$u_n = w_n\ ,\quad m_n = M \quad \text{for } n = 2s+1\ , \tag{3}$$

and write the equations of motion for atoms with odd and even indices,

$$m\frac{d^2v_n}{dt^2} + A(2v_n - w_{n+1} - w_{n-1}) + C(v_n - w_{n-1})^3 + C(v_n - w_{n+1})^3 = 0\ , \tag{4}$$

$$M\frac{d^2w}{dt^2} + A(2w_n - v_{n-1} - v_{n+1}) + C(w_n - v_{n-1})^3 + C(w_n - v_{n+1})^3 = 0\ . \tag{5}$$

First of all, let us briefly analyze the well-known linear limit of these equations. The dispersion relation of linear waves of the kind

$$(v_n, w_n) = (v_0, w_0)\cos(kn - \omega t)$$

has two branches:

$$\omega_{1,2}^2 = A\left[\frac{m+M}{mM} \mp \frac{1}{mM}[m^2 + M^2 + 2mM\cos(2k)]^{1/2}\right]\ , \tag{6}$$

where the plus sign corresponds to the low-frequency acoustic branch and the minus sign to the optical branch (see Fig. 1). It is well known that the possible existence and the character of soliton excitations are determined by the dispersion relation of the system. Usually, for a fixed sign of the anharmonic term, the existence of the dynamical envelope soliton is determined by the sign of the linear wave dispersion $D = d^2\omega/dk^2$. In particular, for hard nonlinearity ($C > 0$), the dispersion should be negative ($D < 0$). In the case of a diatomic chain, $D < 0$ for the whole lower acoustic branch and for the upper branch for small values of the wave number $k < k_0$. The region of ω and k in which solitons can exist for hard nonlinearity is shown as dashed one in Fig. 1. The most interesting part

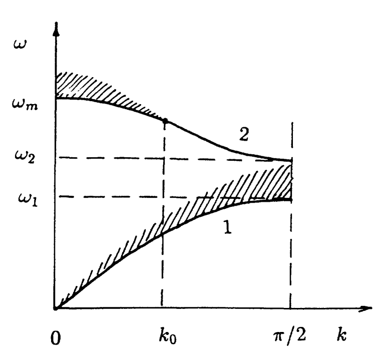

FIG. 1. Linear wave spectrum (1) acoustic g branch, (2) quasioptical f branch.

of the spectrum is in the vicinity of the maximum value of k (at $k \simeq \pi/2 - \kappa$, with $\kappa \ll 1$) where those two branches with opposite signs of dispersion are close to each other. The lower branch has the asymptotic form $\omega_{(1)}^2 = \omega_1^2 - 2A\kappa^2/(m+M)$ and ends at the point $\omega_1 = \sqrt{2A/M}$. At the vicinity of this point, heavy particles oscillate with higher amplitudes than those of light ones $[v_0/w_0 = M\kappa/(M-m)]$ and, at $\kappa = \pi/2$, light particles are at rest ($w_0 = 0$) and the heavy ones oscillate with opposite phases. The asymptotic behavior of the upper branch at $k \simeq \pi/2$ is $\omega_{(2)}^2 = \omega_2^2 + 2A\kappa^2/(M-m)$, where $\omega_2^2 = 2A/m > \omega_1^2$. In this case, the heavy particles essentially do not move, while the light atoms vibrate with opposite phases. In the limit $M = m$, the form of Eq. (6) reduces to $\omega_{1,2}^2 \simeq 2A(1 \mp \kappa)/m$ and the gap in the spectrum disappears.

III. CLASSIFICATION OF SOLITON EXCITATIONS IN NONLINEAR EVOLUTIONAL SYSTEMS

It is well-known that solitonlike excitations in nonlinear systems[3,12,13] may be of the following main types: topological solitons (e.g., kinks in the sine-Gordon equation), one-parameter dynamical solitons (solitons of Korteweg–de Vries and Boussinesq equations), and dynaminal two-parameter solitons [appearing, e.g., in the nonlinear Schrödinger equation (NSE)]. In our case there are no topological solitons due to the absence of degeneracy of the main state and one-parameter solitons are the limiting case of dynamical two-parameter solitons of the general type. Their structure depends essentially on the character of a linear wave dispersion and the type of nonlinearity. The simplest situation appears in the case of cubic anharmonicity in the dynamical equation, which corresponds to the natural interactions of elementary excitations in the system: interaction of the "density-density" type (in our case, we mean phonon-phonon pair interaction). It is well known [3,14] that spatially homogeneous nonlinear waves are modulationally unstable when the condition $(\partial^2\omega/\partial k^2)\partial\omega/\partial a^2 < 0$, where ω, k, and a are the frequency, wave number, and amplitude of the nonlinear wave, is satisfied. In the case of a hard nonlinearity ($\partial\omega/\partial a^2 > 0$), a homogeneous wave is unstable for negative dispersion and this instability leads to soliton creation. When the sign in the criterion is changed, homogeneous nonlinear waves become stable; however, the existence of "dark" solitons then becomes possible. In the first case, we deal with attractive phonons, which form localized many-phonon bound states. In the second example, phonons are repulsive and their coherent motion with an inhomogeneous density is stable. In this case, dark solitons represent bubbles with lower density of phonons in the phonon condensate. To illustrate this we present some results for a one-atomic chain when all the masses in Eq. (2) are equal. In this case the linear spectrum has one branch with negative dispersion.

