On nonlinear waves in media with complex properties

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To the memory of Gérard Maugin – good friend and colleague

Abstract In nonlinear theories the axiom of equipresence requires all the effects of the same order to be taken account. In this paper the mathematical modelling of deformation waves in media is analysed involving nonlinear and dispersive effects together with accompanying phenomena caused by thermal or electrical fields. The modelling is based on principles of generalized continuum mechanics developed by G.A. Maugin. The analysis demonstrates the richness of models in describing the physical effects in media with complex properties.

Key words: nonlinearities, dispersion, microstructures, hierarchies, biomembranes.

1 Introduction

The legacy of G.A. Maugin is huge and has an imprint on many studies on continuum mechanics in the second half of the 20^{th} century. His studies have cast light on many fundamental problems of continua like the principle of virtual power, generalized continuum mechanics, the concepts of internal variables and configurational forces, propagation of waves and fronts – just to name a few (dell'Isola et al., 2014). His sparkling ability to inspire his colleagues to collaborate and find new problems in the field of fundamental understanding of the behaviour of materials has been realized in numerous joint publications. In this paper, the attention is paid to nonlinear wave propagation. G.A. Maugin himself has studied waves in elastic crystals (Maugin, 1999), numerical methods used for the analysis of waves and fronts (Berezovski et al., 2008) and published several overviews on waves (Maugin, 2011; Christov et al. 2007). The cooperation with colleagues in Tallinn has resulted in describing complexities of soliton theory (Salupere et al., 1994; 2001), in nerve pulse

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analysis (Maugin and Engelbrecht, 1994), in elaborating the concept of internal variables (Berezovski et al. 2011a; 2011b), etc. Here we shall present some fundamental ideas from this cooperation and novel results developed recently. The basic problem is how to describe real properties of materials and how these are reflected in wave propagation. The importance of such an analysis is pointed out also by G.A. Maugin (2015).

In what follows, the problems in deriving the governing equations of nonlinear wave motion for describing complicated properties of media (materials) and the corresponding mathematical models are presented in Section 2. The physical effects resulting from these governing equations are analysed in Section 3. Finally, in Section 4 discussion is given together with ideas for the further research.

2 The governing equations

The governing equations for describing wave motion are based on the balance of momentum. Besides classical linear wave equations, the Boussinesq-type models are richer because they account also nonlinear and dispersive effects (Christov et al., 2007). Like classical wave equations in the 1D setting, these equations have bi-directional solutions. Another class of models describing nonlinear waves are evolution equations like the Korteweg-de Vries (KdV) equation and its modifications. Evolution equations describe uni-directional propagation and are usually derived from complicated systems by the reductive perturbation method using the moving frame of reference. Characteristically for both types of equations, the modelling of nonlinear and dispersive effects permits to describe many interesting physical phenomena. Below some results of modelling are briefly described. The 1D set-ups are used in order to reach transparent models where it would be easy to trace the influence of individual terms in models.

A typical form of a Boussinesq-type equation in terms of a displacement u is (Christov et al., 2007):

$$u_{tt} - c_0^2 u_{xx} - [F(u)]_{xx} = (\beta_1 u_{tt} - \beta_2 u_{xx})_{xx}, \tag{1}$$

where c_0 is the wave velocity, F_u is a polynomial and β_1, β_2 are physical constants. As usual, x denotes space and t denotes time. Here and further, indices x and t denote the differentiation with respect to the indicated variable. This equation can be found as in solid mechanics as well as in fluids where it was derived originally. It must be noted that the r.h.s. of Eq. (1) has often an order of $\mathscr{O}(\varepsilon)$ where ε is a small parameter.

The general form of a KdV-type evolution equation in terms of $v \sim u_x$ (or $v \sim u_t$) is (Salupere et al., 2001).

$$v_\tau + [P(v)]_\xi + D(v) = 0, \tag{2}$$

where τ is a scaled coordinate, $\xi = c_0 t - x$ is the moving frame coordinate, $P(v)$ is a polynomial and $D(v)$ is a dispersion operator including the odd derivatives of v with respect to ξ only.

