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LONG-TIME EVOLUTION OF ACOUSTIC SIGNALS IN NONLINEAR CRYSTALS

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ABSTRACT

We show that the well posed continuous model representing the physically appropriate dispersion relation for a discrete lattice must contain higher-order derivatives in space. A strongly implicit conservative difference scheme is designed for solving the resulting generalized Boussinesq equation and the very-long-time evolution and multiple interactions of localized solutions are investigated. The calculations verify that the hump-shaped localized solutions of *sech*-type are solitons. However, for phase velocities that are not close enough to the characteristic velocity the *sechs* evolve into pulses of localized envelopes. Although the pulses are not stationary creatures, they can still be called solitons because the energy and pseudomomentum are perfectly conserved in the course of interaction.

In recent years a marked interest has developed among metallurgists, applied physicists and mathematicians for the continuous or discrete study of changes in the structure of martensitic alloys and ferroelastic materials. In the discrete description, we note the works [1],[2],[3] which consider initially a lattice dynamics approach in one space dimension accounting either for the principal shear deformation alone [1] or for both shear and longitudinal deformations [3], although the latter plays a secondary role only. Further works [4],[5] account in a more satisfactory way for the material symmetry typical of the phases of these materials and various types of interparticle interactions.

1. Posing the Problem

In terms of relative transverse displacements (shear) S_i of atoms in a lattice, the governing equation has the following form [3]:

$$\begin{aligned}\ddot{S}_i = \chi(S_{i+1} - 2S_i + S_{i+1}) + [F(S_{i+1}) - 2F(S_i) + F(S_{i-1})] \\ - \delta(S_{i+2} - 4S_{i+1} + 6S_i - 4S_{i-1} + S_{i-2}) \ ,\end{aligned} \tag{1}$$

where $F(S)$ is the particular nonlinearity of the problem. Respectively χ is proportional to the square of the characteristic speed in the crystal and δ controls the triple interactions. The Tailor-series for the strain in the vicinity of point x_i give

$$(S_{i+1} - 2S_i + S_{i-1}) = a^2 S_i'' + \frac{a^4}{12} S_i^{(4)} + \frac{a^6}{360} S_i^{(6)} + \frac{a^8}{20160} S_i^{(8)} + \frac{a^{10}}{1814400} S_i^{(10)}$$

$$(S_{i+2} - 4S_i + 6S_i - 4S_{i-1} + S_{i-2}) = a^4 S_i^{(4)} + \frac{a^6}{6} S_i^{(6)} + \frac{a^8}{80} S_i^{(8)} + \frac{17a^{10}}{30240} S_i^{(10)}$$

and hence

$$S_{tt} = a^2 \chi S_{x^2} + a^4 \left(\frac{\chi}{12} - \delta\right) S_{x^4} + a^6 \left(\frac{\chi}{360} - \frac{\delta}{6}\right) S_{x^6} + \dots . \quad (2)$$

It is clear that the fourth-order Generalized Wave Equation (GWE) would be proper iff $\delta > \frac{\chi}{12}$, which is hardly the practically important situation. It is the sixth-order GWE which is of practical interest since it is well-posed for $\delta < \frac{\chi}{60}$. The eight-order GWE is similar to the fourth-order one with the only difference that the limitation is not so restrictive, namely $\delta > \frac{\chi}{252}$, but still well above the practical range of parameters. The tenth-order GWE should be used only for very large δ since they are limited there only by $\frac{17\chi}{60}$. We content ourselves with the sixth-order GWE for which the coefficient before the fourth derivative is positive securing the physically acceptable curvature of the dispersion relation (see [3]). After re-scaling the variables, we arrive at the following equation for the transverse strain

$$u_{tt} = \gamma^2 u_{xx} + \frac{d^2 F(u)}{dx^2} - \beta u_{xxxx} + u_{xxxxxx} , \quad F(u) \equiv -\frac{dU(u)}{du} . \quad (3)$$

In what follows we call Eq.(3) Sixth-order Generlized Boussinesq (SGB – for brevity). The same equation was considered in [11] in a fluid dynamics context.

2. Pseudomomentum Formulation

Equation (1.10) is an obvious corollary of the following system

$$u_t = q_{xx} , \quad q_t = \gamma^2 u + F(u) - \beta w + w_{xx} , \quad w = u_{xx} . \quad (4)$$

Different kinds of boundary conditions (b.c. – for brevity) can be imposed. On a finite interval $[-L_1, L_2]$, however, the system (4) admits conservation laws, only for the following b.c.

$$u = 0 , \quad u_x = 0, \quad q_x = 0 \qquad \text{for} \qquad x = -L_1, L_2 , \quad (5)$$

Consider now the quantities

$$M \stackrel{\text{def}}{=} \int_{-L_1}^{L_2} u dx , \quad P \stackrel{\text{def}}{=} \int_{-L_1}^{L_2} u q_x dx , \quad E \stackrel{\text{def}}{=} \int_{-L_1}^{L_2} \frac{1}{2} [\gamma^2 u^2 + q_x^2 - 2U(u) + \beta u_x^2 + w^2] dx . \quad (6)$$

