Numerics of Some Generalized Models of Lattice Dynamics

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A generalized Boussinesq system arising in modelling martensitic alloys is considered. The main equation for the shear-strain component contains both cubic and quintic nonlinearities. The so-called "improved" version of the Boussinesq equation is adopted which allows investigation of super-light solitons. The Hamiltonian formulation of the system is obtained and balance laws for the *mass*, *pseudoenergy* and *pseudomomentum* associated with the solution are derived. The evolution and interaction of systems of solitary waves of *sech* type are tracked numerically by means of a fully implicit difference scheme faithfully representing the balance laws. The *sech* solitons preserve their identities (shapes) in the course of interaction and reemerge virtually unchanged, but the collisions are strongly inelastic exhibiting considerable phase shift and a residual signal of amplitude commensurable with the amplitudes of the incident *seches*. This signal is much more intensive for head-on collisions than for the taking-over ones.

INTRODUCTION

In recent years the study of changes in the structure of martensitic alloys and ferroelastic materials has been intensivelly studied. In the discrete description we note the works [P1],[M1],[MC1] which consider initially a lattice dynamics approach in one space dimension accounting either for the principal shear deformation alone [P1] or for both shear and longitudinal deformations [MC1], although the latter plays a secondary role only. Further works [P2],[P3] account in a more satisfactory way for the material symmetry typical of the phases of these materials and various types of interparticle interactions. However, here we shall content ourselves with the model of [MC1] which, though less elaborate, seems to present a rich dynamical behaviour.

Contrary to common models of nonlinear crystals with weakly nonlocal interactions for which the classical Boussinesq equation for the longitudinal elastic displacement appears to play a fundamental role, in the present case the system resulting from the continuum limit couples a modified Boussinesq equation for a shear strain to a linear wave equation for the longitudinal one. The complete system is conveniently referred to as a generalized Boussinesq system (GBS, for brevity). The "modified" feature comes from the higher-order nonlinearity needed to reproduce the typical ferroelastic behaviour.

These equations were shown in [MC1] to possess solitary wave solutions of various types that are supposed to represent several of the structures existing in real materials (solitons on austenite, and on martenite, kinks between martensitic twins). The conditions of existence of these solitary waves in terms of material parameters and their amplitude were established. The solitonic behaviour of these solutions, however, can only be demonstrated numerically because of the very structure of the high nonlinearity of the system considered here.

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POSING THE PROBLEM

Consider the one- dimensional model of an atomic chain in which the longitudinal displacements x_n couple to the shear strain. Denoting the transverse displacement by y_n the Lagrangian adopts the form (see [3] for details).

$$L = \sum_{i=2}^{N-1} \left[\frac{m}{2}(\dot{x}_i^2 + \dot{y}_i^2) + \frac{1}{2}A(y_{i+1} - y_i)^2 \right. \quad (1)$$

$$-\frac{1}{4}B(y_{i+1} - y_i)^4 + \frac{1}{6}C(y_{i+1} - y_n)^6$$

$$+\frac{1}{2}E(x_{i+1} - x_i)^2 - F(x_{i+1} - x_i)(y_{i+1} - y_i)$$

$$\left. + \frac{1}{2}D(y_{i+1} - 2y_i + y_{i-1})^2 \right] .$$

The variables can be rendered dimensionless according to the scheme

$$L = \frac{B^3}{C^2}L, \tau = \sqrt{\frac{B^2}{mc}}t, (x_i, y_i) = \sqrt{\frac{B}{C}}(u_i, v_i). \quad (2)$$

Upon introducing the relative displacements

$$S_i \equiv v_{i+1} - v_i \;, \;\; T_i \equiv u_{i+1} - u_i \;, \quad (3)$$

the Euler-Lagrange equations resulting from the variation of (1) read

$$\ddot{S}_i = c_T^2(S_{i+1} - 2S_i + S_{i+1}) -$$

$$(S_{i+1}^3 - 2S_i^3 + S_{i-1}^3) + (S_{i+1}^5 - 2S_i^5 + S_{i-1}^5)$$

$$-\chi(S_{i+2} - 4S_{i+1} + 6S_i - 4S_{i-1} + S_{i-2})$$

$$-2\gamma(S_{i+1}T_{i+1} - 2S_iT_i + S_{i-1}T_{i-1}), \quad (4)$$

$$\ddot{T}_i = c_L^2(T_{i+1} - 2T_i + T_{i-1}) - \gamma(S_{i+1}^2 - 2S_i^2 + S_{i-1}^2), \quad (5)$$

