One-Dimensional Microstructure Dynamics

Arkadi Berezovski, Jüri Engelbrecht, and Gérard A. Maugin

Abstract. Dispersive wave propagation in solids with microstructure is discussed in the small-strain approximation and in the one-dimensional setting. It is shown that the generalizations of wave equation based on continualizations of discrete systems as well as on homogenization methods can be recovered in the framework of the internal variable theory in the case of non-dissipative processes.

1 Introduction

It is well known that the propagation of linear elastic waves in a homogeneous medium is governed by the wave equation, which in the one-dimensional case reads

$$u_{tt} = c^2 u_{xx}, \tag{1}$$

where u is the displacement, c is the elastic wave speed.

If the medium is non-homogeneous, i.e. there is a certain microstructure, the wave propagation is accompanied by wave dispersion. Historically, the dispersion

Arkadi Berezovski
Centre for Nonlinear Studies, Institute of Cybernetics at Tallinn University of Technology, Akadeemia tee 21, 12618 Tallinn, Estonia
Tel.: +372-620-4264
Fax: +372-620-4151
e-mail: Arkadi.Berezovski@cs.ioc.ee

Jüri Engelbrecht
Centre for Nonlinear Studies, Institute of Cybernetics at Tallinn University of Technology, Akadeemia tee 21, 12618 Tallinn, Estonia
e-mail: je@ioc.ee

Gérard A. Maugin
Institut Jean Le Rond d'Alembert, Université Pierre et Marie Curie, UMR 7190,
4 Place Jussieu, 75252, Paris Cédex 05, France
e-mail: gam@ccr.jussieu.fr

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effects were also investigated in the non-linear framework (cf. [3, 9], where many possible generalizations are outlined).

In the linear case, the simplest generalization of the wave equation was obtained by the homogenization of a periodically inhomogeneous medium [6, 17]

$$u_{tt} = c^2 u_{xx} + c^2 l^2 A_{22} u_{xxxx}, \tag{2}$$

where l is an internal length parameter and A_{22} is a dimensionless coefficient.

Later on the same model was derived by a standard continualization procedure of the equations of motion for a system of discrete particles [16, 1].

Another modification of the wave equation was pointed out in [9] again on the basis of the continualization

$$u_{tt} = c^2 u_{xx} + l^2 A_{21} u_{xxtt}, \tag{3}$$

and it was repeated later by means of homogenization methods [19, 5].

The combination of the two dispersion models gives (see also derivation in [4])

$$u_{tt} = c^2 u_{xx} + l^2 A_{21} u_{xxtt} + c^2 l^2 A_{22} u_{xxxx}. \tag{4}$$

This model was also derived from a discrete model by means a non-standard continualization procedure [13].

Recently, a ”causal” model for dispersive wave propagation is proposed [14]

$$u_{tt} = c^2 u_{xx} + l^2 A_{21} u_{xxtt} + c^2 l^2 A_{22} u_{xxxx} - \frac{l^2}{c^2} A_{23} u_{tttt}, \tag{5}$$

in order to avoid an infinite speed of propagation in the absence of higher-order time derivatives. The most general one-dimensional model based on the Mindlin theory of microstructure [15]

$$u_{tt} = \left(c^2 - c_A^2\right) u_{xx} - p^2 \left(u_{tt} - c^2 u_{xx}\right)_{tt} + p^2 c_1^2 \left(u_{tt} - c^2 u_{xx}\right)_{xx}, \tag{6}$$

was discussed in [2]. Here c_A, c_1 and p are coefficients discussed in Section 4. It is clear that the last model includes all the previous ones.

Another approach to the description of microstructural effects is provided by the internal variable theory [12]. In this paper, we explain how the internal variable approach is generalized to the description of non-dissipative processes of linear dispersive wave propagation.

The paper is organized as follows. In the next Section we remind the reader of the canonical formulation of thermomechanics, which is applied even when no thermal effects are included. Then we present the internal variable theory specified to the non-dissipative processes. First we consider the case of one weakly non-local internal variable in the Section 3. In Section 4 we introduce an additional internal variable, which is necessary to obtain higher-order time derivatives.

2 Canonical Thermomechanics

The existence of the microstructure generally means that the medium is inhomogeneous. Therefore, we apply the canonical form of balance equations [8], where the inhomogeneities are treated in the most consistent way.