Boussinesq-type models. In modelling of microstructured solids, it is possible to distinguish macro- and microstructure that must be taken into account in modelling the wave motion. Based on the Mindlin (1964) micromorphic theory, the governing equations can be derived for both coupled structures. The existence of the microstructure leads to dispersive effects while nonlinearity is of the physical character. The free energy W is assumed to have a form:

$$W = \frac{\rho_0 c^2}{2} u_x^2 + A_1 \varphi u_x + \frac{1}{2} B \varphi^2 + C \varphi_x^2 + \frac{1}{6} N u_x^3 + \frac{1}{6} M \varphi_x^3, \tag{3}$$

where ρ_0 and c are the density and the sound velocity of the macrostructure, u is the macrodisplacement, φ is the microdeformation in the sense of Mindlin (1964), and A, B, C, N, M are material parameters. The kinetic energy K is

$$K = \frac{\rho_0}{2} u_t^2 + \frac{I}{2} \varphi_t^2, \tag{4}$$

where I is the measure of microstructure inertia.

Then the governing equation in terms of the macrodisplacement u is (Engelbrecht et al., 2005; Berezovski et al., 2013):

$$\begin{aligned} u_{tt} - (c^2 - c_A^2) u_{xx} - \frac{1}{2} k_1 (u_x^2)_x = {} & p^2 c_A^2 \left(u_{tt} - c_1^2 u_{xx} \right)_{xx} \\ & - \frac{1}{2} k_2 (u_{xx})_{xx}, \end{aligned} \tag{5}$$

where $c_A^2 = A^2/\rho_0 B$, $C_1^2 = C/I$, $p^2 = I/B$ and k_1, k_2 are the coefficients of nonlinearities.

It must be stressed that Eq. (5) reflects the following: (i) the nonlinearities are of the deformation-type as usually in solid mechanics; (ii) microinertia of the microstructure is taken into account; (iii) the second wave operator at the r.h.s has a parameter p^2 which is usually small and therefore Eq. (5) is a hierarchical equation. In addition, the velocity of the wave operator for the macrostructure at the l.h.s is influenced by the properties of the microstructure. In such a way, the governing equation reflects real properties of the microstructured material.

In case of a multiscale (the scale in the scale) microstructure, the governing equation involves two wave operators reflecting the properties of microstructures (Engelbrecht et al., 2007). In the linear case this equation is:

$$\begin{aligned} u_{tt} - (c^2 - c_{A1}^2) u_{xx} = {} & p_1^2 c_{A1}^2 \left[u_{tt} - \left(c_1^2 - c_{A2}^2 \right) u_{xx} \right]_{xx} \\ & - p_1^2 c_{A1}^2 p_2^2 c_{A2}^2 \left(u_{tt} - c_2^2 u_{xx} \right)_{xxxx}, \end{aligned} \tag{6}$$

where indices 1 and 2 denote the microstructures. The smaller scales bring in higher order dispersive terms. Like the macrostructure, the level 1 microstructure is also influenced by the level 2 microstructure. Two wave operators at the r.h.s. of Eq. (6) indicate the hierarchical structure the governing equation.

If internal variables are considered to include nonlinearities in the microscale then the structure of governing equations becomes even more complicated compared to Eq. (3) as shown by Berezovski (2015).

The asymptotic analysis demonstrates also the hierarchies for waves in Cosserat media and ferroelectrics, analysed by Maugin (1999). In the linear case, the governing equations are similar to those for microstructured solids (Salupere and Engelbrecht, 2014).

In biomechanics, the character of nonlinearities can be different from what is typical in solid mechanics. Based on experiments, it has been shown that in biomembranes where the microstructure is built up by lipid molecules, the nonlinearity of mechanical waves can be accounted in the effective velocity (Heimburg, Jackson, 2005).