where c_T, c_L, χ, γ are dimensionless combination of the original paremeters A, B, C, D, E, F. The continuum limit of system (4),(5) adopts the form ([MC1])

$$S_{tt} = c_T^2 S_{xx} - (S^3)_{xx} + (S^5)_{xx}$$

$$+\alpha S_{xxxx} - 2\gamma(ST)_{xx} \;, \quad (6)$$

$$T_{tt} = c_L^2 T_{xx} - \gamma(S^2)_{xx} \;. \quad (7)$$

The differential form hints at the the name "generalized Boussinesq system" for the system, because it contains a generalized equation (7) in the sense of involving more complicated nonlinearities than the original Boussinesq equation.

The coefficient α contains contributions from the three-point difference and from the five-point one which contributions are of opposite signs. In the physically important cases the contribution from the three-point difference dominates (see, e.g., [CM2]) and hence $\alpha > 0$. It is known that the Boussinesq equation with positive coefficient of the fourth derivative is instable with respect to linear disturbances (short-wave instability) and cannot be solved directly. It only can be considered as a certain heuristic truncation of an equation of infinite order with respect to the spatial derivative. One of the ways to tackle the ill-posedness of the mathematical problem is to retain some of the higher-order derivatives (See [CM2]). The other way around is to use the so-called "improved" equation in which the fourth-order spatial derivative is replaced by a fourth-order mixed derivative. This is known in the theory of shallow fluid layers as RLW (Regularized Long-Wave equations) and has been succesfully used in computation of the so-called undular bore by Peregrine [PE1]. In solid mechanics it was employed in [B1],[I1]. There are differnt ways to justify the RLW assumption (see, e.g. [B1]) but all of them are more or less heuristic arguments. The simplest argument is just to express the second spatial derivative by means of the original equation namely

$$S_{xx} = c_T^{-2}[S_{tt} + (S^3)_{xx} - (S^5)_{xx} - \alpha S_{xxxx}] \;,$$

and to retain in the brackets just the second time derivative on the grounds that the characteristc speed is much larger than the other coefficients. Without going into further details we apply the above argument in order to get the following governing system

$$S_{tt} = c_T^2 S_{xx} - (S^3)_{xx} + (S^5)_{xx}$$

$$+\beta S_{xxtt} - 2\gamma(ST)_{xx} \;, \quad (8)$$

$$T_{tt} = c_L^2 T_{xx} - \gamma(S^2)_{xx} \;. \quad (9)$$

where $\beta = \alpha c_T^{-2}$. We call it in what follows the "improved" system (IGBS, for brevity).

HAMILTONIAN FORMULATION

Following [MOS1], [C1], [CM2] we show that the system under consideration could also be represented as Hamiltonian system, namely by means of introducing auxiliary functions Q, R as follows

$$S_t = Q_{xx} \;,$$

$$Q_t = c_T^2 S - S^3 + S^5 - 2\gamma ST + \beta S_{tt} \;, \quad (10)$$

$$T_t = c_L R_x \;, \;\; R_t = T_x - \frac{\gamma}{c_L}(S^2)_x \;. \quad (11)$$

It is readily shown that the original equation is a straightforward corollary of the last system provided that the auxiliary functions are eliminated.

We consider a finite interval $x \in [-L_1, L_2]$ where we define the quantities:

$$M = \int_{-L_1}^{L_2} S(x,t)dx \,, \qquad (12)$$

$$E = \int_{-L_1}^{L_2} \left[\frac{c_T^2}{2} S^2 - \frac{1}{4} S^4 + \frac{1}{6} S^6 + \frac{\beta}{2} Q_{xx}^2 + \frac{1}{2} Q_x^2 + c_L^2 (R^2 + T^2) - \gamma T S^2 \right] dx \,, \qquad (13)$$

$$P = \int_{-L_1}^{L_2} (S Q_x + c_L T R) dx \,, \qquad (14)$$

called respectively *mass, pseudoenergy* and *pseudomomentum* . For these we derive the following balance laws

$$\frac{dM}{dt} = Q_x|_{-L_1}^{L_2} \,, \quad \frac{dE}{dt} = Q_x Q_t|_{-L_1}^{L_2} \,,$$

$$\frac{dM}{dt} = -Q_x^2|_{-L_1}^{L_2} + c_L^2(T^2 + R^2)|_{-L_1}^{L_2} - 2\gamma S^2 T|_{-L_1}^{L_2} \,.$$

The above equalities clearly indicate the type of boundary conditions we are to impose in order to have conservation laws over the finite interval. The physically most natural set is

$$S = 0 \,, T = 0 \;\text{ for }\; x = -L_1, L_2 \,, \qquad (15)$$

which also yields the condition $Q = 0$ provided that the latter holds in the initial time moment.