In the case of the thermoelastic conductors of heat, one-dimensional motion is governed by local balance laws for linear momentum and energy (no body forces)

$$\frac{\partial}{\partial t}(\rho_0 v) - \frac{\partial \sigma}{\partial x} = 0, \tag{7}$$

$$\frac{\partial}{\partial t}(\rho_0 v^2/2 + E) - \frac{\partial}{\partial x}(\sigma v - Q) = 0, \tag{8}$$

and by the second law of thermodynamics

$$\frac{\partial S}{\partial t} + \frac{\partial}{\partial x}(Q/\theta + K) \geq 0. \tag{9}$$

Here t is time, ρ_0 is the matter density, $v = u_t$ is the physical velocity, σ is the Cauchy stress, E is the internal energy per unit volume, S is the entropy per unit volume, θ is temperature, Q is the material heat flux, and the ”extra entropy flux” K vanishes in most cases, but this is not a basic requirement.

Canonical form of the energy conservation. The canonical energy equation is obtained by introducing the free energy per unit volume $W := E - S\theta$ and taking into account the balance of linear momentum (7)

$$\frac{\partial (S\theta)}{\partial t} + \frac{\partial Q}{\partial x} = h^{int}, \quad h^{int} := \sigma \dot{\varepsilon} - \frac{\partial W}{\partial t}, \tag{10}$$

where the right-hand side of eqn. $(10)_1$ is formally an *internal heat source* [11].

In the case of non-zero extra entropy flux, the second law of thermodynamics gives

$$-\left(\frac{\partial W}{\partial t} + S\frac{\partial \theta}{\partial t}\right) + \sigma\dot{\varepsilon} + \frac{\partial}{\partial x}(\theta K) - (Q/\theta + K)\frac{\partial \theta}{\partial x} \geq 0, \tag{11}$$

where $\varepsilon = u_x$ is the one-dimensional strain measure. The dissipation inequality (11) can be also represented in the form

$$S\dot{\theta} + (Q/\theta + K)\frac{\partial \theta}{\partial x} \leq h^{int} + \frac{\partial}{\partial x}(\theta K). \tag{12}$$

Canonical (material) momentum conservation. Multiplying eqn. (7) by u_x we then check that eqn. (7) yields the following material balance of momentum (cf. [8])

$$\frac{\partial P}{\partial t} - \frac{\partial b}{\partial x} = f^{int} + f^{inh}, \tag{13}$$

where the *material momentum* P, the material *Eshelby stress* b, the material *inhomogeneity force* f^{inh}, and the material *internal force* f^{int} are defined by [8]

$$P := -\rho_0 u_t u_x, \quad b := -\left(\rho_0 v^2/2 - W + \sigma\varepsilon\right), \tag{14}$$

$$f^{inh} := \left(\frac{1}{2}v^2\right)\frac{\partial\rho_0}{\partial x} - \left.\frac{\partial W}{\partial x}\right|_{expl}, \quad f^{int} := \sigma u_{xx} - \left.\frac{\partial W}{\partial x}\right|_{impl}. \tag{15}$$

Here the subscript notations *expl* and *impl* mean, respectively, the derivative keeping the fields fixed (and thus extracting the explicit dependence on x), and taking the derivative only through the fields present in the function. The canonical equations for energy and momentum (10) and (13) are the most general expressions we can write down without a postulate of the full dependency of the free energy W [11].

3 Single Internal Variable

Up to now the microstructure was not specified. It can be prescribed by the specification of location, shape, and properties of inclusions, as, for example, in the case of periodic structures. If the microstructure is irregular, such a prescription is impossible. In the framework of the phenomenological continuum theory it is assumed that the influence of the microstructure on the overall macroscopic behavior can be taken into account by the introduction of an internal variable φ which we associate with the integral distributed effect of the microstructure. Then the free energy W is specified as the general sufficiently regular function of the strain, temperature, the internal variable, and its space gradient [11]

$$W = \overline{W}(u_x, \theta, \varphi, \varphi_x). \tag{16}$$

The *equations of state* (in a sense, mere definition of the partial derivatives of the free energy) are given by

$$\sigma = \frac{\partial\overline{W}}{\partial u_x}, \quad S = -\frac{\partial\overline{W}}{\partial\theta}, \quad \tau := -\frac{\partial\overline{W}}{\partial\varphi} \quad \eta := -\frac{\partial\overline{W}}{\partial\varphi_x}. \tag{17}$$

Following the scheme originally developed in [7] for materials with *diffusive* dissipative processes described by means of internal variables of state, we chose the non-zero extra entropy flux K in the form

$$K = -\theta^{-1}\eta\dot{\varphi}. \tag{18}$$

In this case, the ”internal” material force and heat source each split in two terms according to

$$f^{int} = f^{th} + \widetilde{f}^{intr}, \quad h^{int} = h^{th} + \widetilde{h}^{intr}, \tag{19}$$

where the *thermal sources* and the *”intrinsic” sources* are given by [11]

$$f^{th} := S\frac{\partial}{\partial x}\theta, \quad h^{th} := S\dot{\theta}, \quad \widetilde{f}^{intr} := \widetilde{\tau}\frac{\partial\varphi}{\partial x}, \quad \widetilde{h}^{intr} := \widetilde{\tau}\dot{\varphi}, \tag{20}$$