$$c_e^2 = c_0^2 + pu + qu^2, \tag{7}$$

where c_0 is the velocity in the unperturbed state and u is the density change along the axis of the biomembrane, while p, q are material coefficients. Substituting c_e^2 into the balance of momentum and the adding dispersive terms, the governing equation for longitudinal waves in biomembranes takes the form

$$u_{tt} = \left[\left(c_0^2 + pu + qu^2\right) u_x\right]_x - h_1 u_{xxxx} + h_2 u_{xxtt}, \tag{8}$$

where h_1, h_2 are constants. This equation was proposed by Heimburg and Jackson (2005) with $h_2 = 0$ and later improved by Engelbrecht et al. (2015). This improvement with $h_2 \neq 0$ is important because it accounts for the microstructure of the biomembrane made of lipids and removes the discrepancy that at higher frequencies the velocities are unbounded. This is a physically admissible situation as stressed by Maugin (1999). It must be stressed that as noted above, in Eq. (5) the nonlinearities are of the deformation-type, then in Eq. (8) they are of the displacement-type.

Evolution-type (KdV-type) models. These one-wave asymptotical models have gained wide attention because of the iconic status of several nonlinear evolution equations like the KdV equation, Schrödinger equation a.o. which permit in some cases also analytical solutions (for example, Maugin, 1999; 2011; Ablowitz, 2011). The classical KdV equation combines the quadratic nonlinearity and cubic dispersion:

$$v_\tau + v v_\xi + d v_{\xi\xi\xi} = 0, \tag{9}$$

where d is the dispersion parameter. The numerical analysis of the KdV equation has revealed many details including the behaviour of multi-recurrence of solitons forming from a harmonic excitation (Salupere et al., 2002), the explanation of the importance of hidden solitons (Salupere et al., 2003; Engelbrecht, Salupere, 2005) and the influence of an additional force (Engelbrecht, Salupere, 2005). The modifications of the KdV equations involve more physical effects. For example, for martensitic shape-memory alloys the governing equation takes the form (Salupere et al., 2001):

$$v_\tau + [P(v)]_\xi + dv_{\xi\xi\xi} + bv_{5\xi} = 0, \tag{10}$$

$$P(v) = -\frac{1}{2}v^2 + \frac{1}{4}v^4, \tag{11}$$

where d and b are the third- and the fifth-order dispersion parameters, respectively. The quartic potential (11) corresponds to the two-well energy distribution which has a direct influence on nonlinear effects. Equations (10), (11) are able to describe several solitonic structures (Ilison, Salupere, 2006).

It is also possible to derive an evolution equation from the bi-directional model (5). However, in this case the result is a modified KdV equation (Randrüüt, Braun, 2010).

$$v_\tau + a_1 v v_\xi + d_1 v_{\xi\xi\xi} + a_2 (v_\xi^2)_{\xi\xi} = 0, \tag{12}$$

where a_1 describes the nonlinearity of the macrostructure, $a_2 \sim \mathscr{O}(\varepsilon)$ - the nonlinearity of the microstructure and d_1 denotes the joint influence of dispersive terms (cf. Eq. (5)). It means that both of the effects – inertia of the microstructure (term u_{ttxx} in Eq. (5)) and elasticity of the microstructure (term u_{xxxx} in Eq. (5)) are involved in the dispersive term in Eq. (12), reflected by the sign of d_1 (Randrüüt, Braun, 2010).

More detailed analysis of nonlinearities in the microscale demonstrates that also Benjamin-Bona-Mahoney or Camassa-Holmb equations can be derived (Berezovski, 2015).

Like for the Boussinesq-type equations, the evolution equations may also have a hierarchical character reflecting the scale effects. This is the case of granular materials when the evolution equation can be written in the form (Giovine, Oliveri, 1995):

$$v_\tau + v v_\varsigma + \alpha_1 v_{\xi\xi\xi} + \beta \left(v_\tau + v v_\xi + \alpha_2 v_{\xi\xi\xi} \right)_{\xi\xi} = 0, \tag{13}$$

where α_1 and α_2 are macro- and microlevel nonlinearities and β is a parameter involving the ratio of the grain size and the wavelength. The solutions of Eq. (13) involve beside single solitons also soliton ensembles. This is a typical example of two concurrent dispersive effects (Ilison, Salupere, 2009).

