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Polish Academy of Sciences
Institute of Fundamental Technological Research

Archives of Mechanics

Archiwum Mechaniki Stosowanej

volume 50 issue 3

FIFTY YEARS OF THE ARCHIVES OF MECHANICS

Polish Scientific Publishers PWN
Warszawa 1998

ARCHIVES OF MECHANICS IS DEVOTED TO Theory of elasticity and plasticity • Theory of nonclassical continua • Physics of continuous media • Mechanics of discrete media • Nonlinear mechanics • Rheology • Fluid gas-mechanics • Rarefied gas • Thermodynamics

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Printed in Poland, Editorial Office: Świętokrzyska 21,
00-049 Warszawa (Poland)

e-mail: publikac@ippt.gov.pl

Arkuszy wydawniczych 23. Arkuszy drukarskich 20,75.
Papier offset. kl. III 70 g. B1.
Oddano do składania w maju 1998 r.
Druk ukończono w lipcu 1998 r.
Skład i łamanie: "MAT-TEX"
Druk i oprawa: Drukarnia Braci Grodzickich, Żabieniec ul. Przelotowa 7

Professor HENRYK ZORSKI

Arch. Mech., 50, 3, p. 343, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

Preface

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

THIS VOLUME of the Archives of Mechanics contains papers presented at the Fourth Meeting on Current Ideas in Mechanics and Related Fields held in Kraków, at the Collegium Maius of the Jagiellonian University, from August 25-th through 28-th, 1997. Following in format and in spirit the previous three meetings (Portland – 1991, Banff – 1993 and Segovia – 1995) this symposium was of a special character, as its main feature was the celebration of the 70-th birthday of Professor HENRYK ZORSKI.

HENRYK ZORSKI, who formally retired from the Department of Mechanics of Liquids and Gases of the Institute of Fundamental Technilogical Research of the Polish Academy of Sciences, obtained his PhD in 1955. He joined the Institute in 1957 becoming in 1960 the head of the Theory of Elasticity Division. He received his promotion to the rank of Professor in 1962 and in 1969 was appointed to the chair of the Department of the Theory of Continuous Media. After eleven years at the helm of this department he moved in 1980 to chair the Department of Mechanics of Liquids and Gases. Over the period of his tenure at IFTR he supervised 18 PhD students, a number of DSc (habilitation) candidates and served on numerous PhD thesis and DSc dissertation committees. These and many more colleagues have been greatly influenced by HENRYK ZORSKI; his research, his enthusiasm and, in perticular, his leadership.

His research interests range from the theory of plates and shells, elasticity and thermoelasticity to mechanics of media with microstructure and the theory of defects in solids. He has published to date about 100 papers and has edited several conference proceedings. HENRYK ZORSKI has also been very active in promoting mechanics on both the domestic and the international arena. Together with R.S. RIVLIN and G. FICHERA he founded in 1977 the International Society for the Interaction of Mechanics and Mathematics, becoming its first Secretary and Treasurer and later its Vice-President. In 1975, also with RONALD RIVLIN, he organized at Jodłowy Dwór the first International Symposium on Continuous Models and Discrete Systems starting a series of regularly held meetings known as CMDS's, the most recent one held in St. Constantine in 1995. His extensive contributions to different areas of mechanics were recognized by his election to a number of Polish and international scientific societies, to the Academy of Sciences in Bologna and to the General Assembly of the International Union of Theoretical and Applied Mechanics. In 1989 HENRYK ZORSKI was elected a Corresponding Member of the Polish Academy of Sciences.

All participants would like to dedicate this volume to HENRYK ZORSKI in celebration of his work.

Marek Elżanowski (Portland) *Marcelo Epstein* (Calgary) *Romuald Kotowski* (Warsaw)

Arch. Mech., 50, 3, pp. 345–365, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

Lagrangian field theory of plasticity and dislocation dynamics
Attempts towards unification with thermodynamics of irreversible processes (*)

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

K.–H. ANTHONY and A. AZIRHI (PADERBORN)

WITHIN THE LAGRANGE FORMALISM, a mechanical continuum theory of dislocation dynamics is presented, which results in a phenomenological, unified description of elastic and plastic deformations of a crystal. Further developments towards a thermo-mechanical theory including dissipation are methodically envisaged. The theory is based on complex matter fields and vortex potentials as fundamental field variables. Especially the dislocation network is divided into different classes of equal dislocations, giving rise to a more refined description of the dislocation dynamics as traditionally can be done by the well-known dislocation density tensor. Each class of dislocations is associated with a complex dislocation field. The elastic interaction between dislocations of different classes results in correlational effects which cannot be described by means of the traditional continuum theory of dislocations. Whereas in traditional approaches the plastically deforming body is formally looked upon as an elastic solid with inherent flow properties, we are looking at such a system in a reverse manner: The plastically deforming body is formally regarded as a fluid with inherent solid properties. Formally the plastically deforming body is associated with a generalized Cosserat fluid based on matter and dislocation fields. In this way we overcome the difficulties due to the deformation chaos produced by dislocation motion.

1. The aim

WITHIN THE FRAMEWORK of Lagrange formalism (LF) we aim at a phenomenological plasticity theory based on dislocation dynamics. The theory is intended as a *methodical unification of elasticity and plasticity.* It will be a dynamical generalization of the well-established eigenstress theory of dislocations. Plasticity being extremely dissipative we finally intend to include thermodynamics of irreversible processes (TIP) along the unifying procedure of LF. With regard to

(*) Conventions: Tensors are marked by bold-type symbols. If not stated otherwise, indices occurring twice in a product imply summation over the range of the index.

TIP the theory of plasticity will be formulated in quite a different manner as compared with traditional attempts.

Roughly speaking, the whole information on static elasticity of a deformable body is contained in an elastic potential $W(\nabla\vec{u}) = W(\mathbf{e})$, W being the density of elastic energy, $\vec{u}$ the elastic displacement field and $\mathbf{e}$ the associated strain tensor. The function W is the kernel of the elastic energy functional U, which in statics defines the fundamental variational principle of minimal energy:

$$U = \int_V W\, dV = \text{minimum}, \tag{1.1}$$

by free variation of $\vec{u}$.

The associated Euler–Lagrange equations (ELEqs.),

$$\nabla\cdot\boldsymbol{\sigma} = 0, \tag{1.2}$$

are the equilibrium conditions, i.e. the fundamental dynamical equations in the case of statics.

$$\boldsymbol{\sigma} = \frac{\partial W}{\partial \mathbf{e}} \tag{1.3}$$

defines the constitutive equations for the stress tensor $\boldsymbol{\sigma}$.

The dynamical generalization of Eq. (1.1) is *Hamilton's variational principle*:

$$J = \int_{t_1}^{t_2}\int_V l(\vec{u}, \partial_t\vec{u}, \nabla\vec{u})\, dV\, dt = \text{extremum}, \tag{1.4}$$

by free variation of $\vec{u}$.

Now the total information on the processes is involved in the Lagrangian l. The ELEqs. as the fundamental field equations are the *equations of motion*:

$$\partial_t \frac{\partial l}{\partial(\partial_t\vec{u})} + \nabla\cdot\frac{\partial l}{\partial(\nabla\vec{u})} - \frac{\partial l}{\partial\vec{u}} = 0\,. \tag{1.5}$$

Obviously, there are two remarkable features involved in the theory: There are *universal structures* (Eqs. (1.1)–(1.5)), which apply in the same way to all elastic materials, whereas the particular forms of the functions $W(\mathbf{e})$ and $l(...)$ are *individual structures*, which depend on the particular material. They have to be fitted to experimental data (elastic moduli)([1]).

([1]) It should be mentioned that the frequently used formula "kinetic minus potential (elastic) energy" for l is but a dogma, which belongs to the individual structures insofar, as it only approximately describes the dynamics of an elastically deformed body. An exact Lagrangian for this case will be given in this paper, too.

We aim at a generalization of this unifying procedure in such a way as to imply the dynamics of plasticity. From the very beginning this theory will be based on dislocation dynamics. In this paper we shall confine our considerations to pure mechanics, adding perspectives for the inclusion of TIP. Single crystals are the systems we have in mind. Dissipation, which is a main feature of plasticity, will be involved in a future step.