Soliton solutions for small-amplitude excitations can be easily obtained with the help of an asymptotic approach,[15] according to which we can look for a solution as a Fourier expansion in the periodic phase of the wave, and the amplitude is represented as a power series. In this approach the amplitude of a soliton or, equivalently, the difference between parameters of nonlinear and linear waves (or the deviation of the frequency from a linear dispersion relation for fixed wave number) can be chosen as a small parameter of the power expansion.

For a one-atomic chain in the continuum limit ($k \to 0$), Eq. (2) is reduced in the dimensionless variables $x = y/\sqrt{12}$, $t = \tau\sqrt{m/12A}$, and $u = v\sqrt{a/36C}$ to the form (in this notation the lattice constants are set equal to unity)

$$v_{\tau\tau} - v_{yy} - v_y^2 v_{yy} - v_{yyyy} = 0 \ . \quad (7)$$

In the linear limit, Eq. (7) possesses wave solutions with the dispersion relation $\omega^2 = \omega^2(k) = k^2 - k^4 (D<0)$. In order to find soliton solutions [with frequencies $\omega > \omega(k)$ corresponding to the dashed region in Fig. 1], let us represent them in the form

$$v(y,\tau) = \sum_{n=1}^{\infty}{}' f_n(y - V\tau)\cos(n\vartheta) + \phi_n(y - V\tau)\sin(n\vartheta) \ , \quad (8)$$

where

$$\vartheta = ky - \omega\tau \ ,$$

$$f_n = \sum_{s=n}^{\infty}{}' f_{ns}\varepsilon^s \ ,$$

$$\phi_n = \sum_{s=n}^{\infty}{}' \phi_{ns}\varepsilon^s \ ,$$

$$\varepsilon^2 = \omega^2 - \omega^2(k) \ ,$$

and the primes mean summing over unity. The value ε is the expansion parameter: $\varepsilon \ll \omega(k)$. If in addition we expand the velocity V in a power series in ε^2 in the vicinity of the group velocity for a given k, it is easy to obtain the soliton solution to an accuracy of any power of ε. The main approximation gives the standard soliton form

$$v \cong \frac{2\sqrt{2}\varepsilon}{k^2} \frac{\cos(ky - \omega\tau)}{\cosh\{\varepsilon(y - V\tau)/\sqrt{|D|\omega}\}} \ . \quad (9)$$

It is obvious that, as the value k decreases, the region of applicability of Eq. (9) and the region of existence of small-amplitude solitons become narrower.

In a diatomic chain in the long-wave limit when $\lambda \ll 2a$ the soliton has qualitatively the same form as that in a one-atomic chain but with an average mass. An approximate solution for it in the framework of nonlinear Schrödinger equation has been given in Ref. 11.

For $k \approx \pi$, i.e., near the Brillouin-zone edge, it is also possible to use long-wave approximation for a wave of opposite-phase vibrations of the nearest-neighbor atoms. if we introduce opposite-phase displacements $w_n = (-1)^n u_n$, then in the continuum limit for a function $w(x)$, we obtain

$$m w_{tt} + 4Aw + A w_{xx} + 16 C w^3 = 0 \ . \quad (10)$$

If the deviation of the soliton frequency from the upper edge of the spectrum of linear waves, $\omega_m = \sqrt{4A/m}$, is small, so is the soliton amplitude, and the stationary soliton solutions can be easily determined by use of the following expansion:

$$w(x,t) = \sum_{n=1}^{\infty}{}' \sin(n\omega t) \sum_{s=n}^{\infty}{}' \varepsilon^s f_{ns}(\varepsilon x) \ , \quad (11)$$

where the small expansion parameter $\varepsilon = [(\omega/\omega_m)^2 - 1]^{1/2} \ll 1$. The main order of this expansion has the following solution:

$$w \approx \sqrt{2A/3C} \frac{\varepsilon \sin(\omega t)}{\cosh\{2\varepsilon(x - x_0)\}} \ , \quad (12)$$

where x_0 is arbitrary parameter describing the soliton-center position. The solution (12) describes localized (in the length $\Delta x \sim 1/2\varepsilon$) opposite-phase, small-amplitude nonlinear vibrations. Since Eq. (10) is invariant with respect to transformations $x \to (x - Vt)/[1 + V^2]$ and $t \to (t + Vx)/[1 + V^2]^{1/2}$, it is easy to construct a propagating-soliton solution,

$$w = \sqrt{2A/3C} \frac{\varepsilon_1 \sin(\omega t - kx)}{\sinh\{2\varepsilon_1(x - Vt)/[1 + V^2]^{1/2}\}} \ , \quad (13)$$

where $V = -k/\omega$, and $\varepsilon_1^2 = (\omega^2 - \omega_m^2 + k^2)/\omega_m^2$. This solution represents localized, almost-opposite-phase vibrations propagating with the group velocity of a linear wave with the same value of the wave number k.