Coupled fields. Several physical situations need accounting for coupled fields. For example, in mechanics of solids, the presence of heat sources lead to coupling of deformation fields and temperature fields. For microstructured materials the processes in macro- and microstructures are influenced by both fields. Besides the deformations of macro- and microstructures, the temperature fields can also be divided: macrotemperature and microtemperature (fluctuation of temperature in microstructural elements). The corresponding governing equations can be derived by using the concept of internal variables (Berezovski et al., 2011a; 2011b). However, due to the complicated structure of these equations, it is impossible to derive a single governing equation like it is done for elastic waves in microstructured solids (see above). In this coupled case the governing system of equations is (Berezovski et al., 2014):

balance of linear momentum:

$$v_{tt} - c_o^2 u_{xx} = m_1 \theta_x + m_2 \alpha_x + m_3 \varphi_{xx}; \tag{14}$$

balance of energy:

$$\theta_t = n(k\theta_x)_x + m_4 u_{xt} + r_1 \varphi_t^2; \tag{15}$$

governing equation for microdeformation:

$$\alpha_{tt} - c_d^2\, \alpha_{xx} = -m_2 u_x - m_3 \alpha; \tag{16}$$

governing equation for microstructure:

$$\varphi_{tt} - c_t^2 \varphi_{xx} = m_5 u_{xx} - r_2 \varphi_t, \tag{17}$$

where u is the macrodisplacement, φ - the microdeformation, θ - the macrotemperature, α - the microtemperature; c_0, c_d, c_t denote velocities, k is the thermal conductivity and m_1, m_2, m_3, m_4, m_5, r_1, r_2, n are coefficients. If conditions $\theta = const, \alpha = const$ are satisfied then Eqs. (14) and (16) can be reduced to the linear form of Eq. (5). The full system of Eqs. (14) – (17) includes three hyperbolic equations (Eqs. (14), (16), (17) and one parabolic equation (Eq. (15)). The coupling of physical effects is complicated – microdeformation and microtemperature are not coupled but both are coupled to the balance of linear momentum while macrostructure is affected by the macrodisplacement (like in the usual theory of thermoelasticity) and microtemperature.

In biophysics, a theoretical model for nerve signal propagation including all the physical effects is still a challenge calling "to frame a theory that incorporates all observed phenomena in one coherent and predictive theory of nerve signal propagation" (Andersen et al., 2009). The phenomena are following: the action potential (the electrical pulse) in a nerve fibre which carries the signal, generates also mechanical waves in the axoplasm within a fibre and in the surrounding biomembrane. The longitudinal wave in the biomembrane leads to the transverse displacement which is measurable. Leaving aside the detailed description on the origin of physical effects and corresponding models, a possible mathematical model uniting all the processes into one system has recently been proposed in the following form (Engelbrecht et al., 2016).

First, the action potential can be modelled by the simplified FitzHugh-Nagumo (FHN) equation governing the propagation of an electrical pulse z (Nagumo et al., 1962):

$$z_{txx} = z_{tt} + \mu(1 - a_1 z + a_2 z^2) z_t + z, \tag{18}$$

where a_1, a_2, μ are parameters and z is the scaled voltage.

Second, the pressure wave in axoplasm may be governed by a 1D Navier-Stokes model

$$\rho(V_t + V V_x) = -p_x + \mu_v V_{xx} + F_1(z), \tag{19}$$

where V is the velocity, ρ – the density, p – the pressure and μ_v – the viscosity. The force acting from the action potential is denoted by $F_1(z)$.

Third, the longitudinal wave in the biomembrane is modelled by Eq. (8)

$$u_{tt} = \left[\left(c_0^2 + pu + qu^2\right) u_x\right]_x - h_1 u_{xxxx} + h_2 u_{xxtt} + F_2(z,V), \tag{20}$$

where $F_2(z,V)$ is a force from other waves. The system of equations (18), (19), (20) is solved for the initial condition

$$z\big|_{t=0} = f(x) \tag{21}$$

and the transverse wave (horizontal displacement w of the biomembrane) is calculated by

$$w = -kru_x, \tag{22}$$

like in rods (Porubov, 2003). All the governing equations are nonlinear and demonstrate explicitly the complexity of the process. The nature of forces $F_1(z), F_2(z,V)$ must be determined by experiments.