so that we have the following consistent canonical equations of momentum and energy:

$$\frac{\partial P}{\partial t} - \frac{\partial \widetilde{b}}{\partial x} = f^{th} + \widetilde{f}^{intr}, \quad \frac{\partial (S\theta)}{\partial t} + \frac{\partial \widetilde{Q}}{\partial x} = h^{th} + \widetilde{h}^{intr}, \tag{21}$$

with dissipation

$$\Phi = \widetilde{h}^{intr} - \left(\frac{Q - \eta\dot{\varphi}}{\theta}\right)\frac{\partial \theta}{\partial x} \geq 0, \tag{22}$$

where we have introduced the new definitions [11]:

$$\begin{aligned} \widetilde{\tau} &\equiv -\frac{\delta \overline{W}}{\delta \varphi} := -\left(\frac{\partial \overline{W}}{\partial \varphi} - \frac{\partial}{\partial x}\left(\frac{\partial \overline{W}}{\partial \varphi_x}\right)\right) = \tau - \eta_x, \\ \widetilde{b} &= -\left(\rho_0 v^2/2 - W + \sigma u_x - \eta\varphi_x\right). \end{aligned} \tag{23}$$

In this formulation the Eshelby stress $\widetilde{b}$ complies with its role of grasping all effects presenting gradients since the gradient of φ plays a role parallel to that of the deformation gradient u_x. The dissipation inequality (22) is automatically satisfied in the isothermal case if $\widetilde{\tau} = k\dot{\varphi}$ with $k \geq 0$ since

$$\Phi = k\dot{\varphi}^2 \geq 0. \tag{24}$$

The fully non-dissipative case corresponds to $k = 0$.

The simplest free energy dependence is a quadratic function [2]

$$\overline{W} = \frac{\rho_0 c^2}{2}u_x^2 + A\varphi u_x + \frac{1}{2}B\varphi^2 + \frac{1}{2}C\varphi_x^2. \tag{25}$$

Accordingly, the stress components $(17)_{3,4}$ are determined as follows:

$$\sigma = \frac{\partial \overline{W}}{\partial u_x} = \rho_0 c^2 u_x + A\varphi, \quad \eta = -\frac{\partial \overline{W}}{\partial \varphi_x} = -C\varphi_x, \tag{26}$$

and τ coincides with the interactive internal force

$$\tau = -\frac{\partial \overline{W}}{\partial \varphi} = -Au_x - B\varphi. \tag{27}$$

Consequently, the balance of linear momentum is rewritten as

$$u_{tt} = c^2 u_{xx} + \frac{A}{\rho_0}\varphi_x, \tag{28}$$

and the evolution equation for the internal variable in the fully non-dissipative case (with $k = 0$) reduces to

$$C\varphi_{xx} - Au_x - B\varphi = 0. \tag{29}$$

Evaluating the first space derivative of the internal variable from the last equation

$$\varphi_x = \frac{C}{B}\varphi_{xxx} - \frac{A}{B}u_{xx}, \tag{30}$$

and its third space derivative from eqn. (28)

$$\frac{A}{\rho_0}\varphi_{xxx} = \left(u_{tt} - c^2 u_{xx}\right)_{xx}, \tag{31}$$

we will have, inserting the results into the balance of linear momentum

$$u_{tt} = c^2 u_{xx} + \frac{C}{B}\left(u_{tt} - c^2 u_{xx}\right)_{xx} - \frac{A^2}{\rho_0 B} u_{xx}. \tag{32}$$

It is clear that the obtained equation covers the first three models of the dispersive wave propagation mentioned in the Introduction. Equation (32) is the most general model for the dispersive wave motion provided by the standard internal variable theory. To go further, we need to introduce one more internal variable following [18].

4 Dual Internal Variables

Now we suppose that the free energy depends on the internal variables φ, ψ and their space derivatives $W = \overline{W}(u_x, \varphi, \varphi_x, \psi, \psi_x)$. Then the constitutive equations follow

$$\sigma := \frac{\partial \overline{W}}{\partial u_x}, \quad \tau := -\frac{\partial \overline{W}}{\partial \varphi}, \quad \eta := -\frac{\partial \overline{W}}{\partial \varphi_x}, \quad \xi := -\frac{\partial \overline{W}}{\partial \psi}, \quad \zeta := -\frac{\partial \overline{W}}{\partial \psi_x}. \tag{33}$$

