Self-localization of vibrations in a one-dimensional anharmonic chain

A. M. Kosevich and A. S. Kovalev

Physico-technical Institute, Ukrainian Academy of Sciences
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An asymptotic method is proposed for determining the long-wave localized characteristic vibrations of a one-dimensional anharmonic chain in the case when nonlinear stationary waves in such a chain are unstable. The frequencies of the self-localized vibrations can lie both below and above the band of vibrational frequencies of the corresponding harmonic chain. The magnitude of the splitting of the vibration frequency from the edge of the continuous harmonic-approximation spectrum is the small parameter that makes it possible to obtain an asymptotic expansion of the solution of the nonlinear vibration equations.

INTRODUCTION

Crystal-lattice mechanics often reduces to the analysis of one-dimensional models, both because of the simplicity of obtaining exact results and in connection with the study of objects for which one-dimensional dynamics is a very good and adequate approximation. In particular, the widely-known one-dimensional model of Frenkel and Kontorova[1] for a dislocation in a crystal is used for the first reason, and a model of kinks in dislocations that is practically equivalent to the latter model in the mathematical sense is usually considered for the second reason.

In the Frenkel-Kontorova model a one-dimensional atomic chain is assumed to be situated in an external periodic potential field, which models the influence of the three-dimensional crystal on the selected row of atoms. If u_n is the displacement of the atom with label n, then in the approximation of a harmonic interaction between nearest neighbors the equation of motion of the atom considered has the form

$$\frac{d^2u_n}{dt^2}+\varkappa^2(2u_n-u_{n+1}-u_{n-1})-F_n=0,\quad mF_n=-\frac{\partial U}{\partial u_n}$$

where m is the mass of the atom and U(u) is a periodic function whose period is taken to be equal to the equilibrium distance a between neighboring atoms. We denote

$$F_n=a\omega_0^2 f(u_n/a),$$

thus introducing a minimum frequency ω_0 of the harmonic vibrations of the chain, and a dimensionless force f. We shall measure the displacements in units of a, and the time in units of $1/\omega_0$. Then the equation of motion of the chain can be written in dimensionless variables:

$$\frac{d^2u_n}{dt^2}+b^2(2u_n-u_{n+1}-u_{n-1})-f(u_n)=0, \tag{1}$$

where $b=\kappa/\omega_0$ is the characteristic dimensionless parameter defining the ratio of the forces of the interatomic interaction along the chain to the force of the external potential.

The entire nonlinearity of the model formulated is contained in the function f(u). We shall assume that for small displacements ($u \ll 1$) the function f(u) is linear: $f(u)=-u$. In this case, small harmonic vibrations of the chain under consideration have the dispersion law

$$\omega^2=2b^2+1-2b^2\cos k. \tag{2}$$

The dispersion law (2) describes the band of frequencies of the optical vibrations of a one-dimensional crystal, and therefore the presence of a gap is characteristic for it: $\omega(0)\equiv\omega_0=1$.

Being interested in vibrations with frequencies near the lower band-edge (i.e., the long-wave vibrations), we can replace the difference equation (1) by a nonlinear Klein-Gordon differential equation:

$$\frac{\partial^2u}{\partial t^2}-\frac{\partial^2u}{\partial x^2}-f(u)=0, \tag{3}$$

where x is the coordinate along the chain, in units of $ba=\kappa a/\omega_0$. Equation (3) is widely discussed in the theory of crystal lattices, in nonlinear optics[2], field theory[3] and other branches of physics. In crystal-lattice mechanics one is usually interested in the solutions of the nonlinear equation (3) that describe displacements of the order of the lattice constant[4], i.e., $u\sim 1$. However, for small displacements too ($u\ll 1$), Eq. (3) can describe essentially nonlinear phenomena, e.g., the self-localization of the characteristic vibrations. We shall be interested only in solutions of this type, and, therefore, shall assume the displacements u to be small.

Taking into account the smallness of the displacements, we expand f(u) in a series in powers of u, confining ourselves to the first terms of this expansion:

$$f(u)=-u+\alpha u^2+\beta u^3. \tag{4}$$

It is clear that all the results look simplest for a symmetric potential U(u), when $\alpha=0$, but we shall also discuss the general case in which the chain has no center of inversion, when $\alpha\neq 0$.

In Sec. 1 an asymptotic method is proposed for finding the localized vibrations of Eq. (3) with the force (4). The frequencies of these vibrations lie in the forbidden band of the spectrum of the harmonic vibrations ($\omega<\omega_0=1$), and the amplitudes of the corresponding vibrations are smaller the smaller is the quantity $\sqrt{1-\omega}$. It is shown that such vibrations are possible only for $\beta>0$, if $\alpha=0$. In Sec. 2 we formulate an effective equation describing the motion of a self-localized vibration in the leading approximation with respect to the size of its amplitude. In Sec. 3 we consider the localized vibrations whose frequencies lie above the upper edge of the harmonic-vibration spectrum (2) ($\omega>\omega_m=\sqrt{1+4b^2}$). Such vibrations are possible only for $\beta<$, if $\alpha=0$. There too it is shown that the appearance of self-localized vibrations can be associated with the anharmonicity in the interaction between neighboring atoms in the chain (even for $f(u)\equiv 0$).