3 Physical effects

The model equations described in Section 2 give an idea about how to account for complicated physical effects reflecting the properties of nonlinear media. In this Section, the most typical effects are described which have resulted from recent studies (many in cooperation with G.A. Maugin). As typical for the complex world, the interactions of effects lead to new phenomena.

Most of the mathematical models described above are the soliton-bearing systems. The nonlinear Boussinesq-type model like Eq. (5) demonstrates the emergence of soliton trains. Note that here the nonlinearity is of the deformation type. An initial condition produces left- and right-propagating trains of deformation solitons (Berezovski et al., 2013) where, as expected, the higher the amplitude, the faster the soliton. The interaction of solitons governed by non-integrable equation (5), however, is not fully elastic and produces some radiation explained already by Maugin (1999). Due to the nonlinearity at the microlevel, the emerging solitons are not fully symmetric (Salupere et al. 2008). By solving the corresponding evolution equation (12), the same effect is demonstrated (Randrüüt, Braun, 2010).

Another Boussinesq-type equation (8) involves displacement-type nonlinearities. It possesses a soliton solution and from an initial input, the soliton trains can be formed. Given the signs of the coefficients from experiments ($p < 0$) contrary to the previous case, the soliton trains have an interesting property – the smaller the amplitude, the faster is the soliton. The analysed improved model (8) demonstrates clearly that the existence of the inertial term $h_2 u_{xxtt}$ leads to a narrower pulse which is important in determining its value from experiments by measuring the width of the pulse. The full analysis of Eq. (8) is given by Engelbrecht et al. (2017) together with the demonstration of the existence of periodical waves (cf cnoidal waves for the KdV equation) governed by this equation. Like in the previous case, the interaction of solitons is not fully elastic resulting in some radiation during interactions.

The existence of solitary solutions or the emergence of regular soliton trains are like benchmarks of solitonics. However, due to complicated physics, the governing equations are different from well-studied classical models and interest should also be focused to the complicated solitonic structures. Such structures may emerge in phase memory alloys (Eq. (10)), in granular media (Eq. (13)) and forced KdV models. In order to understand properly the mechanisms of emerging solitonic structures, one should determine the number of possible emerging solitons. This depends on the energy sharing and redistribution between solitons. In general terms, starting from the seminal paper by Zabusky and Kruskal (1965) this problem has been analysed using various estimations (see references in Salupere et al., 2014). A detailed analysis of interaction of solitons shows that besides visible solitons there exist also hidden (or virtual) solitons (Salupere et al., 1996; Christov, 2012). The hidden solitons can be detected from the changes they cause in trajectories of other solitons during interactions and can be visible during the short time intervals due to the fluctuations of the reference level. What is important, is that these hidden solitons may serve as "energy pockets" which may become visible if an external force acts in a system (Engelbrecht, Salupere, 2005). This effect has been analysed for the KdV equation with the periodic external force (Engelbrecht, Salupere, 2005). Depending on the strength of the force, several features were established: weak, moderate, strong and dominating external fields. In the case of the weak field all hidden and smaller visible solitons are suppressed; in the case of the moderate field the resulting solitons include all visible and some hidden solitons; in the case of the strong field the number of emerging solitons is higher than in the corresponding conservative case; and in the dominating field no soliton complexes but wave packets are formed. If the external force has a polynomial character with one maximum and one minimum then a single soliton may be suppressed or amplified depending on its amplitude (Engelbrecht, Khamidullin, 1988). This phenomenon could explain the possible amplification of the precursors to seismic waves generated by earthquakes. The hierarchical KdV equation (13) governs beside a single soliton several types of soliton complexes: a KdV soliton ensemble with or without a weak tail; a soliton with a strong tail; a solitary wave with a tail and wave packets (Ilison, Salupere, 2009; Salupere et al., 2014). Here the hidden solitons play a role in the emergence of soliton complexes.

It is obvious that the soliton "menagerie" is rich and above only a part of phenomena was described related to microstructured solids. For a more detailed review the reader is referred to Maugin (2011).