The expression (13) for small-amplitude solitons remains valid only for small values of ε. With increasing frequency, the effects of discretization increase. This manifests itself in the appearance of soliton-energy dependence on its center position (analogous to the Peierls potential for dislocations). If in Eq. (12) we make the transformation $x - x_0 \to n - x_0$ and calculate the energy summing over all integer values of n, then in the main approximation in parameter ε, we obtain

$$\begin{aligned} E &\cong \sum_{n=-\infty}^{\infty} \left[\frac{m}{2} \left[\frac{du_n}{dt} \right]^2 + \frac{A}{2}(u_n - u_{n-1})^2 \right] \\ &\cong \frac{m}{2} \sum_n \left[\left[\frac{d}{dt} w(n) \right]^2 + \omega_m^2 w^2(n) \right] \\ &\cong (4A^2/3C)\varepsilon[1 + (2\pi^2/\varepsilon)\cos(2\pi x_0)\exp(-\pi^2/2\varepsilon)] \ . \end{aligned} \quad (14)$$

As usual, the energy is proportional to the small parameter ε but contains an exponentially small term, periodically changing with the soliton-center position. We should note that the situation when the center is placed between two neighboring atoms ($x_0 = \frac{1}{2}$) corresponds to the energy minimum, and the energy has a maximum when the soliton center is situated on the atom.

If the frequency increases further, the soliton becomes localized in several interatomic distances and long-wave approximation is no longer valid. Nevertheless, as it was shown in Ref. 16, dynamical solitons of type (11) (but localized in several atoms) exist in the region of large frequencies $\omega \gg \omega_m$. In this limit, the value ε is not a small parameter and a Fourier expansion in harmonics of the main frequency ω is not related to the smallness of some physical parameter. The amplitude decrease with increasing harmonic number n is determined only by the numerical value $(1/n)^2$. If we introduce the amplitude of the opposite-phase atom displacement for the main harmonic,

$$u_n \cong \sqrt{8A/3C}(-1)^n a_n \sin(\omega t) ,$$

we obtain for a_n the following system of difference equations:

$$-4(\omega/\omega_m)^2 a_n + (2a_n + a_{n+1} + a_{n-1}) \times \{1 + 2(a_{n+1}^2 + a_{n-1}^2 + a_n^2 + a_n a_{n+1} + a_n a_{n-1} - a_{n-1} a_{n+1})\} = 0 . \quad (15)$$

The numerical solution of such a system gives two types of localized solitonlike states, which differ by the soliton-center displacement by half the interatomic distance. The solution in which practically two atoms vibrate with the same amplitude has the minimum energy, which is in agreement with the long-wave case. The maximum energy corresponds to a state with amplitude localization in one atom. In the limit of large amplitude this solution was obtained in Ref. 16. For $\omega \gg \omega_m$ the atoms amplitudes are the following: $a_n = (\omega/\omega_m) b_n$, where $b_0 \cong 0.53$, $b_{\pm 1} \cong 0.28$, $b_{\pm 2} \sim 10^{-3}$, and $b_{\pm 3} \sim 10^{-6}$. In the solution of the first type[17] two central atoms vibrate with amplitude $a_{0,1} \cong 0.47\omega/\omega_m$, and the amplitudes of their neighbors are $a_{-1} = a_2 \cong a_0/9 \ll a_0$. Of course, the smallness of the amplitude $u_n \ll a$ gives the limit for the soliton frequency growth $(\omega - \omega_m) \leq \omega_m$. Nevertheless, high-frequency, strongly localized excitations are observed in numerical simulations (see Ref. 18).

Finally, we would like to discuss nonlinear vibrations near the Brillouin-zone edge ($k \cong \pi$) with the opposite sign of nonlinearity—"soft" nonlinearity ($C<0$). In this case, Eq. (10) is not localized and vanishes at infinity. However, there are localized states of different types. If we use expansion (11) for vibrations with frequency ($\omega < \omega_m$) and introduce the small parameter $\tilde{\varepsilon} = [1 - \omega^2/\omega_m^2]^{1/2}$, we can easily obtain the inhomogeneous solution, which in the main approximation may be written as follows:

$$w \cong \tilde{\varepsilon} \sqrt{A/3|c|} \tanh[\sqrt{2}\tilde{\varepsilon}(x - x_0)] \sin(\omega t) . \quad (16)$$

Such a solution in the theory of solitons is usually called a dark soliton. It represents a localized decrease of density of opposite-phase phonons, localized in the region $l \cong 1/\tilde{\varepsilon}$ near point x_0. A dark soliton can be considered as a hole in the phonon condensate with a finite density, $A\tilde{\varepsilon}^2/3|C|$.