1. ASYMPTOTIC METHOD FOR INVESTIGATING LOCALIZED VIBRATIONS

We shall start the analysis of the self-localized characteristic solutions of the nonlinear equation (3) using the simplest form of the force (4), when $\alpha = 0$ and Eq. (3) takes the form

$$\frac{\partial^2 u}{\partial t^2}-\frac{\partial^2 u}{\partial x^2}+u-\beta u^3=0. \quad (5)$$

If we neglect higher harmonics, the "solutions" of Eq. (5) are nonlinear stationary waves

$$u=a_0 \cos(\omega t-kx) \quad (6)$$

with the dispersion law

$$\omega^2=1-\frac{3}{4}\beta a_0^2+k^2. \quad (7)$$

In accordance with Lighthill's criterion[5], for $\beta > 0$ the stationary waves (6) are unstable. But we shall imagine that the amplitude a_0 is a slowly-varying function of the coordinate x and is nonzero in a certain restricted interval of the x-axis. Then, for $\beta > 0$, in this interval the lower edge of the allowed band of frequencies drops below the edge of the frequency spectrum in the harmonic approximation, i.e., into the region $\omega < 1$. Vibrations with frequencies $\omega < 1$ can arise in this spatial interval. It is clear that such vibrations will be stable against decay into small harmonic vibrations. Indeed, for $\omega < 1$ a harmonic system only permits vibrations that fall off with distance like $\exp(-\epsilon|x|)$, where $\epsilon = \sqrt{1-\omega^2}$.

The localized vibrations corresponding to Eq. (5) are studied most easily by a method analogous to the asymptotic method of Bogolyubov and mitropol'skiĭ[6], which was proposed for the analysis of nonlinear systems with many degrees of freedom. In our case, the system formally possesses an infinite number of degrees of freedom, since it is described by a differential equation in partial derivatives, but this does not hinder the development of the corresponding method[7].

We shall seek the solution of (5) in the form of the following series:

$$u(x,\ t)=A(x)\cos\omega t+B(x)\cos 3\omega t+\ldots, \quad (8)$$

where A(x) and B(x) are functions of the coordinate that vanish at infinity. Naturally, such a procedure has meaning only in the case when the expansion coefficients fall off sufficiently rapidly with the label of the harmonic. In particular, it is necessary to assume that $B(x) \ll A(x)$. We substitute (8) into Eq. (5) and equate the expressions multiplying $\cos\omega t$ and $\cos 3\omega t$ to zero. With allowance for the inequality $B(x) \ll A(x)$ this gives us, in the leading approximation, the following system of equations for A(x) and B(x):

$$\frac{d^2A}{dx^2}-(1-\omega^2)A+\frac{3}{4}\beta A^3=0, \quad (9)$$

$$\frac{d^2B}{dx^2}+(9\omega^2-1)B=-\frac{1}{4}\beta A^3. \quad (10)$$

The only solution of Eq. (9) that falls of at infinity is the function

$$A(x)=\left(\frac{8}{3\beta}\right)^{1/2}\frac{\varepsilon}{\operatorname{ch}\varepsilon x},\quad \varepsilon=(1-\omega^2)^{1/2}. \quad (11)$$

Inasmuch as Eq. (5) was itself obtained under the assumption $\beta u^3 \ll u$, the inequality $\beta A^2(0) \ll 1$ must be fulfilled, and from this it follows that $1-\omega^2 \ll 1$. Thus, the small parameter of the theory ($\epsilon^2 \ll 1$) arises in a natural way.

We turn to the inhomogeneous equation (10) for the function B(x). Since the corresponding homogeneous equation has no solutions vanishing simultaneously both for $x \to \infty$ and for $x \to -\infty$, we must select the necessary particular integral of the inhomogeneous equation. But in this case,

$$\frac{d^2B}{dx^2}\Big/B \sim \frac{d^2A}{dx^2}\Big/A \sim \varepsilon^2 \ll 1$$

and the derivative in the left-hand side of (10) can be omitted. Then, in the leading approximation in the small parameter, we obtain

$$B(x)=-\frac{1}{12}\left(\frac{8}{3\beta}\right)^{3/2}\frac{\varepsilon^3}{\operatorname{ch}^3\varepsilon x}. \quad (12)$$

We emphasize that the small parameter whose powers determine the contribution of the temporal harmonics with the corresponding labels is ϵ, i.e., the magnitude of the splitting of the localized-vibration frequency from the lower edge of the continuous spectrum of frequencies in the harmonic approximation.