2. The physical situation – fundamental ideas

2.1. Deformation chaos

On the microscale, the phenomenological plasticity is based on dislocation dynamics. *Dislocation motion*, however, *is associated with deformation chaos* [1]. The situation is demonstrated by means of the cartoon in Fig. 1:

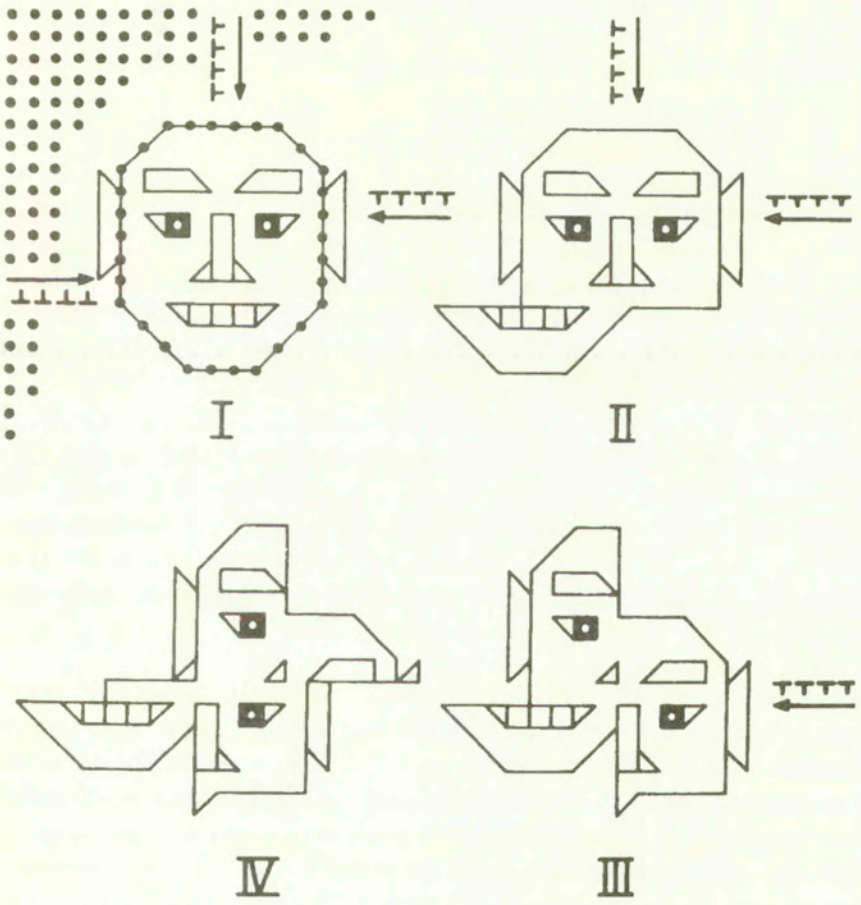

FIG. 1. Deformation chaos due to dislocation motion.

One after the other, three dislocation cascades are running through the crystal. The crystal lattice remains almost perfect except for the actual sites of the dislocations. Nevertheless the crystal gets chaotically torn; material neighbourhoods get completely destroyed. The scales relevant for this chaos are given by the relevant scales of the dislocation network, i.e. by the distances of the active glide planes and by the lengths of the running dislocation cascades. This means, however, that the relevant scales reach from micro to macro-dimensions. In this context one should keep in mind the sliplines and Lüders-bands which can be seen on the surface of a plastically torn specimen nearly with naked eyes.

As a consequence of this situation the traditional concepts for the deformation of solids have to be left. Neither a displacement field nor a material coordinate system dragged along with a deformation makes physical sense; *the plastically deformed body is not a material manifold!*

■ We look at the plastically deforming body by means of *mass densities* and *fluxes*. That's the point of view of TIP, which will be a guide-line throughout our whole approach. Within Lagrange formalism this sight will be realized by means of complex *matter fields*. ■

2.2. Correlational effects

Traditional dislocation theory is based on the *dislocation density* tensor α which geometrically is associated with torsion of the dislocated crystal lattice. This tensor, however, is locally but an averaged measure of the dislocation arrangement. It might vanish even though a vivid dynamics of dislocations of opposite signs takes place in plasticity. So, correlational effects, kinematical as well as dynamical ones, have to be taken into account in plasticity by means of non-traditional tools.

■ We look at dislocation dynamics in a more refined way by dividing the dislocation network into different *classes of equal dislocations* [1, 2, 3, 22]. Within LF each class will be associated with a *complex dislocation field*. Along this line we are particularly able to introduce into LF the interactions between dislocations of different types; we thus take account of correlations within the dislocation network. For realistic plasticity problems only a few classes are really relevant. ■

2.3. Thermodynamics and plasticity

The dislocation network is *far away from thermal equilibrium*. The energy of a dislocation per atomic unit length is 1 ... 10 eV, whereas the thermal energy at room temperature is $kT \sim 1/20$ eV. Dislocation dynamics is extremely dissipative, even at a very low plastic deformation rate. As a consequence there is *no reversible plastic deformation process*, i.e. there is *no thermostatics of plasticity available* which could be extrapolated into the regime of non-equilibrium thermodynamics, e.g. along the line of Onsager's approach to TIP [4].

■ Lagrange formalism allows for any dynamics, even far away from equilibrium. So, especially with regard to thermal effects, we describe dislocation dynamics and plasticity within the framework of LF [1, 2, 3, 22].

It has been shown that TIP can be involved in LF, too [5, 6, 7]. As an essential feature of this theory each degree of freedom, which gives rise to entropy production, has to be represented by a complex field variable. Especially this holds for disipative degrees of freedom. The entropy concept, which is involved in the theory in a natural and straightforward way, is associated with the invariance of the Lagrangian with respect to a common gauge transformation of all complex field variables [8]. As a methodical consequence, all dissipative processes have to be described by means of complex field variables. This is the reason for introducting complex matter and dislocation fields into our approach to plasticity, as has been mentioned above.

LF as applied to TIP is based on the most fundamental, *complex field of thermal excitation* or the *thermion field*(2) ψ. Dissipation of mechanical energy during plastic deformation will be modelled in LF as an irreversible energy transfer from mechanical degrees of freedom, i.e. from matter and dislocation fields, to thermal degrees of freedom, i.e. to the thermion field [22]. ■

2.4. Creation and annihilation processes in plasticity

There are essentially three regions in the stress-strain curve of a plastically deformed body [11, 12]: Increasing the external load of a body, the initial elastic region is followed by an extended region of plastic softening which finally is followed by a region of plastic hardening. The dynamics of dislocations, i.e. dislocation motion, dislocation reactions, creation and annihilation of dislocations, pinning and depinning of dislocations, are responsible with different relevance for the various regions. Especially the plastic softening is related to a dramatic increase of dislocations due to the activities of Frank — Read sources. Except for the motion of dislocations, all these elementary processes can be looked upon as creation and annihilation processes of mobile and immobile dislocations. They are essentially dissipative.

■ In LF the various *elementary processes of dislocation dynamics will be modelled* step by step by an *appropriate coupling of the various fundamental fields in the Lagrangian.*

With regard to motion, creation and annihilation there are *close analogies between the dynamics of dislocations and ordinary chemical reactions* [13]. The latter ones have already been successfully involved into LF by means of complex matter fields associated with the chemically reacting species [7]. They are physically related with point-like objects like atoms or molecules. Dislocations, however, are line-shaped objects. We take account of this peculiarity by means of the geometrical concept of torsion in a *generalized Cosserat-continuum* [1, 2,

(2) This nomenclature is due to the quantization of the thermal excitation field [9, 10].

3, 14, 22], whereas the complex dislocation fields associated with different dislocation classes are directly analogous to the matter fields of chemical species. ■

2.5. Stability theory and dislocation dynamics

It is quite evident that *stability and instability considerations of dislocation dynamics*. We refer to plane pinning and depinning of dislocations and to the bow-out threshold of Frank–Read sources. So, the modelling of plastic behaviour has to take into account stability considerations from the very beginning.

■ *In LF there is involved a stability theory in the sense of Lyapunov's direct method* [8]. This holds in a particular manner in the case of TIP based on complex fundamental field variables. A Lyapunov functional can be established from the Lagrangian in an easy and straightforward manner. This structure will play an important role in our future efforts to model plasticity. ■

Summing up the preceding arguments one can say, that Lagrange formalism is an appropriate tool to describe plasticity from the mechanical as well as from the thermodynamical point of view. Looking further at elasticity, which in the past has more or less successfully been established with LF, a methodically unified description of both deformation modes, the elastic and the plastic one, is a most attractive feature of LF.

3. Design of the theory – formal ingredients ([3])

3.1. The Cosserat-fluid as a model for plasticity

Traditionally a plastically deforming crystal has *formally* been looked upon as an elastic solid with particular (plastic) flow properties. We adopt an alternative view: *A plastically deforming crystal will formally be looked upon as a fluid with particular solid (elastic) properties*! In this way we avoid the concept of a material manifold ([4]) from the very beginning, i.e. we get rid of the difficulties associated with the deformation chaos of a plastically deformed body. One should keep in mind, that the deformation of a solid may equally well be looked upon as a material flow!

THE MODEL:

Formally we introduce the concept of a *generalized Cosserat fluid* [2, 3, 14, 22]. This is the quintessence of a *flowing, material carrier*, the elements (mass points) of which are endowed with an *internal structure in the form of deformable triads of Cosserat directors. The flow of the carrier is physically associated with the phenomenological material flow of the deforming crystal*, whereas the *directors*

([3]) The subsequent Subsecs. 3.1–3.3 refer to the Subsecs. 2.1–2.3, respectively.