IV. QUALITATIVE ANALYSIS OF SOLITONS IN DIATOMIC CHAIN NEAR THE GAP OF PHONON SPECTRUM

To our mind, the most interesting case is the behavior of solitons in a diatomic chain near the Brillouin-zone edge in the gap of the phonon spectrum with $\omega \sim \omega_1, \omega_2$, where two interacting branches with opposite signs of dispersion are close to each other. Near the value $k \simeq \pi/2$, either heavy (lower branch) or light (upper branch) atoms vibrate almost with opposite phases and the long-wave approximation may be used for these opposite-phase vibrations.

Let us introduce normalized displacements for an arbitrary particle

$$v_{2s} = (-1)^s v(2s,t)\sqrt{4A/3C} ,$$
$$w_{2s+1} = (-1)^s w(2s+1,t)\sqrt{4A/3C} , \quad (17)$$

and let us change the discrete argument n by the continuum coordinate x, expanding the functions v and w in Taylor series. For wave numbers $k \simeq \pi/2$, it appears to be enough to leave only the first space derivative; Eqs. (4) and (5) in this case are reduced to the following system of partial differential equations:

$$\frac{1}{\omega_2^2}\frac{\partial^2 v}{\partial t^2} + \frac{\partial w}{\partial x} + v + \frac{4}{3}v(v^2 + 3w^2) - 0 ,$$
$$\frac{1}{\omega_1^2}\frac{\partial^2 w}{\partial t^2} - \frac{\partial v}{\partial x} + w + \frac{4}{3}w(w^2 + 3v^2) = 0 . \quad (18)$$

Below we consider the simplest case of stationary small-amplitude solitons. For the small parameter of expansion it is convenient to choose the value $\varepsilon^2 = (\omega^2 - \omega_1^2)/\omega_1^2$. If the atomic masses are close, i.e., $(M - m) \ll m$, then $\omega_1 \approx \omega_2$ and the parameter ε remains small everywhere inside and near the gap of linear spectrum. Let us represent the periodic in time with the frequency ω solutions as an expansion in Fourier series

$$\begin{bmatrix} v \\ w \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix} \sin(\omega t) + \begin{bmatrix} f_3 \\ g_3 \end{bmatrix} \sin(3\omega t) , \quad (19)$$

where $f, g \sim \varepsilon$, $f_3, g_3 \sim \varepsilon^3$. To the lowest-order ε approximation for the amplitude of the main harmonic, we obtain the system of ordinary differential equations of the first order,

$$\frac{df}{dx} = g(\delta + (g^2 + 3f^2)) , \quad (20)$$

$$\frac{dg}{dx} = f(-\mu - (f^2 + 3g^3)) , \quad (21)$$

where $\delta = 1 - \omega^2/\omega_1^2$, $\mu = 1 - \omega^2/\omega_2^2$ (for $\omega > \omega_1$, we have $\delta = -\varepsilon^2$ and $\mu = ((M - m)/M - m\varepsilon^2/M)$.

Equations (20) and (21) describe the dynamics of Hamiltonian system with one degree of freedom and the following integral of motion:

$$G = 2\mu f^2 + 2\delta g^2 + (f^4 + 6f^2 g^2 + g^4) . \quad (22)$$

Its existence allows one to integrate the system exactly. But first it is useful to use the methods of qualitative analysis of dynamical systems and consider possible solutions of the system, (20) and (21), in the phase plane (g, f). Attention should be paid to separatrixes, which correspond to soliton solutions of different kinds. The phase portrait of the system depends on the signs and on the values of the parameters δ and μ, which change with increasing ω. As ω increases, a number of subsequent bifurcations in phase plane take place.

(a) For $\omega < \omega_1$, both parameters μ and δ are positive and the only fixed point in the phase plane is the center at

$g = f = 0$. In this case the separatrixes and, subsequently, soliton solutions are absent.

(b) At $\omega = \omega_1$, the first bifurcation occurs: The center is split and for the frequency range in $\omega_1 < \omega < \omega_2$, where $\delta < 0$ and $\mu > 0$, the system possesses a saddle point at $g = f = 0$ and two centers at points $f = 0$, $g = \pm\sqrt{|\delta|}$. The phase portrait for this case is sketched in Fig. 2(a) and the corresponding functions $f(x)$ and $g(x)$ in Fig. 2(b). Note that in Fig. 2(b) only the solid curve for the field $g(x)$, i.e., for heavy atoms, has the standard soliton form. This is reasonable, since for $k = \pi/2$ the lower branch of the spectrum corresponds to opposite-phase vibrations of particles with mass M, while the light ones are stationary. The soliton can be considered as bound vibrations of the lower branch of the spectrum. In this case, they are accompanied by localized light-atom vibrations, i.e., a soliton of the lower branch localizes phonons of the upper branch.