Besides solitons and soliton complexes, the microstructured solids reveal other interesting phenomena. In the case of multiscaled hierarchical microstructures (see Eq. (6)) the effect of the negative group velocity may appear (Peets et al., 2013). This phenomenon is related to the coupling effects between the two scales. In terms of dispersion analysis, this is a case when two optical branches of dispersion curves are very close to each other at certain frequencies. As far as the optical modes represent non-propagating oscillations, such a situation can be considered as a pre-resonant one.

The processes in thermoelastic microstructured solids are described by Eqs. (14) – (17). The numerical simulation shows that even in the absence of effects of the microdeformation, the wave propagation process is strongly influenced by the microtemperature (Berezovski, Engelbrecht, (2013). Namely, although the leading terms in the balance of energy (15) reflect the parabolicity as expected, the macrotemperature is affected by the microtemperature changes (hyperbolic equation (17)) and demonstrates the wave-like behaviour. This result casts surely more light on the behaviour of microstructured solids.

The joint model of a nerve signal propagation (Eqs. (18) – (20)) is an attempt to explain this fascinating process by including all the possible waves into an ensemble where the nonlinearities play a decisive role. The waves in the ensemble interact with each other through the coupling forces. Certainly, the description of the electrical signal is here simplified because the FHN model takes into account only one (generalized) ionic current. This current plays a crucial role in the energy balance of the electrical pulse dictating its asymmetric shape. It would better to account for specified currents of Na and K ions but the more complicated models like the Hodgkin-Huxley model (1952) taking these ionic currents into account need many more physical parameters. So at this stage we limit ourselves to the simple FHN equation (18). The pressure wave in the axoplasm is described by the classical Navier-Stokes equation. Finally, the longitudinal waves in the surrounding biomembrane are described by a recently derived equation (20). To make this model work, two important physical phenomena must be properly understood: (i) the mechanisms of opening the ion channels; (ii) the nature of coupling forces. It means that in Eq. (18) the parameters a_1 and a_2 should be carefully estimated and the forces $F_1(z)$ and $F_2(z,V)$ determined. This work is in progress. A special challenge is to understand the synchronization of velocities and the possible phase-shifts between the waves in an ensemble.

4 Discussion

What has been described above, is the description of complexity in wave motion. Indeed, the main features of complex systems are (Érdi, 2008): (i) complex systems are comprised of many different constituents which are connected in multiple ways; (ii) complex systems produce global effects including emergent structures generated by local interactions; (iii) complex systems are typically nonlinear; (iv) emergent structures may occur far from the equilibrium. The need for the inevitable introduction of complexity in the mechanics of real materials has been suggested also by Maugin (2015). The list of effects in nonlinear wave motion includes many fundamental phenomena such as the balance of nonlinear and dispersive effects, scale effects and hierarchies, coupling of different fields, etc. As a result, special wave structures could emerge and the interaction of waves may lead to amplification, instability and energy redistribution. The coupling of several fields like in thermoelasticity and biophysics leads to completely novel physical effects which can explain the behaviour of materials or systems in a more informative way. In general terms, the corresponding mathematical models are non-integrable (Maugin, 2011) and that is why numerical methods are used in the analysis. Most of the results described above are obtained either by using the finite volume (Berezovski et al, 2008) or the pseudospectral (Salupere, 2009) methods. A special attention is paid to the accuracy and convergence of numerical simulations.

The analysis of complexity of wave motion demonstrates clearly that the mechanical behaviour (stresses, velocities, deformation, temperature) of continua depends on the interactions of constituents and fields. From another point of view, the waves are the carriers of information and energy reflecting so the interaction processes. By measuring the physical properties of waves (amplitudes, velocities, spectra, shapes), this information can be used for the determining the properties of fields or internal structures, i.e. for solving the inverse problems (Janno, Engelbrecht, 2011).

There are many unsolved problems in the complexity of wave motion. One could ask about the soliton management, soliton tunability (generation of solitons with predetermined amplitudes or spectral densities), soliton turbulence (self-organization into spatially localized solitonic structures), etc. An interesting question is whether intuitively well understood microtemperatures in microstructured materials can be measured. Metamaterials and nanomaterials need more attention because of their properties which must be reflected also in wave motion.

The impact of G.A. Maugin in generating novel ideas is enormous.

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