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# NONLINEAR LOCALIZATION OF ULTRASONIC WAVES IN MEDIA WITH THE MICROSTRUCTURE

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*The chain consisting of particles is considered, each of which has an internal degree of freedom. Transfer of excitation from one particle to another occurs on account of interatomic and dipole-dipole interactions. It is shown that localized wave trains can be excited in it and their parameters are determined. The obtained information can be used for exposition of an anharmonicity influence on oscillatory excitations transmission in long molecules.*

Elastic chains are the popular object for study of nonlinear dynamics in physics and mechanics. Despite of the simplicity, they make clear the physical nature of the composite phenomena in media with microstructure. One of such effects is existence of the standing or running nonlinear localized modes – envelop-solitons which frequency lies in the forbidden area of a spectrum of the linear oscillations [1-6].

In the work the one-dimensional chain consisting of particles-molecules is considered. Each of particles has an internal oscillatory degree of freedom. Transfer of oscillatory excitation from one molecule to another is carried out due to internuclear and a dipole of interactions [4, 7]. The interaction potential depends linearly on value of the dipole moment of each interacting molecule and rapidly decreases with distance that allows taking advantage of approximation of the nearest neighbours. With account of mentioned above one can write down Lagrangian of dipoles chains as

$$L = \sum_n \left\{ \frac{m}{2}\left(\dot{x}_n^2 - \omega_0^2 x_n^2 + \beta x_n^4\right) + Q x_n x_{n+1} \right\} \qquad (1)$$

Here $x_n$ is length of a dipole, $m$ is effective mass of an oscillatory degree of freedom, $Q$ is a constant of dipole-dipole interaction which is plus if the dipole moments are excited along a line pairing them. At the negative $Q$ all results stated below remain valid if to rename variable: $x_n \to (-1)^n x_n$. Equations of motion for a Lagrangian (1) are

$$\frac{d^2 x_n}{dt^2} + \omega_0^2 x_n - 2\beta x_n^3 - Q\left(x_{n+1} + x_{n-1}\right) = 0\,. \qquad (2)$$

Further we shall use dimensionless quantities $x_n = r_0 b_n$, $\tau = \omega_0 t$. For the dimensionless variable we shall receive the equation

$$\frac{d^2 b_n}{d\tau^2} + b_n - q\left(b_{n+1} - b_{n-1}\right) - 4 g b_n^3/3 = 0\,, \qquad (3)$$

where the following labels $q = Q/m\omega_0^2$, $g = 3\beta r_0^2/m\omega_0^2$ are entered. Continual analog (3) is the equation

$$\frac{\partial^2 b}{\partial \tau^2} - q\frac{\partial^2 b}{\partial n^2} + (1-2q)b - 4 g b^3/3 = 0\,. \qquad (4)$$

The equation (4) has the solution as a solitary wave (kink) [8]

$$b(n,\tau) = \pm(2/\kappa)^{1/2}\sec\left[\theta(n - \upsilon\tau)\right],$$

where υ is the kink's velocity, $\theta = \Omega_0\left(q - \upsilon^2\right)$ is the kink's inverse width, $\kappa = 4g/3\Omega_0^2$, $\Omega_0^2 = 1 - 2q$. Such wave is unstable under small perturbations and collapses at collisions with other solitary wave.

## Quasiharmonic approach

Oscillations of molecules are almost harmonic ones for weak nonlinearity and dispersion:

$$b_n(\tau) = 0{,}5\left[a_n(\tau)e^{-i\Omega\tau} + c.c\right], \qquad (5)$$

where Ω is frequency, $a_n(\tau)$ is complex amplitude of *n-th* molecule's vibration. Substitution of (5) into (2) and neglecting non-resonant terms lead to the following equation

$$\frac{d^2 a_n}{d\tau^2} - 2ia_n + \left(1-\Omega^2\right)a_n - q\left(a_{n+1} + a_{n-1}\right) - g\left|a_n\right|^2 a_n = 0 \tag{6}$$

As we shall be interested excitations, enveloping some the next molecules, we shall take advantage of continual approach

$$a_{n\pm1} \approx \exp\left[ik(n\pm1)\right]\left(A \pm \frac{\partial A}{\partial n} + 0{,}5\frac{\partial^2 A}{\partial n^2}\right)$$

