NONLINEAR COLLECTIVE EXCITATIONS IN QUASI–ONE-DIMENSIONAL STRUCTURES WITH SPATIAL DISPERSION

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It is demonstrated that a description of the effects of higher-order dispersion of continuous oscillations calls for a consideration of interactions with the nearest and more distant neighbors in a crystal lattice. Exact soliton and periodic solutions of the nonlinear equation with fourth-order derivatives describing long-wavelength collective excitations in a quasi–one-dimensional chain have been found.

Interest in the study of special features of nonlinear excitation propagation in systems with dispersion has quickened in the past few years [1–3]. These investigations find application, for example, in the theory of structural phase transitions in ferroelectrics caused by displacements of the equilibrium positions of atoms [4–7]. Frequencies of oscillatory modes in these systems decrease sharply when the temperature of the system approaches the critical one. As a result, ordered local regions arise that manifest themselves as additional peaks in neutron scattering [8].

A theoretical description of such systems is based on the model of quasi–one-dimensional chain of identical oscillators [4]. The model suggests that each oscillator corresponds to a particle of mass m moving in a symmetric external potential field. Below we consider two sublattices, with heavy atoms of the first sublattice spaced at distance a and light atoms of mass m of the second sublattice displaced by u_n from the heavy atoms.

As is well known, the long-wavelength limit in the description of mechanics of a discrete system based on the use of differential equations with the second-order spatial derivatives remains unchanged for arbitrary number of interacting neighbors. Therefore, this approximation can be developed on the basis of the model considering interactions with the nearest neighbors with inclusion of the interparticle interaction parameter. If higher-order dispersion is considered, it will be described by an independent parameter. This parameter arises if we consider interactions with the nearest and more distant neighbors in the crystal lattice. This approach was first examined in [9, 10].

With allowance for the foregoing, we now include terms describing the potential energy of interactions with the second neighbors into the Hamiltonian. Then the model Hamiltonian of the examined system assumes the form

$$H = \frac{1}{2}\sum_n \left\{ m\left(\frac{du_n}{dt}\right)^2 + \chi_1 (u_{n+1} - u_n)^2 + \chi_2 (u_{n+2} - u_n)^2 + 2U(u_n) \right\}, \tag{1}$$

where χ_1 and χ_2 are force constants of interactions with the first and second neighbors, respectively. We now take advantage of the potential corresponding to the u-four model:

$$U(u_n) = U_0 (1 - u_n^2 / d^2)^2 \tag{2}$$

that is often used for a theoretical description and has minima at $u_n = \pm d$ and a potential barrier of height U_0 at $u_n = 0$.

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The properties of the system described by Hamiltonian (1) depend significantly on relationships of the potential barrier energy U_0 with the binding energies of displacements of the first ($\sim a^2\chi_1$) and second neighbors ($\sim a^2\chi_2$). If $U_0 >> a^2\chi_1$ and $U_0 >> a^2\chi_2$, the main role is played by almost independent particle motion in the field of its potential and by the probability of hopping to the next well. If $U_0 << a^2\chi_1$ and $U_0 << a^2\chi_2$, the main role is played by coordinated collective excitations of many lattice sites. This situation describes structural phase transitions of the displacement type [7] realized, for example, in $SrTiO_3$, $BaTiO_3$, and $KNbO_3$ crystals. We are interested in the dynamics of nonlinear collective excitations exactly in these systems.

The discrete system state causes the dispersion law of small oscillations to deviate from its continuous description for quasi–one-dimensional systems. In the long-wavelength approximation, the difference is reduced to allowance for higher-order dispersion, that is, for higher powers of wave numbers q in the expansion of frequency ω in powers of aq. In the coordinate representation, inclusion of higher-order dispersion implies additional consideration of spatial derivatives, for example, of the fourth order in the conventional differential equations of mathematical physics.

Of independent interest is derivation of exact solutions (both soliton and periodic ones) of high-order nonlinear equations. For example, soliton solutions of the sine-Gordon dispersion equation were obtained in [2], solutions of the generalized Boussinesq and Korteweg–de Vries equations were obtained in [3], soliton solutions of the generalized Kuramoto–Sivashinskii equations were obtained in [11], and periodic and soliton solutions of the generalized Kuramoto–Sivashinskii equations with power-law nonlinearity were obtained in [12].