The above conditions secure the conservation of energy but not the conservationn of mass. Both quantities M, E could be conserved if another set of b.c is used, namely $S_x = 0$, $R = 0$, but then the expression for the pseudoforce (the r.h.s. of the balance law for the pseudomomentum) becomes more complicated, showing the term proportional to γ. In addition, a gradient condition of the last kind is hardly justified physically. For this reason we resort to the first set of b.c. It is to be mentioned that for symmetric wave systems, the two terms in the r.h.s. of the balance law for the mass cancel each other due to symmetry. So do the terms comprising the pseudoforce. Then one has conservation laws for the three quantities, but in the general case only the energy is strictly conserved.

THE SOLITARY WAVES

An important feature of the IGBS under consideration is that an analytical expression is available for solutions of type of solitary waves [MC1]. This makes it especially suited for investigating the innate features of more complicated generalized wave equations. In fact Maugin & Cadet [MC1] gave an expression for the solitary waves of the coupled system. Reducing their formula to the case of sole GBE and taking into account the necessary changes related to the "improved" equation we derive the respective expression. Without loosing the generality we consider only waves of positive amplitudes. Then the solution reads

$$S(x - ct) = \frac{s_m}{1 + \nu(s_m, c)\sinh^2(Q(x - ct))} \,,$$

where

$$Q^2 = \frac{c^2 - c_T^2}{\beta c^2} \,, \quad \nu(s_m, c) = \frac{3 - 4s_m^2}{3 - 2s_m^2} \,.$$

Respectively, the amplitude s_m is related to the phase velocity (celerity) of the wave c through the pseudo "dispersion relation"

$$s_m = \frac{1}{2}\sqrt{3 + \sqrt{9 + 48(c^2 - c_T^2)}} \,.$$

It is clear that the condition $Q^2 > 0$ is satisfied only for super-light solitons (tachyons).

DIFFERENCE SCHEME

The scheme follows the development in [C1], [CV1] with the neccesary modifications due to the different type of nonlinearity considered here. The mesh is chosen to be uniform

$$x_i = (i - 1)h - L_1 \,, \quad h = \frac{L_2 + L_1}{N - 1} \,,$$

where N stands for the total number of grid points. The approximation is staggered in time in order to achieve second order of approximation with the least possible number of arithmetic operations per node of mesh. The nonlinear version of the scheme reads

$$\frac{S_i^{n+1} - S_i^n}{\tau} = \frac{1}{h^2}\left[Q_{i+1}^{n+1/2} - 2Q_i^{n+1/2} + Q_{i-1}^{n+1/2} \right] \,,$$

$$\frac{Q_i^{n+1/2} - Q_i^{n-1/2}}{\tau} = \frac{c_T^2}{2}\left[S_i^{n+1} + S_i^{n-1} \right]$$
$$-\frac{1}{4}\left[S_i^{n+1^3} + S_i^{n+1^2} S_i^{n-1} + S_i^{n+1} S_i^{n-1^2} + S_i^{n-1^3} \right]$$
$$+\frac{1}{6}\left[S_i^{n+1^5} + S_i^{n+1^4} S_i^{n-1} + S_i^{n+1^3} S_i^{n-1^2} + S_i^{n+1^2} S_i^{n-1^3} + S_i^{n+1} S_i^{n-1^4} + S_I^{n-1^5} \right]$$
$$+\beta \frac{S_i^{n+1} - 2S_i^{n+} + S_{i-1}^{n-1}}{\tau^2} \,, (16)$$

with boundary conditions $S_0^n = S_N^n = 0$ and initial conditions at the boundary for $Q_0^{1/2} = Q_N^{1/2}$.