Here $A(n,\tau)$ is slowly varying with the number $n$ a real-valued function, depending on one "running" variable $\xi = n - n_0 - \upsilon\tau$. In this case we shall receive from (6)

$$\left(q\cos k - \upsilon^2\right)\frac{d^2 A}{d\xi^2} + \left(\Omega^2 - 1 + 2q\cos k - gA^2\right)A = 0 \tag{7}$$

where $\upsilon = q\Omega^{-1}\sin k$ is velocity of a wave train. Quantities $\xi$ and $A$ are playing role of time and coordinates of an "imaginary" particle with mass $m^* = q\cos k - \upsilon^2$. In this sense the equation (7) describe its motion under forces with potential

$$U(A) = gA^4/4 - \left(1 - 2q\cos k - \Omega^2\right)A^2/2$$

The solution satisfying a condition of localization $A(\xi) \to 0$ at $|\xi| \to \infty$; exists only at $\Omega^2 < 1 - 2q\cos k$, when the potential has two stable positions, separated by a maximum (fig. 1).

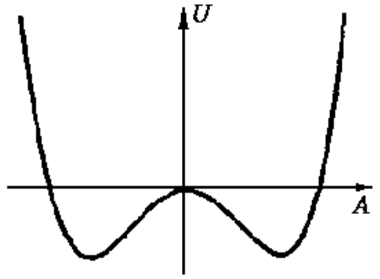


*Fig. 1.*

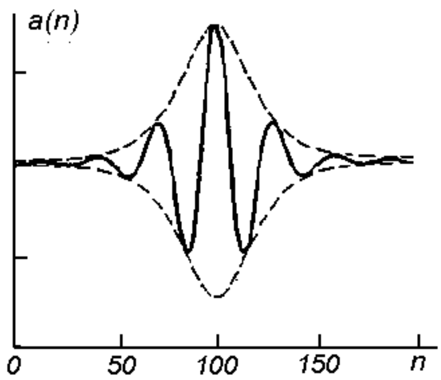


*Fig. 2.*

It is described by two-parametrical expression:

$$A = A_0 \sec \theta\xi \;,$$

and refers as *envelope soliton* [8]. Depending the frequency Ω and wave number $k$ versus amplitude $A_0$ and inverse width $\theta$ of envelope soliton looks like [4]:

$$\Omega^2 = 1 - 2q\cos k - gA_0^2/2\,, \qquad \theta^2 = gA_0^2/2\left(q\cos k - \upsilon^2\right). \tag{8}$$

For complex amplitudes we have the next expression (fig. 2)

$$a_n(\tau) = A_0 \exp\left[ikn + i\delta\right]\sec\left[\left(n - n_0 + \upsilon\tau\right)\theta\right] \tag{9}$$

in which $n_0$, δ are the initial position and phase of soliton. The wave number accepts values from 0 up to 2π, and $k$ and $2\pi - k$ corresponds to the waves traveling in opposite directions. Hence, it is enough to consider interval $0 \le k < \pi$. The real values $\theta$ are possible at $0 \le k < \pi/2$, and the real values Ω are possible at amplitudes, smaller critical $A_{max} \sim g^{-1/2}$ At large amplitudes $A_0 \sim A_{max}$ become essential non-resonant terms rejected in (6). Note, that the solution (9) is valid if $k$ is not close to π/2. It is caused by a requirement of applicability of continual approximation. Stationary value

$$N_0 = 0{,}5\sum_n \left|a_n\right|^2 \approx \int_{-\infty}^{\infty} 0{,}5\left|a_n\right|^2 dn$$

is meaningful the complete number of "quantums" of oscillations excited in a chain and accepts the whole positive number. This requirement can be viewed as normalization leading to the following relation between width and amplitude of the soliton:

$$A_0^2 = N_0\theta \quad (10)$$

If the value $N_0$ is set, the envelope soliton is characterized by only one parameter – wave number *k*. If the wave number grows, the soliton's width decreases, while its amplitude and velocity increase. For frequency validly approximate (at $N_0 g < q\cos k << 1$) expression

$$\Omega = 1 - q\cos k - g^2 N_0^2 / 8q\cos k\,, \quad (11)$$

which plays a role of the nonlinear dispersion equation. Spectrums of the linear waves *(g=0)* and envelope solitons at $g$=0,005, $q$=0,01 and $N_0$ =1,2,3 are represented in fig. 3. For all values of a wave number they parted by a "energy" gap, and solitons implement energy more favourable state of a chain.