(c) At $\omega = \omega_2$, the parameter μ changes its sign and the second bifurcation occurs: the singular point ($g = 0$, $f = 0$) splits into a center at the point ($f = 0$, $g = 0$) and two new saddle points ($g = 0$, $f = \pm\sqrt{|\mu|}$). In the frequency region

$$\omega_2 < \omega < \omega_* = \sqrt{2}\omega_1\omega_2 / [3\omega_1^2 - \omega_2^2]^{1/2}$$

the phase portrait has the form presented in Fig. 3(a). Now separatrixes of two types [S and C in Fig. 3(b)] exist. The S soliton again is the bound phonon state of the lower branch but now it is accompanied by vibrations of light atoms with finite amplitude at infinite density. Close to the frequency $\omega = \omega_2$, the amplitude of the g field exceeds the amplitude of the f field and thus the S soliton can be considered as a soliton of the lower branch. The C soliton has a different form. For $\omega - \omega_2 \ll \omega_2 - \omega_1$, the amplitude of the f field is essentially larger than that for

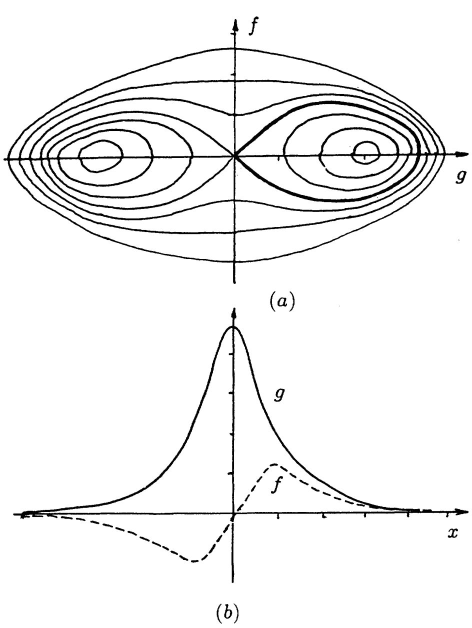

FIG. 2. The phase portrait and field distribution in soliton for $\omega_1 < \omega < \omega_2$.

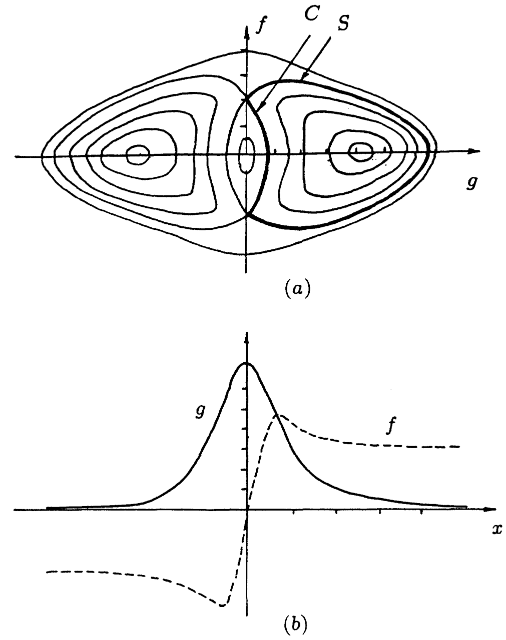

FIG. 3. The phase portrait and field distribution in soliton for $\omega_2 < \omega < \omega_*$.

the g field and, in this sense, this is a soliton of the upper branch. In this latter case, the envelope for light-atom vibrations [dashed line in Fig. 3(b)] has the form of a kink. This result is in complete agreement with the analysis of the dynamics of a one-atomic anharmonic chain.[19] Indeed, in this case, for the upper branch of the spectrum, the dispersion $\partial\omega/\partial k$ is positive, which implies the existence of dark solitons.

(d) Finally, at frequency $\omega = \omega_*$, at which the last bifurcation occurs, each of the saddle points ($g = 0, f = \pm\sqrt{|\mu|}$) splits into the center and two new saddle points. For $\omega > \omega_*$ the positions of these new saddle points are still determined by the parameter μ and four additional saddle points are situated at

$$g_0^2 = \tfrac{1}{8}(3|\mu| - |\delta|) \ , \quad f_0^2 = \tfrac{1}{8}(3|\delta| - |\mu|) \ . \tag{23}$$

The corresponding phase portrait is sketched in Fig. 4(a). An analysis shows that for $\omega > \omega_*$ four different types of separatrixes, S, C, S^*, and C^*, coexist. The separatrixes of S and C type are continuously derived from ones considered for the previous case and the lines S^* and $^*C$ correspond to new solitons. The main feature of the latter appears to be the fact that now none of the field vanishes at infinity. In addition, the principal field difference between S and C solitons disappears; they differ only qualitatively by the amplitude of the field at the soliton center. Thus, a symmetry between the g and f fields arises: In S and C solitons, the soliton of the g field is accompanied by the kink of the f field and, in S^* and C^* solitons the soliton for f fields is accompanied by the kink of the g field.