The nonlinear terms are treated iteratively by means of an "inner" iteration. after the inner iterations are converged (of order of 5-6 in our simulations) the above nonlinear scheme is effected for which is proved that it conserves the difference approximation of the pseudoenergy in the sense that $E^{n+1/2} = E^{n-1/2}$ where

$$E^{n+1/2} \equiv c_T^2 \sum_1^N \left[\frac{S_i^{n+1^2} + S_i^{n^2}}{2} - \frac{S_i^{n+1^4} + S_i^{n^4}}{4} + \frac{S_i^{n+1^6} + S_i^{n^6}}{6} + \beta \left(\frac{S_i^{n+1} - S_i^n}{\tau} \right)^2 \right] + \sum_1^{N-1} \left[\left(\frac{Q_{i+1}^{n+1/2} - Q_i^{n+1/2}}{h} \right)^2 \right]. \quad (17)$$

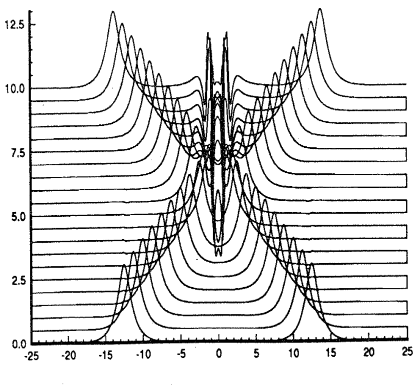

Figure 1: Time evolution of the interacting system of two seches. $c_{left} = 5., c_{right} = -5., c_T = 1.$

RESULTS AND DISCUSSION

As above mentioned, the main purpose of the present work is to investigate the supersonic *seches* of the "improved" equation, viz., the case when $c > c_T$. It is interesting to note that for the equation under consideration, the region of virtually linear behaviour of *seches* is confined to the interval $c \leq 1.001 c_T$. At the same time for the quadratic and cubic improved Boussinesq equations [CV1] found that the essentially linear interaction was confined to the region $c \leq 1.05 c_T$. This difference is explained by the higher-order nonlinearity of the problem considered here. At the same time, the picture of strong nonlinear interaction of solitary waves remains quantitatively the same for all celerities which we investigated (up to $20 c_T$) provided that the time and spatial variable are scaled accordingly. Fig.1 shows the evolution and interaction of the *seches* for the case $c = 5, c_T = 1, \beta = 1$. It is clearly seen that the interaction of the solitary waves is inelastic and a sizable residual signal is excited in the place of the head-on collision. The number of points used for the spatial resolution was $N = 2001$, spacing $h = 0.025$ and time increment $\tau = 0.01$.

Then arises the question whether we can call these solitary waves solitons or not? Basing upon the notion of Zabusky and Kruskal (see [K1] for the story) it is possible to call solitons all waves which behave as particles. As far as the inelastic collision is known in elementary-particle physics then it remains to verify only whether our solutions preserve their shapes. In Fig.2 is shown the comparison between the initial profile of the wave system under consideration (two superimposed *seches*) and the profile attained after 5 dimensionless time units. The parameters are the same as in Fig.1 Here we point out the fact that the *seches* are virtually unchanged by the evolution, despite the sizable non-elastic effects of the collision. The *seches* themselves reemerge virtually unchanged from the interaction, but experience phase shift in a simmilkar fashion as known for KdV and Bousiinesq equaitons. The occurrence of a residual signal is conspicuous. It is excited from the vacuum state and sustained by the nonlinearity, and lives a life on its own after the two solitons have long left the stage. In a sense, the residual can be considered as new particles born out from the vacuum state. Here is to be mentioned that the "pseudoenergy" is conserved in our calculations within 12 significant digits, i.e., the inelastic collision is not an artifact of the numerical scheme. If there could have been some doubts abouth the same result obtained by [B1], [IJ1] because of the non-conservativeness of their schemes now these doubts are dissolved. In addition, because of the better stability properties of our scheme, we were able to treat cases of order of magnitude larger phase velocities than the mentioned works when the nonlinearity is much more important. As already mentioned, the behaviour is essentially the same, even quantitatively, for all values of the phase velocity considereed here. The phase-shift effect is qualitatively the same as for the Improved Boussinesq equation ([CV1]). Fig.3 shows

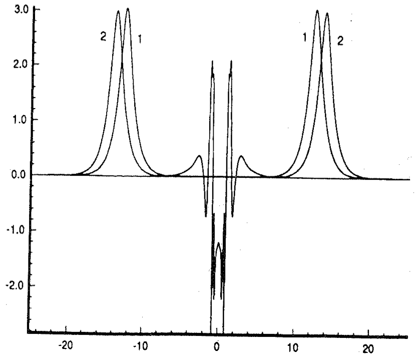

Figure 2: Comparison of the actual wave system (2) and the projected configuration of solitons without interaction(1)