In the long-wavelength approximation, continuous dynamic equations were derived in [9]. It has been demonstrated that whereas differential equations with second-order spatial derivatives can be always used as a long-wavelength approximation of discrete equations, the applicability of equations with the fourth-order spatial derivatives is limited by stringent requirements imposed on the parameters of the initial equation. In particular, continuous equations with the fourth-order spatial derivatives can be subsequently derived for stationary oscillations with allowance for interactions with not only the first but also with the second neighbors in the atomic chain. The problem of allowance for interactions with the second neighbors was also examined in [1] in the study of the dispersion effects in soliton dynamics.

After replacement of the site positions na by the continuous coordinate x, Hamiltonian (1) in the long-wavelength approximation assumes the form

$$H = \frac{m}{2a}\int\{u_t^2 + s^2u_x^2 + \beta u_{xx}^2 + 2U_0/m(1-u^2/d^2)^2\}dx\,, \tag{3}$$

where $s^2 = a^2(\chi_1 - 4\chi_2)/m$, s is the phase velocity of sound waves in the linear chain, and $\beta = a^4(16\chi_2 - \chi_1)/12m$ is the dispersion parameter. Since $s^2 > 0$, the force constants are related by the inequality $\chi_2 < \chi_1/4$. The sign of the dispersion parameter is plus or minus. The positive dispersion is characterized by $\beta > 0$, which is provided by the inequality $\chi_1/16 < \chi_2 < \chi_1/4$. The negative dispersion is characterized by $\beta < 0$, which is provided by the inequality $\chi_2 < \chi_1/16$.

The equation of motion in partial fourth-order derivatives corresponding to Hamiltonian (3) is

$$u_{tt} - s^2u_{xx} + \beta u_{xxxx} - \omega_0^2 u(1-u^2/d^2) = 0\,, \tag{4}$$

where $\omega_0^2 = 4U_0/md^2$.

Consideration of interactions with the second neighbors in the discrete chain influences significantly the long-wavelength oscillations. The law of linear wave dispersion $\omega^2(q) = s^2q^2 + \beta q^4 - \omega_0^2$ follows from Eq. (4), where q is the wave number and $aq << 1$. From here it follows that the equation with the fourth-order derivative in the long-wavelength approximation describes stationary oscillations of the discrete chain only at frequencies $\omega^2 + \omega_0^2 << |\beta|$; to this end, the inequality $a^2s^2 << |\beta|$ must be valid for the chain parameters. But in this case, $\beta = a^4\chi_2/m - a^2s^2/12 \approx a^4\chi_2/m$, and the use of Eq. (4) is justified only with allowance for the interaction with the second neighbors in the atomic chain [9].

Equation (4) with the fourth-order derivative also describes the dynamic excitations of the chain moving stationary with velocity V, when its solution is $u(x, t) = u(x - Vt)$. The long-wavelength approximation in this case is applicable to excitations whose velocities V satisfy the inequality $\left|s^2 - V^2\right| << |\beta|$; in this case, the condition $\omega_0^2 << |\beta|$ must be valid. We are interested exactly in these excitations with stationary moving profiles.

Equation (4) has exact partial soliton solutions vanishing at infinity. They satisfy the boundary conditions $u = 0$ and $u_x = 0$ when $x \to \pm\infty$.

For $\beta > 0$, there exists the soliton solution

$$u(x, t) = A\sinh\{(x - Vt)/l\}\text{sech}^2\{(x - Vt)/l\}, \tag{5}$$

where

$$A = \pm 2d(30/11)^{1/2},\ V^2 = s^2 + 10\omega_0(\beta/11)^{1/2},\ l^2 = (11\beta)^{1/2}/\omega_0. \tag{6}$$

For $\beta < 0$, there exists the soliton solution

$$u(x, t) = A\text{sech}^2\{(x - Vt)/l\}, \tag{7}$$

where

$$A = \pm d(15/8)^{1/2},\ V^2 = s^2 + 5\omega_0|\beta|^{1/2}/2,\ l^2 = 8|\beta|^{1/2}/\omega_0. \tag{8}$$

In these formulas, A is the soliton amplitude, V is its propagation velocity, l is the width of the excitation localization zone. The plus sign in formulas for the amplitude corresponds to the soliton, and the minus sign corresponds to the antisoliton.