([4]) In the usual mathematical sense, of course!

are physically associated with the elementary lattice vectors of the crystal. The elastic response of the crystal is locally modelled by the deformation status of the director triad. In a generalized Cosserat-continuum [14] *the deformations of the material carrier and of the director triads are in principle independent.* However, with regard to plasticity of a crystal and depending on the actual deformation modus of the crystal, *there will be particular kinematical couplings between the flow of the material carrier and the deformation of the director triads.* Especially *in the case of dislocation motion*, i.e. of plastic deformation of the crystal, *the dislocation fields will be involved in these kinematical couplings.* It is evident, that this concept takes account of elastic and of plastic deformation simultaneously and in a methodically unified way.

All relevant physical structures of the crystal are embedded in the material carrier. In the case of plasticity this will happen with the dislocation fields, and – taking account of thermo-mechanical effects (dissipation) – it will happen with the thermion field, too, etc.

The *material carrier* is formally described by means of a *complex matter field* Ψ and a *complex vortex potential* Ω as fundamental field variables:

$$\Psi(x,t) = \sqrt{\varrho(x,t)}\,\exp(i\Phi(x,t)), \tag{3.1}$$

$$\Omega(x,t) = \sqrt{\Lambda(x,t)}\,\exp(iM(x,t)). \tag{3.2}$$

They give rise to the definition of the *mass density*

$$\varrho(x,t) = \Psi^*(x,t)\Psi(x,t) \geq 0, \tag{3.3}$$

of the *flow velocity*

$$\vec{v}_{(f)}(x,t) = \nabla\Phi(x,t) + \Lambda(x,t)\nabla M(x,t), \tag{3.4}$$

and of the *vortex field*

$$\vec{\omega}(x,t) = \frac{1}{2}\nabla\times\vec{v}_{(f)}(x,t) = \frac{1}{2}\nabla\Lambda(x,t)\times\nabla M(x,t) = \frac{1}{2i}\nabla\Omega^*(x,t)\times\nabla\Omega(x,t) \tag{3.5}$$

as secondary field variables, all of them being identified with the respective physical quantities of the crystal.

With regard to the Eqs. (3.4) and (3.5), the quantities Φ, Λ and M are known as *Clebsch* or *Monge potentials* [24]. In three dimensions such a Clebsch-ansatz can always be done. However, the three potentials are not unique; they are associated with a non-Lie gauge group ([5]). It can be shown, that by properly

([5]) This group becomes essential with regard to the definition of area-type balance equations [15]. See also the paper of M. Scholle [16].

regauging of the Clebsch potentials, the property

$$\Lambda(x,t) = \Omega^*(x,t)\Omega(x,t) \geq 0 \tag{3.6}$$

can always be assumed. Thus, the definition of the complex vortex potential Ω is justified.

Let $\vec{e}_i$, $i = 1,2,3$ be the local base vectors of an external, Cartesian coordinate system x^i. Then the *three Cosserat directors*

$$\vec{a}_\kappa(x,t) = A^i_\kappa(x,t)\vec{e}_i\,, \qquad \kappa = 1,2,3, \tag{3.7}$$

are another set of fundamental field variables. They are defined by a non-singular component matrix $A^i_\kappa(x,t)$, the inverse matrix of which is $A^\kappa_i(x,t)$:

$$A^i_\kappa A^\lambda_i = \delta^\lambda_\kappa\,, \qquad A^i_\kappa A^\kappa_j = \delta^i_j\,. \tag{3.8}$$

The Cosserat directors give rise to the definition of secondary quantities such as the *elastic strain tensor* [17]

$$\mathbf{e}(x,t) = (e_{\kappa\lambda}), \qquad e_{\kappa\lambda} = \frac{1}{2}(\vec{a}_\kappa \cdot \vec{a}_\lambda - \delta_{\kappa\lambda}) = \frac{1}{2}\left(A^i_\kappa A^j_\lambda \delta_{ij} - \delta_{\kappa\lambda}\right), \tag{3.9}$$

(6)

and the *affine director connexion* [18]

$$\Gamma(x,t) = \left(\Gamma_{ij}{}^k\right), \qquad \Gamma_{ij}{}^k = A^k_\mu \partial_i A^\mu_j\,, \tag{3.10}$$

which in the Cosserat fluid defines a *director parallelism*. In the associated crystal both quantities are identified with the *elastic lattice strain* and the *lattice parallelism*, respectively. The *torsion* involved in the director parallelism is defined by the *torsion tensor* [17, 18]

$$\mathbf{S} = \left(S_{ij}{}^k\right), \qquad S_{ij}{}^k = \Gamma_{[ij]}{}^k = A^k_\mu \partial_{[i} A^\mu_{j]}\,, \tag{3.11}$$

which in the crystal lattice is identified with the (traditional) *dislocation density tensor* $\boldsymbol{\alpha}$ [17, 19]:

$$\alpha_{ij}{}^k = S_{ij}{}^k. \tag{3.12}$$

Obviously the complete traditional deformation concept of an elastically deformed and dislocated crystal has been taken over into the model of the Cosserat fluid. However, using the complex fields Ψ and Ω, the deformation of the material carrier is considered as a flow (Eqs. (3.4), (3.5)). This holds for *elastic and plastic deformations of the crystal*. We thus get rid of the traditional, conceptual

(6) The Euclidean scalar product is involved.

difficulties associated with the deformation chaos, i.e. *there is no displacement field involved in the theory.*

REMARK. One should keep in mind that the *complex* fields Ψ and Ω fit into the entropy concept of LF as applied to TIP [8]. The dynamics of the directors $\vec{a}_\kappa$, however, gives rise to dissipation too. So, these quantities have finally to be also represented by complex fields. This can be done on the basis of a threefold Clebsch-ansatz

$$\vec{a}^\kappa = \nabla\varphi^\kappa + \xi^\kappa \nabla\eta^\kappa, \qquad \kappa = 1,2,3, \tag{3.13}$$

(7)

with

$$\nabla \times \vec{a}^\kappa = \nabla\xi^\kappa \times \nabla\eta^\kappa \neq 0, \tag{3.14}$$

if the director fields are endowed with torsion, i.e. if dislocations are present in the crystal.

Now we distinguish three deformation modes of the Cosserat fluid:

(I) The compatibly, i.e. elastically deforming crystal containing no dislocations is associated with a Cosserat fluid, the directors of which are completely *substantially dragged along* with the carrier's flow. The Cosserat triads are holonomic [18] and they are deforming holonomically. The reader should imagine a compatibly deforming crystal lattice, the lattice points and lattice vectors of which are identified with the material carrier and the directors of the Cosserat-fluid.

(II) The elastically deforming crystal contains dislocations which are fixed in the crystal lattice. This deformation mode is but *a dynamical generalization of the well-known statical eigenstress problem of dislocations* [19]. It is modelled by a Cosserat-fluid, the directors of which are still substantially dragged along with the carrier's flow. The dislocations are substantially dragged along with the deforming crystal, i.e. with the carrier's flow. Speaking in mathematical terms the director triads are anholonomic; however, they are deforming holonomically.

(III) The plastically deforming crystal is associated with dislocations drifting through the crystal. This deformation mode is modelled by a Cosserat fluid, the director triads of which are anholonomic and which are deforming anholonomically; they are *partially dragged along with the fluid* according to the *drift dislocation flux*, the latter one being exclusively responsible for the plastic flow of the body.

The associated kinematical coupling equations will take into account the matter field Ψ, the vortex potential Ω, the flow field $\vec{v}_{(f)}$, the director fields $\vec{a}_\kappa$, the dislocation density $\boldsymbol{\alpha}$ and its related drift dislocation flux $\mathbf{J}$. These equations will be presented in Sec. 4 (8).

(7) See also M. Scholle: Dissertation [20]. $\vec{a}^\kappa$ are reciprocal vectors associated to $\vec{a}_\kappa$.

(8) Eqs. (4.8)–(4.11), (4.13)–(4.19).

In the cases (I) or (II, III) we call the *Cosserat fluid a compatible* or *incompatible one*, respectively. In any case the deformation state of the Cosserat triads gives rise to a local elastic response of the deforming body.

3.2. Dislocation classes and complex dislocation fields

The dislocation network is divided into different *classes of equal dislocations* (see Fig. 2), which are characterized by the set of three vectors

$$\left\{\vec{l}, \vec{b}, \vec{m}, \right\} = \{\text{line vector of the dislocation lines, Burgers vector, normal vector of the glide plane}\}. \tag{3.15}$$

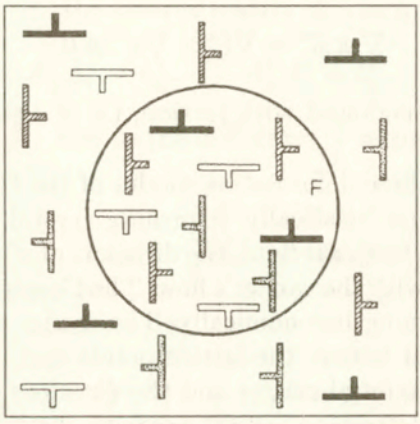

FIG. 2. Different classes of dislocations in the dislocation network.