It follows from (11) and (12) that the amplitude of the vibrations has the order of magnitude of $\epsilon \ll 1$, and the spatial region Δx of localization of the vibrations considered has the order of magnitude of $\sim 1/\epsilon \gg 1$. Both these properties of the localized vibrations justify going over from the system of difference equations (1) to the differential equation (3) or (5).

Having convinced ourselves of the basic consistency of the method of treating the localized vibrations, we pass on to the formulation of a consistent quantitative procedure. We note that since it was found that $B(x) \approx \epsilon^3$, a consistent procedure for finding the solution should give a correction to A(x) of the same order of magnitude. Therefore, we must seek from the outset the coefficients of the different temporal harmonics in (8) by expanding them in powers of ϵ. In principle, such a solution can be obtained to any degree of accuracy in ϵ, but then, naturally, the expansion of f(u) in a series in u would be assumed to be written with the corresponding accuracy. We shall demonstrate the procedure for solving Eq. (3) to order ϵ^5, assuming the force to be

$$f(u)=-u+\beta u^3+\gamma u^5+\delta u^7. \quad (13)$$

We write the solution of (3) in the form

$$u=A(x)\cos\omega t+B(x)\cos 3\omega t+C(x)\cos 5\omega t, \quad (14)$$

where the functions A, B and C of the coordinates have the expansions

$$A=A_1\varepsilon+A_3\varepsilon^3+A_5\varepsilon^5,\quad B=B_3\varepsilon^3+B_5\varepsilon^5,\quad C=C_5\varepsilon^5. \quad (15)$$

Substituting (14) and (15) into Eq. (3) with the force (13) and equating the coefficients of each temporal harmonic and each power of ϵ to zero, we see that the equation for $\epsilon A_1(x)$ coincides with (9), and the following system of equations is obtained for the remaining coefficients in the expansions (15):

$$B_3=-\frac{1}{32}\beta A_1^3,\quad C_5=-\frac{1}{32}\beta A_1^2B_3-\frac{1}{384}\gamma A_1^5, \quad (16)$$

$$A_3''-A_3+\frac{9}{4}\beta A_1^2A_3=-\frac{3}{4}\beta A_1^2B_3-\frac{5}{8}\gamma A_1^5, \quad (17)$$

$$B_5=\frac{9}{8}B_3-\frac{1}{8}B_3''-\frac{3}{32}\beta A_1^2(A_3+2B_3)-\frac{5}{128}\gamma A_1^5, \quad (18)$$

$$A_5''-A_5+\frac{9}{4}\beta A_1^2A_5=-\frac{3}{4}\beta(3A_1A_3^2+A_1^2B_5+2A_1A_3B_3+2A_1B_3^2)-\frac{25}{16}\gamma A_1^4(2A_3+B_3)-\frac{35}{64}\delta A_1^7. \quad (19)$$

In writing Eqs. (16)–(19) we have denoted the derivative with respect to the argument ϵx by a prime.

We note that the last term in the right-hand side of (19) is proportional to δ. It follows from this that to find the solution exactly to order ϵ^n it is necessary to retain terms up to u^{n+2} inclusive in the expansion of the force $f(u)$. After $\epsilon A_1(x)$ has been found in the form (11), the relations (16) determine B_3 and C_5 uniquely. Equally, B_5 is found uniquely when the function $A_3(x)$ is known. However, in solving the inhomogeneous equation (17) we must take into account that the corresponding homogeneous equation

$$A_3''-A_3+\frac{9}{4}\beta A_1^2A_3=0 \tag{20}$$

has an eigen-solution vanishing at infinity:

$$A_3^0(x)=\xi\,\mathrm{sh}\,\varepsilon x/\mathrm{ch}^2\,\varepsilon x, \tag{21}$$

where ξ is an arbitrary constant. Thus, the solution of (17) of interest to us has the form

$$A_3(x)=A_3^0(x)+\left(\frac{8}{3\beta}\right)^{1/2}\frac{1}{36}\left(1-\frac{80}{3}\frac{\gamma}{\beta^2}\right)\left(\frac{2}{\mathrm{ch}\,\varepsilon x}-\frac{1}{\mathrm{ch}^3\,\varepsilon x}\right). \tag{22}$$

After (22) is substituted into (18), it is found that B_5 also contains a term proportional to the arbitrary constant ξ:

$$B_5^0(x)=-\frac{1}{4}\xi\frac{\mathrm{sh}\,\varepsilon x}{\mathrm{ch}^4\,\varepsilon x}. \tag{23}$$

The full expression for B_5 appears in the form

$$B_5=B_5^0-\frac{1}{72}\left(\frac{8}{3\beta}\right)^{1/2}\left(\left\langle 1-\frac{80}{3}\frac{\gamma}{\beta^2}\right\rangle\frac{1}{\mathrm{ch}^3\,\varepsilon x}+\left\langle\frac{11}{2}+\frac{100}{3}\frac{\gamma}{\beta^2}\right\rangle\frac{1}{\mathrm{ch}^5\,\varepsilon x}\right). \tag{24}$$