It should be noted that excitations are propagated with fixed velocities exceeding the phase sound velocity of linear waves. Therefore, these solitons can be called supersonic. As is well known, only solitons whose velocities do not exceed the phase sound velocity of linear waves can propagate in systems without dispersion (at $\beta = 0$). In systems without dispersion, excitation (7) vanishes, and excitation (5) assumes the kink (antikink) form $u(x, t) = \pm d\tanh\{(x - Vt)/l\}$, where $l = 2^{1/2}(s^2 - V^2)^{1/2}/\omega_0$. This excitation propagates with arbitrary velocity V limited by s from above. The velocity V here is a free parameter.

Equation (4) has exact periodic solutions that are expressed through the Jacobi elliptic functions and satisfy the periodic boundary conditions $u(x + L, t) = u(x, t)$, where L is a certain spatial period.

For $\beta > 0$, there exists an exact periodic solution

$$u(x, t) = A\,\text{SN}\{(x - Vt)/l, k\}\text{CN}\{(x - Vt)/l, k\}. \tag{9}$$

Here

$$A = \pm 2d\,(30)^{1/2}k^2/(11k^4 + 64k^2 - 64)^{1/2}, \tag{10}$$

$$V^2 = s^2 + 10\omega_0\beta^{1/2}(2 - k^2)/(11k^4 + 64k^2 - 64)^{1/2},\ l^2 = \beta^{1/2}(11k^4 + 64k^2 - 64)^{1/2}/\omega_0, \tag{11}$$

k is the modulus of the elliptic function. Solution (9) exists only when this modulus lies in the small interval $k_{c1} < k < 1$, where $k_{c1} = 2\{2(3\cdot 3^{1/2} - 4)/11\}^{1/2} \approx 0.932699$. In the limit $k = 1$, solution (9) is transformed into Eq. (5), and its parameters specified by Eqs. (10) and (11) are transformed into the corresponding parameters given by Eq. (6). The expression

$$L = 2K(k)\beta^{1/4}(11k^4 + 64k^2 - 64)^{1/4}/\omega_0^{1/2} \tag{12}$$

follows from the periodic boundary condition and determines in an implicit form the modulus k as a function of L and parameters of Eq. (4), where $K(k)$ is the complete elliptic integral of the first kind. We consider only the roots of Eq. (12) from the interval $k_{c1} < k < 1$.

For $\beta < 0$, there exists an exact periodic solution of the form

$$u(x, t) = A\mathrm{DN}\{(x - Vt)/l, k\}\mathrm{CN}\{(x - Vt)/l, k\}, \tag{13}$$

where

$$A = \pm 2d(30)^{1/2}k^2/(86k^2 - 11k^4 - 11)^{1/2}, \tag{14}$$

$$V^2 = s^2 + 10\omega_0|\beta|^{1/2}(1 + k^2)/(86k^2 - 11k^4 - 11)^{1/2},\ l^2 = |\beta|^{1/2}(86k^2 - 11k^4 - 11)^{1/2}/\omega_0. \tag{15}$$

Solution (13) exists only for modulus k from the interval $k_{c2} < k < 1$, where $k_{c2} = (3\cdot 3^{1/2} - 4)/11^{1/2} \approx 0.360653$. In the limit $k = 1$, solution (13) is transformed into Eq. (7), and its parameters specified by Eqs. (14) and (15) are transformed into the corresponding parameters given by Eq. (8). Expression

$$L = 4K(k)|\beta|^{1/4}(86k^2 - 11k^4 - 11)^{1/4}/\omega_0^{1/2} \tag{16}$$

follows from the periodic boundary condition and determines in an implicit form the modulus k as a function of L and parameters of Eq. (4). Moreover, values k must be taken from the interval $k_{c2} < k < 1$.

These new exact solutions of the nonlinear dispersion equation can be used to describe the propagation of a local deformation along quasi–one-dimensional molecular chains with velocities exceeding the velocity of linear waves.

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