The dislocations are topologically defined with respect to the crystal lattice: The three vectors are constant with respect to the Cosserat triads, i.e. with respect to the lattice geometry:

$$\vec{l} = l^{\kappa}\vec{a}_{\kappa}, \qquad \vec{b} = b^{\kappa}\vec{a}_{\kappa}, \qquad \vec{m} = m^{\kappa}\vec{a}_{\kappa}, \quad \text{all components } l^{\kappa},\ b^{\kappa},\ m^{\kappa} = \text{constants}. \tag{3.16}$$

The line vector $\vec{l}$ is assumed to be a unit vector with respect to the Cosserat triad, i.e. with respect to the lattice geometry; the line vector and the normal vector are by definition perpendicular in the same sense ([9]):

$$\vec{l} * \vec{l} = \delta_{\kappa\lambda} l^{\kappa} l^{\lambda} = 1, \qquad \vec{l} * \vec{m} = \delta_{\kappa\lambda} l^{\kappa} m^{\lambda} = 0\,. \tag{3.17}$$

Each class $\{\vec{l}, \vec{b}, \vec{m}\}$ is associated with two complex fields, with a *complex dislocation field*

$$\psi_{\{l,b,m\}}(x,t) = \sqrt{n_{\{l,b,m\}}(x,t)}\, \exp\left(i\varphi_{\{l,b,m\}}(x,t)\right), \tag{3.18}$$

([9]) i.e. with respect to the lattice metric $\mathbf{a} = (a_{\kappa\lambda} = \delta_{\kappa\lambda})$: $\vec{u} * \vec{v} = a_{\kappa\lambda} u^{\kappa} v^{\lambda}$ [18].

and with a *complex vortex potential*

$$\omega_{\{l,b,m\}}(x,t) = \sqrt{\lambda_{\{l,b,m\}}(x,t)}\exp\left(i\mu_{\{l,b,m\}}(x,t)\right). \tag{3.19}$$

From these fields we define the *scalar dislocation density within the class* $\{\vec{l},\vec{b},\vec{m}\}$,

$$n_{\{...\}}(x,t) = \psi^*_{\{...\}}(x,t)\psi_{\{...\}}(x,t) \geq 0, \tag{3.20}$$

and the *total dislocation flow velocity of class* $\{\vec{l},\vec{b},\vec{m}\}$,

$$\vec{v}_{\{...\}}(x,t) = \nabla\varphi_{\{...\}}(x,t) + \lambda_{\{...\}}(x,t)\nabla\mu_{\{...\}}(x,t). \tag{3.21}$$

$n_{\{...\}}$ is the *number of dislocations of class* $\{...\}$ *intersecting a unit test area perpendicular to the line direction* $\vec{l}$. It may equally well be interpreted as the *total length of dislocations of class* $\{...\}$ *within a unit volume*, i.e. it is also a good *thermodynamical state variable for the dislocated crystal*. Again we may assume $\lambda_{\{...\}}(x,t) \geq 0$ in the Clebsch-ansatz (3.21), which justifies the definition of the complex vortex field (3.19).

The *dislocation density tensor associated with the class* $\{\vec{l},\vec{b},\vec{m}\}$ ([10]) is the dyad

$$\boldsymbol{\alpha}_{\{l,b,m\}} = n_{\{...\}}(x,t)\,\vec{l}\otimes\vec{b}. \tag{3.22}$$

We get the *traditional, total dislocation density tensor* by superposing all classes:

$$\boldsymbol{\alpha} = \sum_{\{l,b,m\}} n_{\{...\}}(x,t)\,\vec{l}\otimes\vec{b}. \tag{3.23}$$

From (3.21) and (3.4) we obtain the *drift velocity of the dislocations of class* $\{\vec{l},\vec{b},\vec{m}\}$:

$$\vec{v}_{(d)\{...\}}(x,t) = \vec{v}_{\{...\}}(x,t) - \vec{v}_{(f)}(x,t). \tag{3.24}$$

It describes the motion of the dislocations with respect to the crystal lattice, i.e. it is associated with plastic deformation.

Having introduced the dislocation classes and its related fields (3.18) and (3.19), we result in a more refined description of dislocation dynamics than in traditional dislocation theory!

Obviously the dislocation classes are handled in an analogous way as before has been done with the carrier of the Cosserat fluid (see the fields Ψ, Ω and $\psi_{\{...\}}$, $\omega_{\{...\}}$, respectively). So, in our model the dynamics of the dislocated crystal can alternatively be looked upon as a sort of *multi-fluid model*. The vectors $\{\vec{l},\vec{b},\vec{m}\}$ are the Cosserat directors of that Cosserat fluid which is associated with the dislocation class $\{\vec{l},\vec{b},\vec{m}\}$.

([10]) Partial torsion due to class $\{\vec{l},\vec{b},\vec{m}\}$.

3.3. Thermodynamics of plasticity within LF

Looking at thermal effects of plasticity, the Cosserat fluid will further be endowed with the complex *thermion field* as the most fundamental variable of TIP within LF [5–10]:

$$\chi(x,t) = \sqrt{T(x,t)}\exp(i\eta(x,t)). \tag{3.25}$$

It gives rise to the definition of the *absolute temperature*

$$T(x,t) = \chi^*(x,t)\,\chi(x,t) \geq 0. \tag{3.26}$$

The phase function $\eta(x,t)$ is associated with the deviation of the irreversible heat transport process from local equilibrium [5, 6, 7]. Dissipation of mechanical energy during plastic deformation will be modelled as an *irreversible energy transfer* from mechanical to thermal degrees of freedom, i.e. from the matter field Ψ (Eq. (3.1)) of the Cosserat fluid and the dislocation fields $\psi_{\{lbm\}}$ (Eq. (3.18)) on the one hand to the thermion field χ (Eq. (3.25)) on the other hand. This transfer can be modelled in different ways: A direct coupling between the dislocation fields and the thermion field is discussed by Azirhi [22]. Another approach takes account of supplementary variables, which we call *transfer variables* [21].

4. The construction of the Lagrangian

4.1. The ideal hydroelastic fluid

Being a constitutive element of our Cosserat fluid, we start from the *Lagrangian of an ideal hydroelastic fluid* [24]:

$$l_{\text{fluid}} = -\varrho\left[(\partial_t\Phi + \Lambda\partial_t M) + \frac{1}{2}(\nabla\Phi + \Lambda\nabla M)^2 + W(\varrho)\right] = l_{\text{fluid}}(\varrho, \partial\Phi, \Lambda, \partial M), \tag{4.1}$$

where $W(\varrho)$ is the specific hydroelastic energy. This Lagrangian can equally well be expressed in terms of the complex matter field Ψ. The difference between both representations becomes essential only with regard to quantization, but not with respect to the present classical field theory. The form (4.1) is the simpler one for our purpose.

The ELEqs. associated with the variation of the variables ϱ, Φ, Λ, M are:

$$\delta\Phi: \quad \partial_t\varrho + \nabla\cdot[\varrho(\nabla\Phi + \Lambda\nabla M)] = 0, \tag{4.2}$$

$$\delta\varrho: \quad (\partial_t\Phi + \Lambda\partial_t M) + \frac{1}{2}(\nabla\Phi + \Lambda\nabla M)^2 - \left(\varrho\frac{\partial W}{\partial\varrho} + W\right) = 0, \tag{4.3}$$

$$\delta\Lambda: \quad [\partial_t + (\nabla\Phi + \Lambda\nabla M)\cdot\nabla]\Lambda = 0, \tag{4.4}$$

$$\delta M: \quad [\partial_t + (\nabla\Phi + \Lambda\nabla M)\cdot\nabla]M = 0. \tag{4.5}$$

Obviously (4.2) is the *mass balance equation* with the *mass flux density*

$$\vec{J}_{(\varrho)} = \varrho(\nabla\Phi + \Lambda\nabla M) \tag{4.6}$$

and the *flow velocity*

$$\vec{v}_{(f)} = \frac{\vec{J}_{(\varrho)}}{\varrho} = \nabla\Phi + \Lambda\nabla M. \tag{4.7}$$

Equation (4.3) is *Bernoulli's law* and (4.4), (4.5) together are equivalent with *Helmholtz's vortex law*. With regard to (4.7) the differential operator [...] in (4.4), (4.5) defines the substantial derivative. One can further easily show, that via Noether's theorem the Lagrangian (4.1) results in the correct balances for energy and momentum. Furthermore the mass balance (4.2) coincides with Noether's balance associated with the gauge group $\Psi \to \Psi e^{i\varepsilon}$, which is an invariance group of the Lagrangian ([11]).

