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Reprint of Nonlinear vector waves of a flexural mode in a chain model of atomic particles ☆

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ABSTRACT

Flexural transverse waves in an anharmonic chain of atoms is considered and the nonlinear vector equation for the phonon modes in the long-wave approximation is derived taking into account the weak dispersion effects. Particular cases of the equation derived are discussed; among them the vector mKdV equation (Gorbacheva and Ostrovsky, 1983) [12], as well as the new model vector equations dubbed here the 'second order cubic Benjamin–Ono (socBO) equation' and 'nonlinear pseudo-diffusion equation'. Stationary solutions to the equation derived are studied and it is found in which cases physically reasonable periodic and solitary type solutions may exist. The simplest non-stationary interactions of solitary waves of different polarisation are studied by means of numerical simulation. A new interesting phenomenon is revealed when two solitons of the same or opposite polarities interact elastically, whereas the interaction of two solitons lying initially in the perpendicular planes is essentially inelastic resulting in the survival of only one soliton and destruction of another one.

1. Introduction

In spite of intensive study of anharmonic chains and lattices in last decades (see, e.g., [21,25,4,27,18,26] and many, many others), the theory of such discrete structures remains very topical due to their numerous applications in theoretical physics (theory of crystal heat transport, termalization in a set of coupled oscillators [10,29]), molecular physics (transport of excitations in long spiral molecules [7,6]), X-ray spectroscopy [3], ultrasound diagnostics of solids, etc. Anharmonic chains and lattices are also studied in application to electric transmission lines ([29]) and even in dusty plasma [11,9].

In the majority of cases either longitudinal modes or mixed longitudinal and transverse modes were studied thus far. In the one-dimensional case in application to a chain of atoms the equation of motion for longitudinal modes is scalar describing atom vibrations in the direction of wave propagation (see, e.g., [10,29]). However, when the transverse modes are considered (see Fig. 1), the equation of motion becomes vector [12,8] describing particle displacements in two perpendicular

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directions transverse to the direction of wave propagation. In both these cases of longitudinal and transverse vibrations the dispersion law of phonon (acoustic) modes in the long-wave approximation is linear, $\omega \sim k$, where ω is the wave frequency and k is the wave number of infinitesimal amplitude perturbations. In the meantime, it is a matter of experimental fact that in many cases the transverse flexural modes in crystals demonstrate the quadratic dispersion law in the long-wave approximation, $\omega \sim k^2$. The quadratic dispersion law is typical for anisotropic crystals with strong difference between the inlayer and interlayer forces; for example, for the graphite (C) see Fig. 2 from [24].

Lifshitz in his pioneering work [20] pointed out at the importance of the quadratic dispersion law for strongly anisotropic crystals and suggested a simplified model for the description of flexural modes in crystal layers by analogy with the vibrations of elastic thin plate. Similar model is applicable for the flexural modes in the chain of atoms when particles interact not only with the nearest neighbours, but also with the next two, at least [3,27].

In what follows we consider flexural transverse waves in an anharmonic chain of atoms and derive the nonlinear vector equation for phonon modes in the long-wave approximation taking into account weak dispersion. Then we analyse the particular cases of the equation derived, study its stationary solutions and simplest interactions of solitary waves of different polarisation.

2. Derivation of the vector equation

Consider the chain of equal mass atoms shown in Fig. 1. The equation of motion for the atom with number n can be written as

$$m\frac{d^2\xi_n}{dt^2} = \mathbf{F}_{n-2} + \mathbf{F}_{n-1} + \mathbf{F}_{n+1} + \mathbf{F}_{n+2}, \tag{2.1}$$

where m is the mass of each atom; $\xi_n = (y_n, z_n)$ is the two-component transverse displacement vector with the y- and z-components orthogonal to the axis x, the axis along which perturbations propagate; and $\mathbf{F}_n$ are transverse forces exerting on the nth atom of the chain from its nearest and next neighbours.Following the approach used in the paper [12], let us write down the transverse force exerting on the atom in the form

$$F_{n\pm j} = \pm\beta_j\left[T + jaK\left(\frac{1}{\cos\alpha_{n\pm j}} - 1\right)\right]\sin\alpha_{n\pm j}, \tag{2.2}$$

where β_j are some coefficients which characterise the strength of the corresponding force, $T > 0$ is the uniform tension of the chain (which is balanced by interaction forces acting between the particles), $K > 0$ is Hooke's constant, α_n is the local angle between the chain and axis x, $j = 1$ for the nearest two neighbouring atoms and $j = 2$ for the next two atoms. Without loss of generality, we can put $\beta_1 = 1$ which is presumed in what follows. Another coupling constant β_2 may be both positive and negative, but apparently, it cannot be less than $-1/2$ (see below).In the case of a plane polarisation when the displacement ξ has only one y component, the angle $\alpha_{n\pm j}$ can be expressed in terms of displacements: $\tan\alpha_{n\pm j} = \pm(y_{n\pm j} - y_n)/(ja)$. With the help of these expressions we can find then:

$$\sin\alpha_{n\pm j} = \frac{\tan\alpha_{n\pm j}}{\sqrt{1+\tan^2\alpha_{n\pm j}}} = \pm\frac{y_{n\pm j} - y_n}{\sqrt{(ja)^2 + (y_{n\pm j} - y_n)^2}}; \tag{2.3a}$$

$$\cos\alpha_{n\pm j} = \frac{1}{\sqrt{1+\tan^2\alpha_{n\pm j}}} = \frac{ja}{\sqrt{(ja)^2 + (y_{n\pm j} - y_n)^2}}. \tag{2.3b}$$

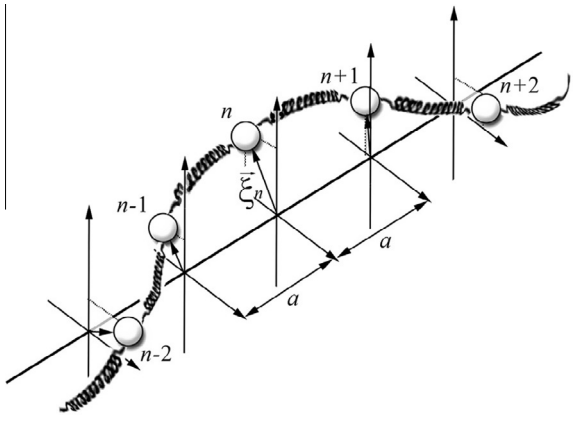

Fig. 1. Longitudinal and transverse oscillations of equal mass particles in an atomic chain.