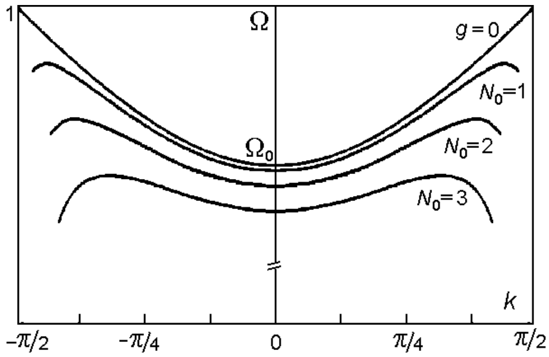


***Fig. 3.***

*Effects of an anharmonicity*. At large amplitudes of excitation the anharmonicity of the molecular oscillations predominates above dipole - dipole interaction and becomes the main process driving dynamics of oscillatory excitations [9]. For small values of constants *q* and *g* there is an area of amplitudes at which expression (1) is still valid, but continual approach is impossible. In this case practically all excitation is focused on one molecule and reminds itself a standing breather [10]. Due to big distinction of vibration amplitudes of neighbours, the frequencies of their oscillations strongly differ. As a result, the dipole-dipole interaction becomes non-resonant and does not provide transfer of excitation along the chain.

**The slow-moving localized excitations**

In the previous section the nonlinear law of dispersion for envelope solitons has been obtained and areas of wave numbers for which they can exist in a discrete chain are indicated. In practice the majority of initial perturbations is smooth enough that corresponds to small values *k*. In this case, we shall carry out more detailed analysis of a problem.

Let's compare real quantities $b_n(\tau)$ with the complex amplitudes $a_n(\tau)$

$$b_n = 0{,}5\left(a_n + a_n^*\right), \quad \frac{db_n}{d\tau} = -0{,}5i\left(a_n - a_n^*\right). \quad (12)$$

In this variables $a_n$ satisfy the conditions

$$\frac{da_n}{d\tau} + \frac{da_n^*}{d\tau} = -i\left(a_n - a_n^*\right). \quad (13)$$

Substitution of (1.12) into (1.3) with account of (1.13) yields

$$i\frac{da_n}{d\tau} - a_n + 0{,}5q\left(a_{n+1} + a_{n-1} + c.c\right) + 1/6\,g\left(a_n^3 + 3\left|a_n\right|^2 a_n + c.c\right) = 0 \quad (14)$$

At $q=g=0$ the function $a_n(\tau)=a_n(0)\exp(-i\tau)$ is fast oscillating. It allows us at $q<<1$ and $g|a_n|^2<<1$ to separate the slow and fast motions and to pass from complete equations (14) to the reduced equations

$$2\left(i\frac{da_n}{d\tau} - a_n\right) + q\left(a_{n+1} + a_{n-1}\right) + g\left|a_n\right|^2 a_n = 0\,. \quad (15)$$

At small velocities of solitons ($k$<<1) the amplitude $a_n$ slowly varies from molecule to molecule. In this case it is possible to put

$$a_{n\pm 1} \approx a_n \pm \partial a_n / \partial n + 0{,}5 \partial^2 a_n / \partial n^2 ,$$

that after substitution

$$a_n(\tau) = \exp[-i(1-q)\tau]\Psi(n,\tau)$$

reduces equation (15) to nonlinear Schrodinger equation (NLS) [8]:

$$2i\frac{\partial \Psi}{\partial \tau} + q\frac{\partial^2 \Psi}{\partial n^2} + g|\Psi|^2 \Psi = 0 . \qquad (16)$$

Soliton solution NLS looks like $A = A_0 \sec \theta\xi$ at $\upsilon = qk$ and

$$2q\theta^2 = gA_0^2, \quad \Omega = 1 - q + qk^2/2 - gA_0^2/4 .$$

The same expressions can be received immediately from (8) at the approaches made above.

Nonlinear Schrodinger equation well describes at small values $k$ oscillations on a basic frequency. The exact solution of the equation (3) contains oscillations of all harmonics that are divisible by the basic frequency. However presence of harmonics does not destroy nonlinear wave packet. This fact can be illustrated by analogy of the localized excitations, which are described by equation (3) with the breather excitations in the sine-Gordon equation [8].

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