4.2. The elastic crystal

We proceed to the Lagrangian of *a compatibly deforming, elastic crystal* without dislocations. Referring to our model of the compatible Cosserat fluid we are dealing with the deformation mode (I) of Subsec. 3.1. The *compatibility conditions for the holonomic and holonomically deforming Cosserat triads* are in compact and component form, respectively([12]):

$$(\vec{a}_\kappa \cdot \nabla\vec{a}_\lambda)_{[\kappa,\lambda]} = 0, \qquad \left(A^m_\kappa \partial_m A^j_\lambda\right)_{[\kappa,\lambda]} = 0, \tag{4.8}$$

$$\partial_t\vec{a}_\kappa + \vec{v}_{(f)} \cdot \nabla\vec{a}_\kappa - \vec{a}_\kappa \cdot \nabla\vec{v}_{(f)} = 0, \qquad \partial_t A^k_\kappa + v^m_{(f)}\partial_m A^k_\kappa - A^m_\kappa \partial_m v^k_{(f)} = 0. \tag{4.9}$$

The volume

$$(\vec{a}_1, \vec{a}_2, \vec{a}_3) = \mathrm{Det}\,(A^i_\kappa) = A \tag{4.10}$$

spanned by the three directors is coupled with the mass density of the material carrier:

$$A(x,t)\varrho(x,t) = m_0\,, \tag{4.11}$$

m_0 being the mass contained in the elementary cell of the crystal (atomic volume A).

([11]) One should keep in mind, that the Lagrangian (4.1) is exact. See footnote 1.

([12]) Latin and Greek indices refer to the external coordinate system x^k and to the internal director basis $\vec{a}_\kappa$, respectively.

By slightly modifying the ansatz (4.1) ([13]) and taking account of the kinematical constraints (4.8), (4.9), (4.11) by means of Lagrange multipliers $\vec{L}^{\kappa\lambda}$, $\vec{M}^{\kappa}$, N, we result in the *Lagrangian of the compatibly deforming, dislocation-free crystal*:

$$
\begin{aligned}
(4.12) \qquad l_{\text{elastic}} = & - \varrho \left[(\partial_t \Phi + \Lambda \partial_t M) + \frac{1}{2} \vec{v}_{(f)}^{\,2} + W(\vec{a}_\kappa) \right] \\
& - \vec{L}^{\kappa\lambda} \cdot (\vec{a}_\kappa \cdot \nabla \vec{a}_\lambda)_{[\kappa,\lambda]} \\
& - \vec{M}^{\kappa} \cdot \left(\partial_t \vec{a}_\kappa + \vec{v}_{(f)} \cdot \nabla \vec{a}_\kappa - \vec{a}_\kappa \cdot \nabla \vec{v}_{(f)} \right) \\
& - N(A\varrho - m_0) \\
& - \vec{K} \cdot \left(\vec{v}_{(f)} - (\nabla \Phi + \Lambda \nabla M) \right) \\
& = l_{\text{elastic}}(\varrho, \partial\Phi, \Lambda, \partial M, \vec{v}_{(f)}, \vec{L}^{\kappa\lambda}, \vec{M}^{\kappa}, N, \vec{K}).
\end{aligned}
$$

It is formulated within the *model of the compatible Cosserat fluid* and is absolutely exact ([14]). The variable $\vec{v}_{(f)}$ in the first and third row on the right-hand side of the equation has to be read as the Clebsch-ansatz (4.7). However, this results in a Lagrangian of the second order ([15]). So, in order to keep the formalism within the first order, we prefer to insert the Clebsch-ansatz by means of another Lagrange multiplier $\vec{K}$ (last row) and to join $\vec{v}_{(f)}$ to the set of independent variational variables. One can show by means of the set of Euler - Lagrange equations and by means of Noether's energy and momentum balances, that (4.12) really describes the dynamics of the dislocation-free, elastically deforming crystal. It is a remarkable fact, that we again result in the mass balance (4.2) and that the velocity field of the deformation process is defined from this balance *without making use of a displacement field* (Eq. (4.7)). From this point of view we are well prepared to proceed to the plastically deformed crystal, i.e. to the incompatible Cosserat fluid.

4.3. The dislocated crystal

In order to take account of dislocations in our Cosserat fluid model we have to liberate the system from the kinematical constraints (4.8), (4.9):

$$
(4.13) \qquad \boldsymbol{\alpha} = (\vec{a}_\kappa \cdot \nabla \vec{a}_\lambda)_{[\kappa,\lambda]} \neq 0, \qquad \alpha_{\kappa\lambda}{}^{j} - \left(A_\kappa^m \partial_m A_\lambda^j \right)_{[\kappa,\lambda]} = 0,
$$

$$
\begin{aligned}
(4.14) \qquad & \mathbf{J}_{(d)} = - \left(\partial_t \vec{a}_\kappa + \vec{v}_{(f)} \cdot \nabla \vec{a}_\kappa - \vec{a}_\kappa \cdot \nabla \vec{v}_{(f)} \right) \neq 0, \\
& J_{(d)\kappa}{}^{k} + \left(\partial_t A_\kappa^k + v_{(f)}^m \partial_m A_\kappa^k - A_\kappa^m \partial_m v_{(f)}^k \right) = 0.
\end{aligned}
$$

([13]) $W(\varrho) \Rightarrow W(\vec{a}_\kappa,\ \kappa = 1, 2, 3)$.

([14]) The most common form "density of kinetic energy minus density of the elastic energy" is but an approximate Lagrangian of the elastically deforming body (see footnote 1).

([15]) Last term in the third row.

Formally $\boldsymbol{\alpha}$ and $\mathbf{J}_{(d)}$ are the *incompatibility tensors* of the system. Physically these quantities have to be identified as follows: $\boldsymbol{\alpha}$ is the *total dislocation density tensor*, which has to be understood as the *superposition* (3.23) *of dislocations of the different dislocation classes*:

$$\boldsymbol{\alpha} = \sum_{\{l,b,m\}} n_{\{\ldots\}}(x,t)\, \vec{l} \otimes \vec{b}, \qquad \alpha^{\mu j} = \sum_{\{l,b,m\}} n_{\{\ldots\}}(x,t)\, l^{\mu} b^{j}. \tag{4.15}$$

The tensor $\boldsymbol{\alpha}$ can be taken as a third rank or a second rank tensor([16]).

$$\alpha^{\mu j} = \varepsilon^{\mu\kappa\lambda}\alpha_{\kappa\lambda}{}^{j}, \qquad \alpha_{\kappa\lambda}{}^{j} = \frac{1}{2}\varepsilon_{\mu\kappa\lambda}\alpha^{\mu j}. \tag{4.16}$$

$\mathbf{J}_{(d)}$ is the density tensor of the *drift dislocation flux*, which together with the *convective flux* $\mathbf{J}_{(f)}$ results in the total dislocation flux $\mathbf{J}$,

$$\mathbf{J} = \mathbf{J}_{(f)} + \mathbf{J}_{(d)}, \tag{4.17}$$

$$\mathbf{J}_{(f)} = -\vec{v}_{(f)} \times \boldsymbol{\alpha}, \qquad J_{(f)\kappa}{}^{j} = -\varepsilon_{\kappa\mu\nu} v^{\mu}_{(f)} \alpha^{\nu j}. \tag{4.18}$$

The drift flux is a *superposition of the partial drift fluxes associated with the dislocation classes*:

$$\begin{aligned} \mathbf{J}_{(d)} &= -\sum_{\{l,b,m\}} \vec{v}_{(d)\{l,b,m\}} \times \boldsymbol{\alpha}_{\{l,b,m\}}, \\ J_{(d)\kappa}{}^{j} &= -\sum_{\{l,b,m\}} \varepsilon_{\kappa\mu\nu} v^{\mu}_{(d)\{l,b,m\}} \alpha_{\{l,b,m\}}{}^{\nu j}. \end{aligned} \tag{4.19}$$

Here $\vec{v}_{(f)}$ and $\vec{v}_{(d)\{l,b,m\}}$ are the *flux velocity of the material carrier* and the *drift velocities of the dislocations of classes* $\{\vec{l},\vec{b},\vec{m}\}$ respectively, defined from the matter and dislocation fields by Eqs. (3.4), (3.24), (3.21).

By means of the kinematical constraints (4.13), (4.14) and using the expressions (4.15), (4.17), (4.18), (4.19) and substituting the definitions (3.4), (3.24), (3.21) for the velocities, we finally result in *kinematical constraints for the dynamical eigenstress problem of a crystal with dislocations as well as for the plastically deforming crystal.* In the case of the dynamical eigenstress problem the dislocation fields $\psi_{\{\ldots\}}$ are different from zero but the dislocation drift velocities $\vec{v}_{(d)\{\ldots\}}$ vanish (sessile dislocations). The Cosserat triads are anholonomic. Furthermore in the case of plastic deformation the Cosserat triads are deforming anholonomically, i.e. they are only partially dragged along with the carrier's flow.