We should also note that, while all the other distinct frequencies ω_1, ω_2 were characteristics of the linear spectrum, the appearance of the frequency ω_* is essentially a

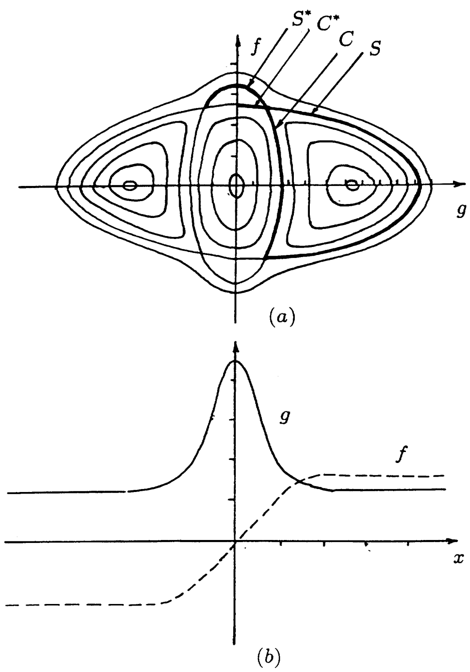

FIG. 4. The phase portrait and field distribution in soliton for $\omega > \omega_*$.

nonlinear effect. As the frequency and the vibration amplitude increase, the interaction of g and f fields becomes increasingly important and the change of their characteristics due to the interaction with one another takes place. If we rewrite the system, (20) and (21), in the form of the equations $d^2g/dx^2 = f\Psi(g^2, f^2)$ for the g field, then the interaction of g and f fields will lead to the appearance in the function Ψ the additional term $3f^2(|\delta| - |\mu| - f^2)$, which describes the interaction of the lower branch of phonons with the upper branch. Taking into consideration that the characteristic amplitude of light-atom vibrations $f \sim \sqrt{|\mu|}$, we obtain, for the g field, the approximate equation

$$\frac{d^2g}{dx^2} = 2|\mu|(|\delta| - 3|\mu|)g + (3|\delta| + 7|\mu|)g^3 - 3g^5 . \tag{24}$$

When the amplitude of the f field (which is related to the upper branch of the spectrum) increases the edge of lower zone is displaced and this becomes more sufficient at $\omega = \omega^*$ than the nonlinear growth of the frequency of the g field soliton.

Finally, we should note that when the sign of nonlinearity is changed ($C \to -C$) the sequence of bifurcations becomes in some sense inverse. For $\omega > \omega_2$, soliton solutions are absent. In the gap $\omega_1 < \omega < \omega_2$, envelope solitons of opposite-phase vibrations of light atoms, i.e., bound phonon states of the upper branch of vibrations are present. For $\omega < \omega_1$, the soliton still represents a bound state of phonons of the upper branch but it is accompanied by opposite-phase vibrations of heavy atoms (lower-branch phonons) not vanishing at infinity. As in the previous case, at $\omega = \omega_{**} = \sqrt{2}\omega_1\omega_2/[3\omega_2^2 - \omega_1^2]^{1/2}$, the last bifurcation occurs after which (for $\omega < \omega_{**}$) the principal difference between S and C solitons disappears and so neither field vanishes at infinity.

V. EXACT SOLITON SOLUTIONS OF EQUATIONS OF LATTICE VIBRATIONS NEAR THE GAP OF PHONON SPECTRUM

The most remarkable property of the system of Eqs. (20) and (21) for diatomic lattice vibrations is that it is completely integrable. This allows to obtain the analytical expression for envelopes of solitons, the forms of which have been predicted in Sec. IV. Indeed, by making the transformation $g = zf$ in Eqs. (20) and (21) and taking into account the value of the integral of motion (22), it is easy to obtain the equation for the function $z(x)$,

$$\frac{dz}{dx} = \pm[(\mu + \delta z^2)^2 + G(z^4 + 6z^2 + 1)]^{1/2} . \tag{25}$$

The value G can be found, for example, from the boundary conditions for functions f and g at $x = \pm\infty$. With that, the function $f(x)$ is calculated to be

$$f^2 = \frac{1}{z^4 + 6z^2 + 1}\{-\mu - \delta z^2 \pm [(\mu + \delta z^2)^2 + G(z^4 + 6z^2 + 1)]^{1/2}\} . \tag{26}$$

In the general case, the solutions of Eq. (26) are expressed in terms of elliptic integrals. However, it is not difficult to find the function $z(x)$ for some particular values of G, corresponding to separatrixes in phase portraits of the system [see Figs. 2(a), 3(a), and 4(a)]. Localized soliton solutions corresponding to these values are expressed in terms of elementary functions.