In an analogous manner we can find the function $A_5(x)$, which, in view of its cumbersome form, we shall not give; we note, however, that it consists of terms with sech ϵx, $\mathrm{sech}^3\,\epsilon x$ and $\mathrm{sech}^5\,\epsilon x$. Therefore, $A_5(x)$ can certainly be represented in the form

$$A_5(x)=\tilde{A}_5(x)\,\mathrm{sech}\,\varepsilon x,\ \text{where}\ \tilde{A}_5(\infty)=\mathrm{const}\neq 0.$$

By considering the structure of the eigen-solutions (21) and (23) it is easy to notice the obvious relations:

$$\varepsilon^2A_3^0=-\varepsilon\xi\left(\frac{3\beta}{8}\right)^{1/2}\frac{dA_1(x)}{dx},\quad \varepsilon^4B_5^0=-\varepsilon\xi\left(\frac{3\beta}{8}\right)^{1/2}\frac{dB_3(x)}{dx}. \tag{25}$$

It follows from (25) that the contribution of the homogeneous solutions to A_3 and B_5 describes a shift of the corresponding first-approximation terms $A_1(x)$ and $B_3(x)$ through a small constant distance $x_0=-\epsilon(3\beta/8)^{1/2}\xi$. Allowance for similar terms in the third-approximation term A_5 leads to a more exact calculation of the shift through the distance x_0 in the terms from the preceding approximations. Thus, allowance for the homogeneous solutions in Eqs. (17) and (19) corresponds to an arbitrary shift of the solution along the x-coordinate. It is clear that invariance with respect to such a shift is embodied in the structure of the initial equation (5), and therefore the solution can always be sought in the form $u=u(x-x_0, t)$, where $x_0=\mathrm{const}$.

Taking into account all that has been said above, we shall give the explicit form of the localized solution of Eq. (5):

$$u=\left(\frac{8}{3\beta}\right)^{1/2}\frac{\varepsilon}{\mathrm{ch}\,\varepsilon x}\left\{\left[1+\frac{\varepsilon^2}{36}\left(1-\frac{80}{3}\frac{\gamma}{\beta^2}\right)\left(2-\frac{1}{\mathrm{ch}^2\,\varepsilon x}\right)+\varepsilon^4\tilde{A}_5\right]\cos\omega t\right.$$
$$-\frac{1}{12}\frac{\varepsilon^2}{\mathrm{ch}^2\,\varepsilon x}\left[1+\frac{\varepsilon^2}{6}\left(1-\frac{80}{3}\frac{\gamma}{\beta^2}\right)+\left\langle\frac{11}{2}+\frac{100}{3}\frac{\gamma}{\beta^2}\right\rangle\frac{1}{\mathrm{ch}^2\,\varepsilon x}\right]\cos 3\omega t$$
$$\left.+\frac{1}{18}\left(\frac{1}{8}-\frac{\gamma}{3\beta^2}\right)\frac{\varepsilon^4}{\mathrm{ch}^4\,\varepsilon x}\cos 5\omega t\right\}. \tag{26}$$

The solution (26) is localized near the point $x = 0$, but again we recall that it can be localized near any point $x = x_0$.

A particular case of Eq. (3) is the so-called sine-Gordon equation[3, 8], in which $f(u)=-\sin u$. For this equation an exact solution corresponding to localized vibrations is known. It was first obtained by Seeger[9] and has been discussed in detail by Lamb[2] and Ablowitz et al.[8]. In our notation, this solution has the following form:

$$u(x,t)=4\,\mathrm{arctg}\left\{\frac{\varepsilon}{\omega}\frac{\cos\omega t}{\mathrm{ch}\,\varepsilon x}\right\}. \tag{27}$$

Inasmuch as (27) is an exact solution, the parameter ϵ can take any values from 0 to 1. Correspondingly, the possible frequencies ω occupy the whole interval from zero to the lower edge ($\omega = 1$) of the harmonic-vibration spectrum. However, we are interested primarily in the solution (27) for small ϵ and, consequently, small displacements . For small u, the values $\beta = 1/6$, $\gamma = -1/120$ and $\delta = 1/5040$ correspond to the series expansion of $f(u) = -\sin u$. Naturally, if these values of β, γ and δ are substituted into (26), then (26) coincides with the first three terms of the expansion of (27) in a series in the argument of the arctangent.

We must say a few words about the stability of the vibrations considered. The numerical experiments of[10] show that the localized vibrations (27) are stable. In addition, in[8] the general solution of the sine-Gordon equation was obtained by a method used in the inverse scattering problem, and it was shown that for arbitrary initial conditions, falling off sufficiently rapidly at infinity, the asymptotic (as $t\to\infty$) solution can contain the localized vibrations (27). Thus, the vibrations (27) are stable with respect to perturbations that fall off sufficiently rapidly at large distances. It may be hoped that, in the general case of an arbitrary function f(u) also, the localized vibrations for which the asymptotic method of description outlined above is valid are stable. In any case, they are stable against decay into small harmonic vibrations.