Upon an appropriate manipulation of system (4), integrating with respect to x and acknowledging the appropriate b.c from (5), one obtains the following conservation and balance laws (see the similar derivation in [6],[7] for the fourth-order BE):

$$\frac{dM}{dt} = 0 , \quad \frac{dP}{dt} = \frac{1}{2} [u_{xx}^2] \Big|_{-L_1}^{L_2} \equiv F , \quad \frac{dE}{dt} = 0 . \quad (7)$$

Here M has an obvious interpretation as the *mass* of wave. Following [8],[9] we call P *pseudomomentum*, and F – *pseudoforce*. Although in [8] a quantity similar to E is called energy, we prefer to use the safer coinage *pseudoenergy* because of the higher-order spatial derivatives.

In the present paper we consider only the case of quadratic nonlinearity $F(u) = -\alpha u^2$. However, any other kind of algebraic nonlinearity (cubic, quintic, etc.) can be treated in absolutely the same manner as in what follows.

3. Difference Scheme

Let us introduce a regular mesh $x_i = -L_1 + (i-1)h$, $h = (L_1 + L_2)/(N-1)$, where N is the total number of grid points. Following [7] we construct an implicit difference scheme which conserves *mass* and *pseudoenergy*.

$$\begin{aligned} \frac{q_i^{n,k} - q_i^n}{\tau} &= \gamma^2 \frac{u_i^{n,k} + u_i^n}{2} - \alpha \frac{u_i^{n,k} u_i^{n,k-1} + u_i^{n,k} u_i^n + (u_i^n)^2}{3} \\ &- \frac{\beta}{2}(w_i^{n,k} + w_i^n) + \frac{1}{2}\left[\frac{w_{i+1}^{n,k} - 2w_i^{n,k} + w_{i-1}^{n,k}}{h^2} + \frac{w_{i+1}^n - 2w_i^n + w_{i-1}^n}{h^2}\right] , \end{aligned} \quad (8)$$

$$\frac{u_i^{n,k} - u_i^n}{\tau} = \frac{1}{2}\left[\frac{q_{i+1}^{n,k} - 2q_i^{n,k} + q_{i-1}^{n,k}}{h^2} + \frac{q_{i+1}^n - 2q_i^n + q_{i-1}^n}{h^2}\right] , \quad (9)$$

$$w_i^{n,k} = \frac{u_{i+1}^{n,k} - 2u_i^{n,k} + u_{i-1}^{n,k}}{h^2} , \quad (10)$$

with b.c.

$$u_N^{n,k} = u_1^{n,k} = u_N^{n,k} - u_{N-1}^{n,k} = u_2^{n,k} - u_1^{n,k} = q_N^{n,k} - q_{N-1}^{n,k} = q_2^{n,k} - q_1^{n,k} = 0 . \quad (11)$$

The multidiagonal system is treated by the solver, developed in [10]. The "inner" iterations are conducted starting from the "initial" conditions $u_i^{n,0} = u_i^n$, $q_i^{n,0} = q_i^n$, and are terminated at a certain $k = K$ after the following criterion is satisfied $\max |u_i^{n,K} - u_i^{n,K-1}| \leq 10^{-11} \max |u_i^{n,K}|$. After the inner iterations have converged one obtains, in fact, the solution of the non-linear conservative difference scheme for the "new" time stage, namely $u_i^{n+1} \equiv u_i^{n,K}$.

Similarly to the way it is done in [7], it can be shown that appropriate difference approximations $\mathcal{M}, \mathcal{E}$ of the *mass* and *pseudoenergy* are conserved by the difference scheme (8)-(10) in the sense that $\mathcal{M}^{n+1} = \mathcal{M}^n$,and $\mathcal{E}^{n+1} = \mathcal{E}^n$. A conservative scheme is obviously stable if the inner iterations converge.

4. Results and Discussion

We set for definiteness $\alpha = -3, \gamma = 10$. Our first objective is the head-on collision of two *sechs*. It is easily verified that the analytical solution found in [11] for a FKdV is also a solution of SGB, namely

$$u = \frac{105}{169}\frac{\beta^2}{2\alpha}\mathrm{sech}^4\left(\frac{x}{2}\sqrt{\frac{\beta}{13}}\right), \qquad \text{and } |c| = \sqrt{\gamma^2 - \frac{36}{169}\beta^2}, \tag{12}$$

where c is the phase velocity or *celerity* of the wave. The above solution exists only for positive β.

In *Fig*.1 is presented the head-on collision of two *sechs*. The soliton interaction is perfectly elastic and the difference approximations $\mathcal{M}$ and $\mathcal{E}$, are conserved in these numerical experiments with an accuracy of 10^{-11}, i.e., within the round-off error of the computer. For the difference approximation of the balance law scaled by the maximum of the solution we obtain quantity of order of 10^{-12}.