([16]) A more refined consideration may distinguish between tensors and tensor densities according to the permutation symbols $\in^{\mu\kappa\lambda}$ and $\in_{\mu\kappa\lambda}$ which – precisely speaking – are no tensors but "tensor densities of weight 1 and -1", respectively [25].

The dislocations are moving with respect to the crystal, i.e. their drift velocities $v_{(d)\{l,b,m\}}$ are different from zero.

We are now prepared to write down the *pure mechanical Lagrangian of the dynamical eigenstress problem* of a crystal with sessile dislocations, and – simultaneously – of a *plastically deforming crystal* with moving dislocations. The Lagrangian (4.12) of the compatible Cosserat fluid will slightly be extended:

$$
\begin{aligned}
(4.20)\qquad l_{\text{plastic}} = &-\varrho\left[(\partial_t\Phi + \Lambda\partial_t M) + \frac{1}{2}\vec{v}^{\,2}_{(f)}\right] \\
&- \varrho\left[\frac{1}{2}\Theta^{\kappa\lambda} D_t\vec{a}_\kappa \cdot D_t\vec{a}_\lambda + W(\vec{a}_\kappa, \nabla\vec{a}_\kappa)\right] \\
&- \sum_{\{l,b,m\}} m_{\{l,b,m\}} n_{\{l,b,m\}}\left[(\partial_t\varphi_{\{l,b,m\}} + \lambda_{\{l,b,m\}}\partial_t\mu_{\{l,b,m\}}) + \frac{1}{2}\vec{v}^{\,2}_{\{l,b,m\}} + \varepsilon_{\{l,b,m\}}\right] \\
&+ L^{\kappa\lambda}{}_j\left[\frac{1}{2}\in_{\kappa\lambda\mu}\sum_{\{l,b,m\}}(n_{\{l,b,m\}} l^\mu b^j) - (A^m_\kappa \partial_m A^j_\lambda)_{[\kappa,\lambda]}\right] \\
&+ M^\kappa{}_j\left[\in_{\kappa\lambda\mu}\sum_{\{l,b,m\}}((v^\lambda_{\{l,b,m\}} - v^\lambda_{(f)}) n_{\{l,b,m\}} l^\mu b^j) - \left(\partial_t A^j_\kappa + v^m_{(f)}\partial_m A^j_\kappa - A^m_\kappa \partial_m v^j_{(f)}\right)\right] \\
&- N\left[A\varrho - m_0\right] \\
&- \vec{K}_1 \cdot \left[\vec{v}_{(f)} - (\nabla\Phi + \Lambda\nabla M)\right] \\
&- \sum_{\{l,b,m\}} \vec{K}_{2\{l,b,m\}} \cdot \left[\vec{v}_{\{l,b,m\}} - (\nabla\varphi_{\{l,b,m\}} + \lambda_{\{l,b,m\}}\nabla\mu_{\{l,b,m\}})\right] \\
&= l_{\text{plastic}}(\varrho, \partial\Phi, \Lambda, \partial M, \vec{a}_\kappa, \partial\vec{a}_\kappa, n_{\{l,b,m\}}, , \partial\varphi_{\{l,b,m\}}, \lambda_{\{l,b,m\}}, \partial\mu_{\{l,b,m\}}, \\
&\qquad \vec{v}_{(f)}, \partial\vec{v}_{(f)}, \vec{v}_{\{l,b,m\}}, \partial\vec{v}_{\{l,b,m\}}, L^{\kappa\lambda}{}_j, M^\kappa{}_j, N, \vec{K}_1, \vec{K}_{2\{l,b,m\}}).
\end{aligned}
$$

The different terms are written in the compact tensor form and in the index form, respectively, depending on the most lucid form of the respective terms. The arguments which will take part in the variational procedure, are listed explicitly in $l_{\text{plast}}(...)$ in the last row. The plus signs in front of the multipliers L and M are chosen in succession to the respective terms in Eq.(4.12). One should keep in mind, that the line vectors $\vec{l}$ and the Burgers vectors $\vec{b}$ of the dislocations (4-th and 5-th row) are involved in the variation of the Cosserat triads according to (3.16) and (3.7). In the 2-nd row there is involved the substantial derivative

$$
(4.21)\qquad D_t = \partial_t + \vec{v}_{(f)} \cdot \nabla\,,
$$

which is necessary according to the Galilean invariance of the Lagrangian.

The theory of elasto-plastic deformation based on the *Lagrangian* (4.20) *is a reversible, pure mechanical theory.* Especially the reversibility is due to the

time reversal invariance of l_{plast} (replace: $t \Rightarrow -t$, complex fields $\Rightarrow$ conjugated complex fields, i.e. phase functions $\Rightarrow$ opposite phase functions, velocities $\Rightarrow$ opposite velocities, multipliers $M, K_1, K_2 \Rightarrow$ opposite multipliers).

The rows in l_{plastic} are in turn associated with the dynamics of the different parts of our model.

1-ST ROW: *The dynamics of the material carrier*:

As compared with (4.12) the elastic potential is now joint with the Cosserat triads. The second term defines the translational kinetic energy. The ansatz describes in the continuum picture the dynamics of a flow of free particles.

2-ND ROW: *The dynamics of the Cosserat directors*:

The first term defines the kinetic energy of the Cosserat triads. It is associated with the micro-inertia of the triads (tensor $\boldsymbol{\Theta}$). W is the elastic potential associated with the elastic energy of the crystal. As compared with l_{elast} (see (4.12)) this potential is supplemented by the lattice curvature – involved in $\nabla \vec{a}_\kappa$ – in order to account for moment stresses, which are a natural ingredient of the theory of Cosserat continua and of the dislocation theory. The 2-nd row describes the elastodynamics of the crystal.

3-RD ROW: *The dislocation dynamics of the different classes*:

For the dislocation dynamics we assume again the continuum model of a flowing medium. As already mentioned at the end of in Subsec. 3.2 we are thus formally dealing with a "multi-fluid" system. The quantity $m_{\{l,b,m\}}$ is the effective mass of the dislocations. It is related with the inertia of dislocations. The quadratic term is the kinetic energy of the dislocations, whereas $\varepsilon_{\{l,b,m\}}$ is the self-energy of the dislocation kernel [12]. The latter one will become important in a later stage of the theory, when creation and annihilation of dislocations will be taken into account.

Using the Lagrange multipliers the next rows take account of the *kinematical couplings* discussed above:

4-TH ROW: The kinematical coupling of the dislocations of all classes with the torsion involved in the field of Cosserat triads.

5-TH ROW: The kinematical coupling between the Cosserat triads and the carrier's flow via the motion of the dislocation of all classes.

6-TH ROW: The kinematical coupling of the triads with the mass of the carrier.

These three terms given rise to a dynamical coupling between the material flow (material carrier) of the medium, its elasticity (Cosserat triads) and its dislocations.

Finally a few more *formal constraints* are involved:

7-TH ROW: A formal variational constraint between the carrier's flow velocity and its Clebsch potentials.

Using this constraint we preserve again a first order Hamilton's principle (see the last term in the 5-th row).

8-TH ROW: A formal variational constraint between the dislocation flow velocities and its Clebsch potentials.

This constraint could be avoided. It is introduced because of a formal symmetry between the velocities of all "partial fluids".

The Lagrangian (4.20) completely describes the unrestricted dynamics of *freely moving dislocations* due to elastic stresses; the *Cosserat triads are the transmitters of the elastic stresses*. Under external load the dislocation motion gives rise to an accelerating flow of the material carrier, i.e. to an accelerating plastic flow of the crystal. For a more detailed discussion we refer to the forthcoming papers [22].

In reality there is a pinning of dislocations due to the discrete crystal lattice (Peierls potential) and due to the pinning of dislocations at a lot of different obstacles disturbing the perfectness of the crystal. So, in order to cause sessile dislocations to move, the local driving forces acting on dislocations (Peach – Koehler force) have to overcome particular thresholds. By means of the following considerations we are able to involve these effects into our Lagrangian field theory of plastic deformation ([17]):

The density of the Peach – Koehler force on dislocations of the class $\{\vec{l}, \vec{b}, \vec{m}\}$ is given by

$$\vec{\Gamma}_{\{l,b,m\}} = n_{\{l,b,m\}} \vec{l} \times (\boldsymbol{\sigma} \cdot \vec{b}); \tag{4.22}$$

$\boldsymbol{\sigma}$ is the local elastic stress tensor (1.3). Projecting $\vec{\Gamma}_{\{l,b,m\}}$ onto the glide plain (normal $\vec{m}$) we result in the relevant driving force acting on these dislocations:

$$\vec{\tau}_{\{l,b,m\}} = \vec{m} \times \vec{\Gamma}_{\{l,b,m\}} \times \vec{m} = (\mathbf{1} - \vec{m} \otimes \vec{m}) \cdot \vec{\Gamma}_{\{l,b,m\}} \,. \tag{4.23}$$

By definition of the P.K. force the vector $\vec{\tau}_{\{l,b,m\}}$ is perpendicular to the dislocation line. This stress gives rise to dislocation motion if and only if it overcomes the critical stress $\tau^c_{\{l,b,m\}} > 0$, which is assumed to be characteristic for each class and for each type of stability barrier:

$$|\vec{\tau}_{\{l,b,m\}}| < \tau^c_{\{l,bm\}} \Leftrightarrow \vec{v}_{(d)\{l,b,m\}} = 0 \Leftrightarrow \text{sessile dislocations}, \tag{4.24}$$

$$|\vec{\tau}_{\{l,b,m\}}| \geq \tau^c_{\{l,b,m\}} \Leftrightarrow \vec{v}_{(d)\{l,b,m\}} \neq 0 \Leftrightarrow \text{moving dislocations}. \tag{4.25}$$

Both cases can be joint together in one equation by means of Heaviside's function ([18]):

$$(\vec{v}_{(d)\{l,b,m\}} \cdot \vec{v}_{(d)\{l,b,m\}}) H({\tau^c_{\{l,b,m\}}}^2 - \vec{\tau}_{\{l,b,m,\}} \cdot \vec{\tau}_{\{l,b,m\}}) = 0 \,. \tag{4.26}$$

Obviously this equation is solved by the inequalities (4.24), (4.25).