Up to now we have considered the case of a symmetric potential U(u). However, the method of finding the localized vibrations is not difficult to generalize to the general case when there is a term with $\alpha\neq 0$ in the expansion (4) for f(u). Naturally, .when terms with u^2 and u^3 are present simultaneously in Eq. (3), the solution will contain all temporal harmonics, including the zeroth:

$$u(x,\ t)=C(x)+A(x)\cos\omega t+D(x)\cos 2\omega t+\ldots \tag{28}$$

As in the preceding case, we shall seek the functions of the coordinate in the form of expansions in powers of ϵ. For A(x) this expansion has the same form as (15), and for C(x) and D(x) it must be represented as

$$C(x)=C_2\varepsilon^2+C_4\varepsilon^4+\ldots,\quad D(x)=D_2\varepsilon^2+D_4\varepsilon^4+\ldots \tag{29}$$

Confining ourselves to the force (4), we obtain the following localized solution, exact to order ϵ^2[1)]:

$$u(x,t)=\frac{2\varepsilon}{5\alpha(1+9\beta/10\alpha^2)}\left\{\frac{3\varepsilon}{\mathrm{ch}^2\,\varepsilon x}-\left[15\left(1+\frac{9}{10}\frac{\beta}{\alpha^2}\right)\right]^{1/2}\times\frac{\cos\omega t}{\mathrm{ch}\,\varepsilon x}+\varepsilon\frac{\cos 2\omega t}{\mathrm{ch}^2\,\varepsilon x}\right\}. \tag{30}$$

It follows from the expression (30) that in the present case localized vibrations exist only when there is a well-defined relationship between the constants α and β–namely, when $\beta > -10\alpha^2/9$. Referring to the work of Grimshaw[11], it is curious to note that when this inequality is fulfilled, nonlinear periodic solutions in the given system are unstable.

2. EFFECTIVE EQUATION OF THE VIBRATIONS IN THE LEADING APPROXIMATION

The regularity of the procedure used in obtaining an expansion of the type (26) or (30) makes it possible to conclude that Eq. (3) always admits a solution in the form of a localized standing vibration with $\omega < 1$. The degree of monochromaticity (discrimination of the fundamental frequency) of such a vibration is uniquely related to its degree of localization. If $1-\omega^2 \ll 1$, i.e., $\epsilon \ll 1$, the first term of the asymptotic expansion, corresponding to the vibration with the fundamental frequency, is the principal term and gives a good approximation for the localized solution. But in this case the region Δx of localization of the vibration turns to be very large, in proportion as the quantity ϵ is small, namely $\Delta x \sim 1/\epsilon$. It should be noted that allowance for subsequent terms in the expansion of the solution under discussion does not widen its region of localization.

If we make use of the expansion (26) or (30) for the qualitative characteristics of the localized vibration for $\epsilon \sim 1$, we see that the standing vibrations turn out to be strongly localized ($\Delta x \sim 1$). But, on the other hand, the contribution of high harmonics then becomes important and in describing a periodic localized vibration we cannot neglect them. The latter circumstance is illustrated by the explicit form of the solution (27) for the sine-Gordon equation. However, in this case we must be cautious in using the differential equation (3), which is a long-wave approximation for the finite-difference equation (1). Only under the condition $b \gg 1$ (see the Introduction), i.e., when the interaction of the atoms along the chain is substantially greater than their interaction with the external potential, can Eq. (3) be used to describe localized vibrations, even for $\Delta x \sim 1$.

Returning to the case for which we shall apply the method developed ($\epsilon \ll 1$), we shall confine ourselves to treating sufficiently small vibrations of a chain with a center of inversion, i.e., a chain describable by Eq. (5). We shall find that effective equation stemming from (5) for which the principal term of the expansion (26), i.e., a function of the type $u(x, t) = A(x)\cos\omega t$, is the exact solution. For this we introduce a complex function $\Psi(x, t)$ such that its real part defines the displacement:

$$u(x,t)=\operatorname{Re}\Psi(x,t). \qquad (31)$$

In proposing an equation for $\Psi(x, t)$, we shall take the dispersion law (7) as the basis of its derivation and use a procedure analogous to that described in the monograph by Karpman[12]–namely, we shall replace k^2 by $-\partial^2/\partial x^2$ and ω^2 by $-\partial^2/\partial t^2$. We then obtain

$$\frac{\partial^2\Psi}{\partial t^2}-\frac{\partial^2\Psi}{\partial x^2}+\Psi-\frac{3}{4}\beta|\Psi|^2\Psi=0. \qquad (32)$$

We note that this equation follows directly from (9). It is easily verified that the exact solution of Eq. (32) that corresponds to localized vibrations is the function

$$\Psi(x,t)=\left(\frac{8}{3\beta}\right)^{1/2}\frac{\varepsilon}{\operatorname{ch}\varepsilon x}e^{i\omega t}. \qquad (33)$$

We see that $\operatorname{Re}\Psi(x, t)$, where $\Psi(x, t)$ is defined by the expression (33), does indeed etermine the leading approximation of the vibrational solution of Eq. (5). However, for small amplitudes ($a_0 \ll 1$) it is usual to represent the dispersion law (7) in the long-wave approximation in the form

$$\omega=1-\frac{3}{8}\beta a_0^2+\frac{1}{2}k^2. \qquad (34)$$

In the sense of establishing the k-dependence of ω for small k, the dispersion laws (7) and (34) are equivalent.