We include into consideration the non-zero extra entropy flux similarly to the case of one internal variable

$$K = -\theta^{-1}\eta\dot{\varphi} - \theta^{-1}\zeta\dot{\xi}. \tag{34}$$

The generalization of the internal variable theory to the case of two internal variables is straightforward. The canonical equations of momentum and energy keep their form with appropriate modifications. It can be checked that in the considered case the intrinsic source terms are determined as follows

$$\widetilde{f}^{intr} := (\tau - \eta_x)\varphi_x + (\xi - \zeta_x)\psi_x, \quad \widetilde{h}^{intr} := (\tau - \eta_x)\dot{\varphi} + (\xi - \zeta_x)\dot{\psi}. \tag{35}$$

The latter means that the dissipation inequality in the isothermal case reduces to

$$\widetilde{h}^{intr} = (\tau - \eta_x)\dot{\varphi} + (\xi - \zeta_x)\dot{\psi} \geq 0. \tag{36}$$

It is easy to see that in the non-dissipative case ($\widetilde{h}^{intr} = 0$) the dissipation inequality (36) can by satisfied by the choice

$$\dot{\varphi} = L(\xi - \zeta_x), \qquad \dot{\psi} = -L(\tau - \eta_x), \tag{37}$$

where L is a coefficient. The latter two evolution equations express the duality between them: one internal variable is driven by another one and vice versa.

Keeping a quadratic function as the free energy dependence

$$\overline{W} = \frac{\rho_0 c^2}{2} u_x^2 + A\varphi u_x + \frac{1}{2}B\varphi^2 + \frac{1}{2}C\varphi_x^2 + \frac{1}{2}D\psi^2, \tag{38}$$

we include for simplicity only the contribution of the second internal variable itself. In this case, the stress components are the same as previously

$$\sigma = \frac{\partial \overline{W}}{\partial u_x} = \rho_0 c^2 u_x + A\varphi, \quad \eta = -\frac{\partial \overline{W}}{\partial \varphi_x} = -C\varphi_x, \quad \zeta = -\frac{\partial \overline{W}}{\partial \psi_x} = 0, \tag{39}$$

as well as the interactive internal force τ

$$\tau = -\frac{\partial \overline{W}}{\partial \varphi} = -Au_x - B\varphi. \tag{40}$$

The only new term is

$$\xi = -\frac{\partial \overline{W}}{\partial \psi} = -D\psi. \tag{41}$$

It follows from eqns. (37), $(39)_3$, and (41) that

$$\dot{\varphi} = -LD\psi, \tag{42}$$

i.e., the dual internal variable ψ is proportional to the time derivative of the primary internal variable $\dot{\varphi}$ in this particular case. It follows immediately from eqn. (42) that the evolution equation for the dual internal variable $(37)_2$ can be rewritten in terms of the primary one as the hyperbolic equation

$$\ddot{\varphi} = L^2 D(\tau - \eta_x). \tag{43}$$

As a result, we can represent the equations of motion in the form, which includes only primary internal variable,

$$u_{tt} = c^2 u_{xx} + \frac{A}{\rho_0}\varphi_x, \quad I\varphi_{tt} = C\varphi_{xx} - Au_x - B\varphi, \tag{44}$$

where $I = 1/(L^2 D)$ is an internal inertia measure.

In terms of stresses introduced by eqn. (33), the same system of equations is represented as

$$\rho_0 \frac{\partial^2 u}{\partial t^2} = \frac{\partial \sigma}{\partial x}, \quad I\frac{\partial^2 \varphi}{\partial t^2} = -\frac{\partial \eta}{\partial x} + \tau. \tag{45}$$

It is worth to note that the same equations are derived in [4] based on different considerations.

Again, we can determine the first space derivative of the internal variable from eqn. $(44)_2$

$$\varphi_x = -\frac{I}{B}\varphi_{ttx} + \frac{C}{B}\varphi_{xxx} - \frac{A}{B}u_{xx}, \tag{46}$$

and its third derivatives from eqn. $(44)_1$

$$\frac{A}{\rho_0}\varphi_{xxx} = \left(u_{tt} - c^2 u_{xx}\right)_{xx}, \quad \frac{A}{\rho_0}\varphi_{ttx} = \left(u_{tt} - c^2 u_{xx}\right)_{tt}. \tag{47}$$

Inserting the results into the balance of linear momentum $(44)_1$, we obtain a more general equation

$$u_{tt} = c^2 u_{xx} + \frac{C}{B}\left(u_{tt} - c^2 u_{xx}\right)_{xx} - \frac{I}{B}\left(u_{tt} - c^2 u_{xx}\right)_{tt} - \frac{A^2}{\rho_0 B} u_{xx}. \tag{48}$$

It is easy to see, identifying $A^2 = c_A^2 B\rho_0, C = Ic_1^2, B = I/p^2$, that the obtained equation is nothing else but the general model of the dispersive wave propagation (6).

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