(a) For $\omega_1 < \omega < \omega_2$, the phase portrait is sketched in Fig. 2(a). The envelopes of the fields $f(x)$ and $g(x)$ tend to zero at $x = \pm\infty$, which gives us the following expression for the function $z(x)$:

$$z = \sqrt{\mu/|\delta|}\coth(\sqrt{\mu|\delta|}x) , \tag{27}$$

while functions $f(x)$ and $g(x)$ can be written in the following form:

$$f^2 = \frac{2(|\delta|z^2 - \mu)}{z^4 + 6z^2 + 1} , \quad g = zf . \tag{28}$$

These forms are presented in Fig. 2(b). The maximum value of the g field is $\sqrt{2|\delta|}$.

(b) For $\omega_2 < \omega < \omega_*$, the f soliton does not vanish at infinity. The boundary conditions $g = 0$, $f = \pm\sqrt{|\mu|}$ at $|x| = \pm\infty$ give the value of the integral of motion $G = -|\mu|^2$. The integration of Eq. (25) gives

$$z = \pm\frac{2\mu}{\sinh(\gamma x)} , \tag{29}$$

$$f^2 = \frac{1}{z^4 + 6z^2 + 1}[|\mu| + |\delta|z^2 \pm |z|(\alpha^2 z^2 + \beta^2)^{1/2}] , \tag{30}$$

where

$$\alpha^2 = |\delta|^2 - |\mu|^2 , \quad \beta^2 = 2|\mu|(|\delta| - 3|\mu|) , \quad \gamma = \beta/\alpha . \tag{31}$$

Taking different signs for the functions $z(x)$ and $f(x)$, one can obtain the solutions, corresponding to S and C separatrixes, and those symmetric to them $(-g(x),-f(x))$. In the limit case $x\to\pm\infty\,(z\to 0)$, the f field tends to the value $\pm\sqrt{|\mu|}$, while the g field vanishes. It is not difficult also to find the maximum value of the function $g(x)$:

$$g^2_{\max}=|\delta|\pm\alpha \ .$$

(c) For $\omega>\omega_*$, neither solution has zero boundary conditions. The integral of motion for these solutions has the value

$$G=\tfrac{1}{8}(|\delta|^2+|\mu|^2-6|\delta||\mu|) \ . \quad (32)$$

Having integrated the equation for the function $z(x)$ we obtain the solution in the following form,

$$z(x)=\begin{cases}\beta\coth(\gamma x) \ , \\ \beta\tanh(\gamma x) \ ,\end{cases} \quad (33)$$

$$f^2=\frac{1}{z^4+6z^2+1}(|\mu|+|\delta|z^2\pm\alpha|z^2-\beta^2|) \ , \quad (34)$$

where

$$\alpha=\frac{1}{\sqrt{8}}(3|\delta|-|\mu|) \ , \quad \beta^2=\frac{3|\mu|-|\delta|}{3|\delta|-|\mu|} \ , \quad \gamma=\alpha/\beta \ . \quad (35)$$

The four types of the solutions (separatrixes C, C^*, S, and S^*) differ by different forms of the function $z(x)$ as well as by different signs in the expression for f^2. The solutions C and S correspond to the first value of $z(x)$, with that for $x\to 0$, $f(x)\to 0$, and

$$g^2=g^2_{\max}=|\delta|\pm\alpha=g^2(-\infty) \ .$$

The second value of $z(x)$ corresponds to C^* and S^* solitons. In this case, at $x\to 0$, $g(x)\to 0$, and

$$f^2=f^2_{\max}=|\mu|\pm\alpha\beta^2>f^2(-\infty) \ .$$

It is necessary to note that the solutions $f(x)$ and $g(x)$ with opposite signs in fact describe the same atom displacements in the chain, since atoms with sites n and $n+2$ vibrate with opposite phases.

VI. OPTICAL HIGH-FREQUENCY SOLITONS

Finally, we study one more case allowing long-wave approximation: nonlinear vibrations with frequencies near the upper edge of the spectrum $\omega\cong\omega_m$. In a one-atomic chain, in this region envelope solitons of the form (12) or dark solitons of the form (16) exist, depending on the nonlinearity sign. In a diatomic chain we start with a system of difference equations (4) and (5), making the following expansions:

$$v_{n\pm 1}=v(x)\pm\frac{\partial v}{\partial x}+\frac{1}{2}\frac{\partial^2 v}{\partial x^2}\pm\cdots \ ,$$
$$w_{n\pm 1}=w(x)\frac{\partial w}{\partial x}+\frac{1}{2}\frac{\partial^2 w}{\partial x^2}\pm\cdots \ . \quad (36)$$