An important feature of the *sechs* is that they appear to be stable only when propagating almost with the characteristic speed, namely when $0.995\gamma \le |c| < \gamma$. This kind of limited structural stability was already discovered in [7] for the "usual" Boussinesq equation. In *Fig*.2 we present the long-time evolution of a *sech* At the beginning it evolves into a pulse with wavy fore-runner of relatively low intensity. Gradually, the fore-runner forms an individual *pulse* propagating with the characteristic speed and breaks away from the *sech*-like reminder which is marginally slower. The celerity of the latter is defined by (12) for $\beta = 5$.

In the case $\beta < 0$, the *sechs* are never stationary. Even if their celerities are very close to characteristic speed, they are not able to preserve their shapes and eventually transform into pulses. In *Fig*.3 is presented a typical case. One sees that the amplitude of the *pulse* decreases with time while its support increases ("red shift"). This self-similar (we call it also "Big-Bang") behaviour of the pulses was observed in our previous calculations [12] for the case of cubic-quintic nonlinearity of fourth-order BE. The "Big-Bang" behaviour can also be traced back to the relevant numerical calculations for KdV (see, the works referred in [13], [14]). Here is to be mentioned that the basin of attraction of *pulse* solution appears to be much larger than the basin of attraction of *sechs*. The latter means that in the experiments one is to expect *pulses* rather than *sechs*.

The limited space does not allow us to present here a picture, but we can say that in the course of interaction the *pulses* pass through each other without changing qualitatively their shapes (save the red-shifting) and the *mass* and *pseudoenergy* of the system of *pulses* are perfectly conserved. This sufficeS to claim that the *pulses* are also solitons in the strict sense.

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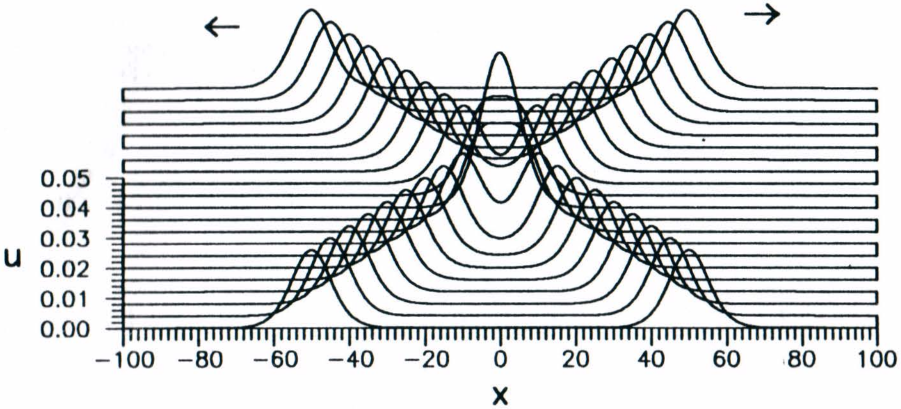

Fig.1 γ=10; β=0.5; τ=0.05; h=0.2; Δt=0.2

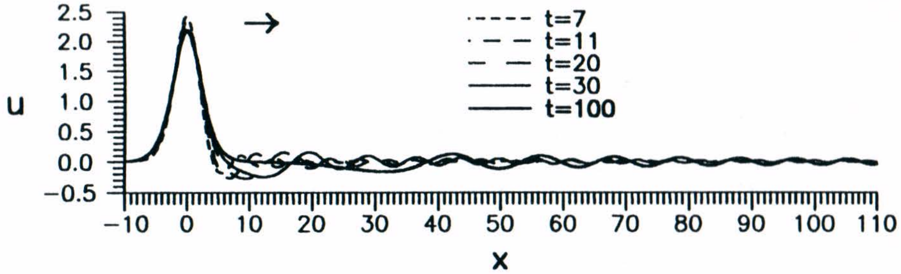

Fig.2 γ=10; β=10(5); h=0.15; τ=0.02

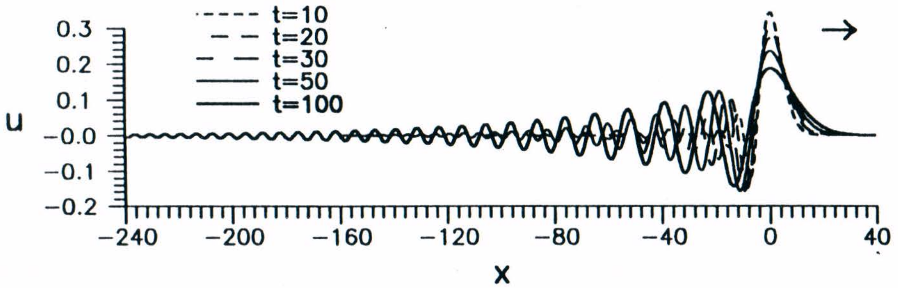

Fig.3 γ=10; β=−2; h=0.2; τ=0.1