On the basis of (34), it is possible by the procedure indicated[12] to re-establish the nonlinear parabolic equation

$$i\frac{\partial\Psi}{\partial t}-\frac{1}{2}\frac{\partial^2\Psi}{\partial x^2}+\Psi-\frac{3}{8}\beta|\Psi|^2\Psi=0. \qquad (35)$$

In the approximation for which the effective equation is written, (32) is equivalent to the nonlinear parabolic equation (35). Indeed, Eq. (35) has the same solution (33), with, however, $\omega = 1 - 1/2\epsilon^2$. But for $\epsilon \ll 1$ this expression coincides with $\omega^2 = 1-\epsilon^2 \approx (1-\epsilon^2/2)^2$. If we separate out explicitly the rapid temporal oscillations of $\Psi(x, t) = \Phi(x, t)e^{it}$, from (35) we obtain for the slowly-varying (with frequency $1/2\,\epsilon^2$) function $\Phi(x, t)$ the well-known[12] nonlinear equation for the envelope waves:

$$2i\frac{\partial\Phi}{\partial t}-\frac{\partial^2\Phi}{\partial x^2}-\frac{3}{4}\beta|\Phi|^2\Phi=0.$$

The properties of this equation and of its solutions are sufficiently fully discussed in the literature, and so we shall not dwell on them.

Up to now we have confined ourselves to considering only those vibrations whose center of localization does not move along the chain. But by virtue of the Lorentz invariance of the nonlinear wave equation (3) or (32), along with the solution $u = u(x, t)$ there always exists the solution

$$u=u\left(\frac{x-vt}{(1-v^2)^{1/2}},\ \frac{t-vx}{(1-v^2)^{1/2}}\right).$$

Therefore, if there exists a stationary localized vibration of the type (26), i.e., a solution with the asymptotic expansion

$$u(x,t)=\sum_n A_n(\varepsilon,x)\cos n\omega t,\qquad \varepsilon=(1-\omega^2)^{1/2},$$

then simultaneously there also exist vibrations of the following form:

$$u(x,t)=\sum_n A_n\left(\varepsilon,\ \frac{x-vt}{(1-v^2)^{1/2}}\right)\cos n(\omega t-kx). \qquad (36)$$

where $v = k/\omega$ and $\epsilon^2 = 1 + k^2 - \omega^2$. The function (36) is a solution of the initial equation for $v < 1$; however, the equation itself was obtained by us to describe long-wave vibrations and, therefore, it must be remembered that $v = k/\omega \ll 1$, and so $1 - v^2 \approx 1$.

The solution (36) has the form of a wave-packet of width $\Delta x \sim 1/\epsilon$, moving with a velocity which coincides with the group velocity $v = \partial\omega/\partial k$ corresponding to the dispersion law (7). A remarkable property of this packet is the fact that it does not spread as a consequence of the dispersion of the waves, although its motion is itself due to this dispersion.

3. SELF-LOCALIZED VIBRATIONS WITH FREQUENCIES NEAR THE UPPER EDGE OF THE SPECTRUM

We have considered self-localized vibrations with frequencies lying below the frequencies of the corresponding waves in the harmonic approximation. The condition for their existence was the fulfilment of certain inequalities relating the coefficients of the nonlinear terms in the expansion of f(u): $\beta > 0$ in (5) or $\beta > 10\alpha^2/9$ in (4). However, it is known from the theory of local vibrations in the harmonic approximation[4] that if for one sign of the perturbation in a one-dimensional system local frequencies appear below the band of frequencies of the unperturbed chain, for the opposite sign they appear above the frequency-band of the ideal system. We should expect, therefore, that when other inequalities relating α and β are fulfilled, self-localized vibrations with frequencies $\omega > \omega_m$, where ω_m is the maximum frequency of harmonic vibrations of the chain of atoms, may turn out to be possible. We recall that it follows from (2) that $\omega_m = (1 + 4b^2)^{1/2}$.