If we limit our calculations by the second spatial derivatives and nonlinear terms, containing only the displacements themselves but not their spatial derivatives, then for relative displacements $\Psi=w-v$ and displacements of the centers of mass of the elementary cell $\Phi=(Mw+mv)/(M+m)$, we obtain the following simple system of equations:

$$\frac{2Mm}{M+m}\frac{\partial^2\Psi}{\partial t^2}+4A\Psi+A\frac{\partial^2\Psi}{\partial x^2}+4C\Psi^3+(M-m)\frac{\partial^2\Phi}{\partial t^2}=0 \ , \quad (37)$$

$$(M+m)\frac{\partial^2\Phi}{\partial t^2}+A\frac{M-m}{M+m}\frac{\partial^2\Phi}{\partial x^2}-2A\frac{\partial^2\Phi}{\partial x^2}=0 \ . \quad (38)$$

Since at $\omega\cong\omega_m$ the ratio of amplitude vibrations is $v/w\cong -M/m$, then the inequality $\Phi\ll\Psi$ (at $\omega=\omega_m$, we have $\Psi=0$) is satisfied and the last term in Eq. (38) can be neglected in comparison with the second. As a result, we come to the following equation for the relative displacements:

$$\frac{2Mm}{M+m}\frac{\partial^2\Psi}{\partial t^2}+\frac{4AMm}{(M+m)^2}\frac{\partial^2\Psi}{\partial x^2}+4A\Psi+4C\Psi^3=0 \ . \quad (39)$$

This equation coincides with Eq. (10) at $M=m$ and may be reduced to the equation for optical-mode vibrations obtained in Ref. 11 by means of a special ansatz.

To solve Eq. (39), we use the asymptotic expansions (11) and obtain the solutions analogous to (12) and (16). In the case of a hard nonlinearity ($C>0$), the solution for high-frequency envelope solitons in the main approximation in the small parameter $\varepsilon=[\omega^2/\omega_M^2 1]^{1/2}$ has the form

$$\Psi=\sqrt{8A/3C}\,\frac{\varepsilon\sin(\omega t)}{\cosh(\varepsilon x(M+m)/\sqrt{Mm}\,)} \ . \quad (40)$$

The difference in atoms masses manifest themselves in the magnitude of the localization region of a soliton. For equal soliton amplitudes in one-atomic and diatomic chains, the ratio of their localization lengths is equal to

$$l/l_0=\sqrt{M/m}\,(2-\sqrt{M/m}\,) \ . \quad (41)$$

As M increases this ratio at first grows and then vanishes at $M\to\infty$.

In the case of soft nonlinearity ($C<0$), the form for dark solitons (16) changes as follows:

$$\Psi=\sqrt{4A/3|C|}\,\bar{\varepsilon}\sin(\omega t)\tanh\left[\frac{\bar{\varepsilon}x(M+m)}{\sqrt{2Mm}}\right] \ , \quad (42)$$

where the small parameter $\bar{\varepsilon}$ is defined as $\bar{\varepsilon}=[1-\omega^2/\omega_m^2]^{1/2}$.

The moving solutions with small k and, consequently, small velocities can be easily obtained from expressions (40) and (42) with the help of the transformations $x\to(x-Vt)/[1+V^2]^{1/2}$ and $t\to(t+Vx)/[1+V^2]^{1/2}$.

VII. CONCLUSIONS

The main result of this paper is the consideration of all kinds of solitonic excitation with frequencies in the region of the gap in the spectrum of linear waves for a diatomic chain. For small mass difference, this gap separating the acoustic and quasioptical spectral regions becomes narrow and phonons of different branches strongly interact with one another. The fact that the gap region is narrow allowed us to obtain, in the long-wave approximation, rather simple equations for chain dynamics, which are valid in the region of frequencies close to the gap. These equations were studied qualitatively and for them the approximate soliton solutions were obtained analytically. If the frequency of localized exitations changes, their structure undergoes a sequence of bifurcations. As the frequency increases, envelope solitons formed by phonons of the lower branch appear at the edge of the lower zone boundary. If the lower edge of the upper branch is reached, this soliton is transformed to a more complicated structure: a combination of an ordinary soliton of the lower branch and a dark soliton of the upper branch of the spectrum. When we further increase the frequency, the next bifurcation occurs and the combined soliton from solitons with nonvanishing boundary conditions of one branch and dark solitons of another branch is formed. This situation is general for physical systems described by two nonlinear interacting fields, which are characterized by the same nonlinearity but with different dispersion signs. The results obtained may be generalized to the case of more complicated nonlinear elastic systems. In particular, if an elementary cell contains more than two atoms with two different masses, then the number of quasioptical branches and the gaps in the spectrum increase. However, near every gap the formalism of this paper can be applied and the combined solitons of phonons of neighboring branches can be constructed. The general structure of the soliton solution will be the same. If we take rather large number of first steps of Fibonacci sequence as an elementary cell, then the complicated one-dimensional chain obtained can be considered as an approximate model of quasicrystals. In this approach, the soliton solution obtained here describes approximately solitons of quasicrystals with frequencies near the main gaps of their phonon spectrum.

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