([17]) In a more general context these questions are related with dynamical stability of the dislocation dynamics. See the remarks in Subsec. 2.5.

([18]) $H(z) = 0$ or 1 for $z \leq 0$ or $z > 0$.

Taking Eq. (4.26) into account by means of another Lagrange multiplier we pass from (4.20) to a *Lagrangian which* – in a first and lump-sum way – *takes account of a critical stress* in the phenomenological stress-strain curve of an elasto-plastic material. Locally a free motion of dislocations takes place whenever and wherever the inequality (4.25) holds. Otherwise the motion of the dislocations stops abruptly; the dislocations are pinned. Phenomenologically there are spatial regions in the deforming material where we get plastic or pure elastic deformations according to the ineqalities (4.25) or (4.24), respectively. Moving dislocations give rise to a reduction of elastic strains till we arrive at the situation (4.24), where the plastic flow stops. However, we are still dealing with a reversible, purely mechanical theory. The thresholds $\tau^c_{\{l,b,m\}}$ are not yet related with dissipation!

5. Perspectives

The theory of elasto-plastic deformation and of dislocation dynamics presented in this paper will be extented towards several goals:

The creation of dislocations *via* the Frank – Read sources can be involved in various ways: With regard to the activation barrier of Frank – Read sources there is an analogy with the relations (4.24-26). Another possibility is due to analogies between a dislocated crystal and a spin system [22, 23].

Dislocation reactions between dislocations of different classes are analogous with chemical reactions. The dynamics of the latter ones is already involved into LF [7]. Furthermore the transition from immobile to mobile dislocations and vice versa can be looked upon as creation and annihilation processes [22].

The Lagrangian (4.20) will be extended towards dissipative dislocation dynamics. A first approach is based on a direct coupling between the dislocation fields and the thermion field: Friction gives rise to a transition of the dislocations from the mobile to the immobile state [22]. Alternatively we shall attack the difficult problem of dislocation motion with friction by means of *transfer variables*, which manage the energy transfer from the mechanical to the thermal degrees of freedom. Using this method we already succeeded in the dissipation problem in point mechanics [21]. A third approach tries to take advantage of the methods of the gauge theory [20].

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FB 6, THEORETISCHE PHYSIK
UNIVERSITÄT-GH PADERBORN

Warburger Str. 100, D-33098 Paderborn, Germany
e-mail: fanth1@Lagrange.uni-paderborn.de
e-mail: azi@Lagrange.uni-paderborn.de

Received October 23, 1997.

Arch. Mech., **50**, 3, pp. 367–376, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

On two reinterpretations of Cosserat continuum: fiber bundle versus the motor calculus

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

J. BADUR (GDAŃSK) and Y. POVSTENKO (LVIV, CZĘSTOCHOWA)

IT IS THE PURPOSE of this paper to reinterprete the original Cosserat continuum from the point of view of both the fiber bundles geometry and the non-Abelian motor calculus. The main ideas of Cosserats are best explained in terms of the moving reper which is synonymous with the procedure of gauging in physics as well as with the procedure of constructing a fiber bundle in pure geometry. On the other hand, the classical (linear) von Mises motor calculus is extended to a non-Abelian case. It also appears that this non-Abelian version of the von Mises concept is fully equivalent with the fiber bundle description.

Notations

A connection,
$\mathbf{b}$ tensor of the second fundamental form,
$\mathbf{D}$ differential operator,
$\mathbf{F}$ curvature,
$\mathbf{I}$ disclination current tensor,
$\mathbf{J}$ dislocation current tensor,
$\mathbf{M}$ motor,
R curvature,
S torsion,
$\mathbf{u}$ translation vector,
$\mathbf{v}$ velocity vector,
$\mathbf{X}$ body force,
$\mathbf{Y}$ body couple,

$\boldsymbol{\alpha}$ dislocation density,
Γ connection,
$\boldsymbol{\gamma}$ strain tensor,
γ time connection,
$\boldsymbol{\varepsilon}$ antisymmetric tensor,
$\boldsymbol{\theta}$ disclination density,
$\boldsymbol{\kappa}$ bend-twist tensor,
$\boldsymbol{\mu}$ couple-stress tensor,
$\boldsymbol{\sigma}$ stress tensor,
$\boldsymbol{\varphi}$ rotation vector,

$\mathcal{A}$ one-form of fiber connection,
$\mathcal{D}$ differential operator,
$\mathcal{F}$ two-form of bundle curvature,
$\mathcal{J}$ base,
$\mathcal{M}$ base manifold,
$\mathcal{P}$ bundle,
$\mathcal{R}$ curvature,
$\mathcal{S}$ torsion.

1. Introduction

STARTING from investigations of KONDO [1] and BILBY *et al.* [2] who identified the Cartan torsion tensor with the dislocation density, development of continuum mechanics is closely associated with differential geometrical ideas and methods. The subject has been extensively developed in Refs. [3–8], among others. The tangent bundle and the connection on it are the fundamental notions of the above-mentioned studies.

The next important step was made by the gauge theory of defects (for example, see [9–11] and others). The gauge theory considers not only the tangent bundle but also more general fiber bundles. It has recently been proposed that a fiber bundle might be of considerable interest in continuum mechanics as a basis for a differential geometrical description of the complex interactions between the recoverable and the dissipative processes.

In order to describe forces and couples, translations and rotations, etc. simultaneously, VON MISES [12, 13] developed the motor algebra, an algebra of vector fields in rigid bodies. OSIPOV [14, 15] and SCHAEFER [16, 17] extended the motor algebra to the motor analysis and introduced the differential operators for motor fields. At the same time, it turns out that there is a close correlation between the motor calculus and the fiber bundle with a group $T(3) \triangleright SO(3)$ as a fiber [18–21].

In COSSERAT pioneering paper [22], the geometrization and gauging play a leading role. Recalling the Cosserat results in contemporary language, one can say that during their treatment, the properties of the mathematical model are strictly separated. All geometrical properties are carried by the base manifold, while all the physical properties are embedded within the standard fiber – structural group $T(3) \triangleright SO(3)$. The consequences of this are valuable indeed. The objects familiar for the Cauchy continuum, such as displacements, measures of deformation and stresses, equations of motion, etc. are now defined within the space of fiber bundle and, what is characteristic for the Cosserat bundle, they are completely separated from the base.

The aim of the present paper is to show the development of ideas and to reinterprete the original Cosserat continuum in terms of both the non-Abelian motor calculus and the fiber bundles geometry.

2. The Abelian motor calculus

For a given point P of a rigid body, infinitesimal translation and infinitesimal rotation are described by the translation vector $\mathbf{u}(P)$ and the rotation vector $\boldsymbol{\varphi}(P)$ forming a motor

$$\begin{pmatrix} \mathbf{u}(P) \\ \boldsymbol{\varphi}(P) \end{pmatrix}, \tag{2.1}$$

i.e. the ordered pair of two vectors which changes according to the rule

$$\begin{pmatrix} \mathbf{u}(Q) \\ \boldsymbol{\varphi}(Q) \end{pmatrix} = \begin{pmatrix} \mathbf{u}(P) + \boldsymbol{\varphi}(P) \times \overrightarrow{QP} \\ \boldsymbol{\varphi}(P) \end{pmatrix} \tag{2.2}$$

when changing a reduction point. For the following matrix notation it is convenient to use such an order of vectors forming a motor as that shown in Eq. (2.1), in contrast to that used in the literature.