Again, we start the analysis of such vibrations from the simplest case, when $f(u) = -u + \beta u^3$, but $\beta < 0$. Then Eq. (1) for the vibrations of the chain has the form

$$\frac{d^2u_n}{dt^2}+b^2(2u_n-u_{n+1}-u_{n-1})+u_n-\beta u_n^3=0. \tag{37}$$

We shall be interested in vibrations with frequencies $\omega > \omega_m$ such that $\omega - \omega_m \ll \omega_m$. Then the displacements are conveniently written in the form $u_n = v_n \cos \pi n$, where the quantity $v_n(t)$ is a slowly-varying function of the label n and can be regarded as a continuous function of the coordinate x: $v_n(t) = v(x, t)$. Therefore, by writing (37) in terms of v_n, we can replace it approximately by the following differential equation in partial derivatives:

$$\frac{\partial^2 v}{\partial t^2}+\frac{\partial^2 v}{\partial x^2}+\omega_m^2 v-\beta v^3=0, \tag{38}$$

where x, as in Sec. 1, is measured in units of $ba = \kappa a/\omega_0$.

It is easy to see that for $\omega > \omega_m$ with $\beta > 0$ Eq. (38) is analogous to Eq. (5) for $\omega < \omega_0$ with $\beta > 0$. Therefore, it has a solution of the self-localized vibration type, similar to (26). The amplitude and degree of localization of these vibrations are determined by the parameter

$$\varepsilon=(\omega^2-\omega_m^2)^{1/2}. \tag{39}$$

The leading term in the expansion of the solution of (38) in ϵ coincides with the leading term of the expansion (26), if for ϵ we take its new value (39).

It is somewhat more complicated to find a solution for the high-frequency localized vibrations in the case when the force f(u) contains both odd and even terms in u, i.e., has the form (4) with $\alpha \neq 0$. We write the equation of the vibrations in this case:

$$\frac{d^2u_n}{dt^2}+b^2(2u_n-u_{n+1}-u_{n-1})+u_n-\alpha u_n^2-\beta u_n^3=0. \tag{40}$$

It is now found that although, as before, the displacements of neighboring atoms are almost opposite in phase, their magnitudes are different because of the asymmetry of the external potential with respect to the direction of displacement of the atom. Therefore, the solution of Eq. (40) must be sought in the form

$$u_n=v_n\cdot\cos\pi n,\quad n=2m,$$
$$u_n=w_n\cdot\cos\pi n,\quad n=2m+1, \tag{41}$$

where v_n and w_n can be regarded as slowly-varying functions of the label n. In the long-wave approximation the following system of equations is obtained for v(x, t) and w(x, t):

$$\frac{\partial^2 v}{\partial t^2}+\frac{\partial^2 w}{\partial x^2}+(1+2b^2)v+2b^2w-\alpha v^2-\beta v^3=0,$$
$$\frac{\partial^2 w}{\partial t^2}+\frac{\partial^2 v}{\partial x^2}+(1+2b^2)w+2b^2v+\alpha w^2-\beta w^3=0. \tag{42}$$

Since in Eq. (40) we have confined ourselves to cubic terms in u, we shall seek the solution of the system (42) to terms of order ϵ^2 inclusive. This solution has the following form:

$$v=\left(\frac{8}{3\eta}\right)^{1/2}\frac{\varepsilon\cos\omega t}{\operatorname{ch}\varepsilon x}+\frac{4\alpha}{3\eta}\frac{\varepsilon^2}{\operatorname{ch}^2\varepsilon x}\left(1-\frac{\cos 2\omega t}{1-4\omega_m^2}\right),$$
$$w=\left(\frac{8}{3\eta}\right)^{1/2}\frac{\varepsilon\cos\omega t}{\operatorname{ch}\varepsilon x}-\frac{4\alpha}{3\eta}\frac{\varepsilon^2}{\operatorname{ch}^2\varepsilon x}\left(1-\frac{\cos 2\omega t}{1-4\omega_m^2}\right); \tag{43}$$
$$\eta=-\beta-\frac{6-16\omega_m^2}{3-12\omega_m^2}\alpha^2.$$

It follows from (43) that localized vibrations near the upper edge of the spectrum exist only for $\eta > 0$, i.e., for

$$\beta<-\frac{6-16\omega_m^2}{3-12\omega_m^2}\alpha^2.$$

In conclusion, we shall discuss the question of the effect of anharmonicity in the interaction of the atoms of the chain with each other on the problem of the appearance of self-localized vibrations with frequencies $\omega > \omega_m$. We denote the anharmonic correction to the interaction energy of the atoms by W:

$$W=\frac{1}{3}\Lambda\sum_n(u_n-u_{n-1})^3+\frac{1}{4}M\sum_n(u_n-u_{n-1})^4. \tag{44}$$