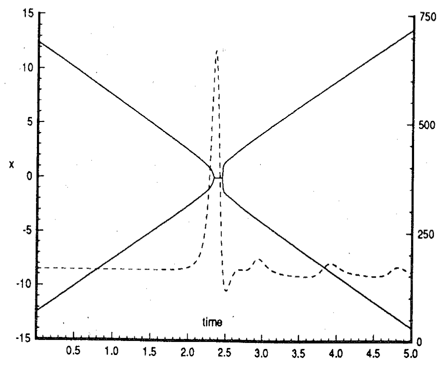

Figure 3: Trajectories of the centres of *seches* (solid line) and evolution with time of the nonlinear part of the pseudoenergy (dashed line)

the trajectories of the centres of *seches* as functions of time (the solid lines). Following the reasoning of [CV1] we can conclude that the "improved" equation can serve adequately as a substitute for the "improper" one, as far as the supersonic solitons are concerned. In the light of the perfect conservation of the pseudoenergy, and the fact of the reemergence of the *seches* virtually unchanged by the interaction, some comments on the residual signal are due. It appears that its energy is not derived from the *seches*. This can be explained by the fact that E is not a positive definite fuinction and allows growing of disturbances, limited only by the requirement that the cubic and quintic powers for the expression of E should balance each other. In this instance, it is interesting to examine the contribution of the nonlinear terms to the expression of the pseudoenergy. The dashed curve in Fig. 3 gives an impression about that effect. One sees that in the region of interaction, the nonlinear part E_n experiences a violent increase and then gradually subsides to its pre-collision value.

Thus we can conclude that similarly to the classical IBE (see [B1], [I1], [CV1]) the supersonic *seches* in the IGBS retain their identities, but the interaction is inelastic. In this sense, they can be called inelastic solitons. Quantitatively, the effect here is more pronounced because of the higher-order nonlinearity. On the other hand, the quintic nonlinearity effectively serves to limit the growth of the disturbances and the blow-up (see [T1]) due to the nonlinearity does not show up in our calculations.

Qualitatively similar is the picture for the taking-over collision (see Fig.4[top]), but the excited residual signal is of much less intensity and is of considerably lesser steepness. In Fig.4 [bottom] are shown the trajectories of the centres of the two *seches*. The dotted lines present the projected trajectories of the solitons without interaction. What is interesting here is that the larger soliton experiences larger phase shift than the smaller one.

The mesh parameters in this case are: $N = 3201, h = 0.025, \tau = 0.01$

CONCLUSION

In the present paper we treate numerically a generelized Boussinesq equation with higher-order (cubic-quintic) nonlinearity. We use the so-called "improved" version of the equation in which the fourth-order spatial derivatives are replaced by a mixed fourth derivative. Such an equation is stable with respect to small disturbances (well posed in the sense of Hadamard).

We investigate the evolution of a system of two solitary waves of type of *sech*, e.g., head-on and taking-over collisions. The two solitons reemerge from the interaction strictly unchanged in form, but with a phase shift which is of the same order of magnitude as for the second-order Boussinesq equation. Similarly, an inelastic character of the interacion is also observed, but in the case under consideration, due to the higher-order nonlinearity, the residual signal excited in the cite of the bygone interaction is of higher amplitude than one observed in the second-order Boussinesq equation. On the other hand, the presence of the quintic term prevents the nonlinear blow-up of the solution in finite time.

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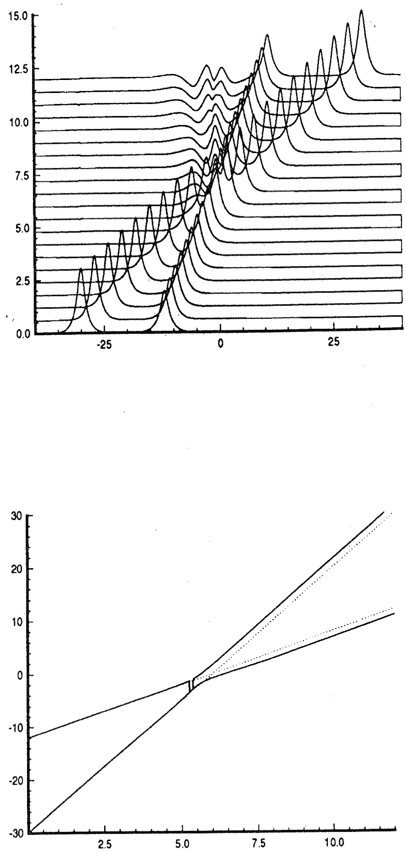

Figure 4: Time evolution of two *seches* in taking-over collision. $c_{left} = 5., c_{right} = 2., c_T = 1.$ [top]; trajectories of the centres of *seches* (solid line) and the projected trajectories without interaction (dotted line) [bottom]

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