Being interested in the role of this nonlinearity, we shall omit the force associated with the external potential U(u), i.e., we shall consider the acoustic vibrations of the chain. Then in place of (1) we obtain the following equation for the vibrations:

$$\frac{d^2u_n}{dt^2}+(2u_n-u_{n+1}-u_{n-1})\{1+\lambda(u_{n+1}-u_{n-1})$$
$$+\mu(u_{n+1}-u_{n-1})^2+\mu(u_n-u_{n+1})(u_n-u_{n-1})\}=0, \tag{45}$$

in which the time is measured in units of $2/\omega_m$ where ω_m is the maximum frequency of the acoustic band in the harmonic approximation, $\lambda = 4a\Lambda/m\omega_m^2$ and $\mu = 4a^2M/m\omega_m^2$. Introducing the new variables v_n and w_n by formula (41), we can obtain for them a system of two differential equations in partial derivatives. However, the explicit form of Eq. (45) leads to the conclusion that it is more convenient to introduce other variables, namely,

$$\chi=v+w,\quad \psi=v-w.$$

Bearing in mind the definition (41), it is easily seen that χ is the difference in the displacements of two neighboring atoms, while ψ defines twice the displacement of the center of gravity of the two neighboring atoms. The system of equations for the new variables χ and ψ has the form

$$\frac{\partial^2\chi}{\partial t^2}+\frac{\partial^2\chi}{\partial x^2}+4\chi-4\lambda\chi\frac{\partial\psi}{\partial x}+4\mu\chi^3=0,$$
$$\frac{\partial^2\psi}{\partial t^2}-\frac{\partial^2\psi}{\partial x^2}+4\lambda\chi\frac{\partial\chi}{\partial x}=0, \tag{46}$$

where both the displacements χ and ψ and the coordinate x are measured in units of a.

The small parameter that makes it possible to formulate a method for constructing the asymptotic solution of this system is, as before, the amplitude of the localized vibrations, which is determined by the same parameter $\epsilon = (\omega^2 - \omega_m^2)^{1/2}$. In the leading approximation in this parameter we obtain

$$\chi=\sqrt{\sigma}\frac{\varepsilon\cos\omega t}{\operatorname{ch}\varepsilon x},\qquad \psi=\lambda\sigma\varepsilon\operatorname{th}\varepsilon x, \tag{47}$$

where $\sigma = 2/(3\mu - 4\lambda^2)$. It can be seen that such a solution exists only for $\sigma > 0$, i.e., when the inequality $\mu > 4\lambda^2/3$ is fulfilled. An interesting feature of the vibrations (47) is the fact that

$$u(+\infty)=-{}^1/_2\lambda\sigma\varepsilon,\qquad u(-\infty)={}^1/_2\lambda\sigma\varepsilon. \tag{48}$$

Thus, in the presence of a nonlinear localized vibration a statistical elongation $\delta u = u(\infty) - u(-\infty) = \lambda\sigma\epsilon$ arises in the chain, i.e., the chain is found to be extended for $\lambda < 0$ or compressed for $\lambda > 0$. The static deformation induced by this elongation is concentrated in the region $\Delta x \sim 1/\epsilon$ in which the vibration itself is localized. Naturally, this effect occurs only for $\lambda \neq 0$, i.e., when the potential W is nonsymmetric with respect to the direction of the mutual displacement of the atoms.

As before, it is natural to seek the asymptotic solution of Eq. (45) in the form of an expansion in powers of ϵ to terms of order ϵ^2 inclusive:

$$\chi=\sqrt{\sigma}\frac{\varepsilon}{\operatorname{ch}\varepsilon x}\left[\left\{1-\frac{\varepsilon^2\sigma}{8}\left\langle\left(\lambda^2+\frac{\mu^2\sigma}{4}\right)-\left(\lambda^2+\frac{\mu^2\sigma}{8}\right)\frac{1}{\operatorname{ch}^2\varepsilon x}\right\rangle\right\}\cos\omega t+\frac{\mu\sigma}{32}\frac{\varepsilon^2}{\operatorname{ch}^2\varepsilon x}\cos 3\omega t\right],$$
$$\psi=\lambda\sigma\varepsilon\operatorname{th}\varepsilon x\left[1-\frac{\varepsilon^2\sigma}{4}\left\langle\left(\frac{5\lambda^2}{2}+\frac{\mu^2\sigma}{3}\right)+\frac{1}{3}\left(\lambda^2+\frac{\mu^2\sigma}{8}\right)\frac{1}{\operatorname{ch}^2\varepsilon x}\right\rangle-\frac{1}{3}\frac{\varepsilon^2}{\operatorname{ch}^2\varepsilon x}\cos 2\omega t\right]. \tag{49}$$

The method of obtaining the solution (49) and its structure are such as to enable us in principle to take simultaneous account both of anharmonicity in the interaction of the atoms in the chain and of an anharmonic external potential U(u). In view of the cumbersome form of the corresponding expressions, we see no need to cite the results for this case.

We note that the presence of self-localized characteristic vibrations of the type (49) can influence the character of the local vibrations in a one-dimensional chain with point defects, if the corresponding frequencies lie near an edge of the frequency spectrum in the harmonic approximation. In addition, it may turn out that kinetic phenomena in a one-dimensional chain that admits stable localized characteristic vibrations are described more conveniently in terms of the dynamics of such moving structures than in terms of scattering of ordinary phonons.

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[1)]In contrast to the preceding case, to find the solution exact to order ϵ^2 it now turns out to be sufficient to keep terms up to u^3 inclusive in the expansion for the force.

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194