The gradient and the curl of a motor field have the following form [17]:

$$\operatorname{grad} \begin{pmatrix} \mathbf{W} \\ \mathbf{V} \end{pmatrix} = \begin{pmatrix} \operatorname{grad} \mathbf{W} - \mathbf{V} \times \mathbf{1} \\ \operatorname{grad} \mathbf{V} \end{pmatrix}, \tag{2.3}$$

$$\operatorname{rot} \begin{pmatrix} \mathbf{W} \\ \mathbf{V} \end{pmatrix} = \begin{pmatrix} \operatorname{rot} \mathbf{W} - \mathbf{V} \overset{\times}{\times} \mathbf{1} \\ \operatorname{rot} \mathbf{V} \end{pmatrix} \tag{2.4}$$

with the well-known relation

$$\operatorname{rot} \operatorname{grad} \begin{pmatrix} \mathbf{W} \\ \mathbf{V} \end{pmatrix} = 0. \tag{2.5}$$

In the case of a two-dimensional surface Σ embedded in a three-dimensional space, we have [23]

$$\operatorname{grad}_\Sigma \begin{pmatrix} \mathbf{W}_\Sigma \\ \mathbf{V}_\Sigma \end{pmatrix} = \begin{pmatrix} \operatorname{grad}_\Sigma \mathbf{W}_\Sigma - \mathbf{V}_\Sigma \times \mathbf{1}_\Sigma \\ \operatorname{grad}_\Sigma \mathbf{V}_\Sigma \end{pmatrix}, \tag{2.6}$$

$$\operatorname{rot}_\Sigma \begin{pmatrix} \mathbf{W}_\Sigma \\ \mathbf{V}_\Sigma \end{pmatrix} = \begin{pmatrix} \operatorname{rot}_\Sigma \mathbf{W}_\Sigma - \mathbf{V}_\Sigma \overset{\times}{\times} \mathbf{1}_\Sigma \\ \operatorname{rot}_\Sigma \mathbf{V}_\Sigma \end{pmatrix}, \tag{2.7}$$

and

$$\operatorname{rot}_\Sigma \operatorname{grad}_\Sigma \begin{pmatrix} \mathbf{W}_\Sigma \\ \mathbf{V}_\Sigma \end{pmatrix} - \boldsymbol{\varepsilon}_\Sigma \cdot \mathbf{b} \cdot \operatorname{grad}_\Sigma \begin{pmatrix} \mathbf{W}_\Sigma \\ \mathbf{V}_\Sigma \end{pmatrix} = 0, \tag{2.8}$$

where $\mathbf{1}$ is the three-dimensional metric tensor, $\mathbf{1}_\Sigma$ and $\mathbf{b}$ are the tensors of the first and the second fundamental forms of a surface, $\boldsymbol{\varepsilon}_\Sigma$ is the surface alternating tensor.

The motor calculus is very effective in various investigations of mechanics and in the theories of defects in Cosserat continua [24–28]. For example, the equilibrium equations, the compatibility conditions and the stress-strain relations for a three-dimensional Cosserat continuum with dislocations and disclinations, can be written in very convenient concise form:

$$\operatorname{div}\begin{pmatrix}\boldsymbol{\mu}\\ \boldsymbol{\sigma}\end{pmatrix} = -\begin{pmatrix}\mathbf{Y}\\ \mathbf{X}\end{pmatrix}, \tag{2.9}$$

$$\begin{pmatrix}\boldsymbol{\alpha}\\ \boldsymbol{\vartheta}\end{pmatrix} = \operatorname{rot}\begin{pmatrix}\boldsymbol{\gamma}\\ \boldsymbol{\kappa}\end{pmatrix}, \tag{2.10}$$

$$\begin{pmatrix}\boldsymbol{\mu}\\ \boldsymbol{\sigma}\end{pmatrix} = \begin{pmatrix}\mathbf{0} & \mathbf{D}\\ \mathbf{C} & \mathbf{0}\end{pmatrix} : \begin{pmatrix}\boldsymbol{\gamma}\\ \boldsymbol{\kappa}\end{pmatrix}, \tag{2.11}$$

$$\frac{d}{dt}\begin{pmatrix}\boldsymbol{\alpha}\\ \boldsymbol{\vartheta}\end{pmatrix} = -\operatorname{rot}\begin{pmatrix}\mathbf{J}\\ \mathbf{I}\end{pmatrix}. \tag{2.12}$$

The corresponding set of equations for a Cosserat surface reads

$$\operatorname{div}_\Sigma\begin{pmatrix}\boldsymbol{\mu}_\Sigma\\ \boldsymbol{\sigma}_\Sigma\end{pmatrix} = -\begin{pmatrix}\mathbf{Y}_\Sigma\\ \mathbf{X}_\Sigma\end{pmatrix}, \tag{2.13}$$

$$\begin{pmatrix}\boldsymbol{\alpha}_\Sigma\\ \boldsymbol{\vartheta}_\Sigma\end{pmatrix} = \operatorname{rot}_\Sigma\begin{pmatrix}\boldsymbol{\gamma}_\Sigma\\ \boldsymbol{\kappa}_\Sigma\end{pmatrix} - \boldsymbol{\varepsilon}_\Sigma\cdot\mathbf{b}\cdot\begin{pmatrix}\boldsymbol{\gamma}_\Sigma\\ \boldsymbol{\kappa}_\Sigma\end{pmatrix}, \tag{2.14}$$

$$\begin{pmatrix}\boldsymbol{\mu}_\Sigma\\ \boldsymbol{\sigma}_\Sigma\end{pmatrix} = \begin{pmatrix}\mathbf{0} & \mathbf{D}_\Sigma\\ \mathbf{C}_\Sigma & \mathbf{0}\end{pmatrix} : \begin{pmatrix}\boldsymbol{\gamma}_\Sigma\\ \boldsymbol{\kappa}_\Sigma\end{pmatrix}, \tag{2.15}$$

$$\frac{d}{dt}\begin{pmatrix}\boldsymbol{\alpha}_\Sigma\\ \boldsymbol{\vartheta}_\Sigma\end{pmatrix} = -\operatorname{rot}_\Sigma\begin{pmatrix}\mathbf{J}_\Sigma\\ \mathbf{I}_\Sigma\end{pmatrix} + \boldsymbol{\varepsilon}_\Sigma\cdot\mathbf{b}\cdot\begin{pmatrix}\mathbf{J}_\Sigma\\ \mathbf{I}_\Sigma\end{pmatrix}, \tag{2.16}$$

where $\boldsymbol{\sigma}$ and $\boldsymbol{\mu}$ are the stress and the couple-stress tensor, $\boldsymbol{\gamma}$ and $\boldsymbol{\kappa}$ denote the strain tensor and the bend-twist tensor, $\boldsymbol{\alpha}$ and $\boldsymbol{\theta}$ are the densities of dislocations and disclinations, $\mathbf{J}$ and $\mathbf{I}$ are the dislocation and disclination current tensors, $\mathbf{X}$ and $\mathbf{Y}$ denote the body force and the body couple, $\mathbf{C}$ and $\mathbf{D}$ are the material constant tensors (for details see [28]).

3. The non-Abelian motor calculus

Let us consider six-parameter local transformations of E_3 consisting of three translational parameters $u_a(x^i)$, $a = 1,2,3$; $i = 1,2,3$, and three rotational parameters $\varphi_A(x^i)$, $A = 1,2,3$; $i = 1,2,3$. As stated above, in the Abelian approach the ordered pair $(u_a(x^i), \varphi_A(x^i))$ is an Abelian motor. To introduce a concept of the non-Abelian motor [18] we consider the local translation Lie group

$T(3)$, the local special orthogonal Lie group $SO(3)$, and the semi-direct product $T(3) \triangleright SO(3)$ [10]. An element $\mathbf{M}$ of this product is represented by a matrix

$$\begin{bmatrix} 1 & \mathbf{u} \\ \mathbf{0} & \mathbf{R} \end{bmatrix}_{4\times 4}, \tag{3.1}$$

where $\mathbf{u} \in T(3)$ is the translation and $\mathbf{R} \in SO(3)$ is the rotation:

$$\mathbf{R}^{\mathrm{T}}\mathbf{R} = \mathbf{1}, \qquad \det \mathbf{R} = 1. \tag{3.2}$$

The Lie algebra $t(3) \triangleright so(3)$ can be described by six matrices

$$\mathbf{T}_a = \begin{bmatrix} 0 & t_a \\ \mathbf{0} & \mathbf{0} \end{bmatrix}_{4\times 4}, \qquad \mathbf{T}_A = \begin{bmatrix} 0 & 0 \\ \mathbf{0} & \mathbf{r}_A \end{bmatrix}_{4\times 4}, \qquad a = 1,2,3, \quad A = 1,2,3 \tag{3.3}$$

with the matrices

$$\mathbf{t}_1 = (1,0,0), \qquad \mathbf{t}_2 = (0,1,0), \qquad \mathbf{t}_3 = (0,0,1), \tag{3.4}$$

$$\mathbf{r}_1 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}, \qquad \mathbf{r}_2 = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \qquad \mathbf{r}_3 = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{3.5}$$

forming the basis of the Lie algebras $t(3)$ and $so(3)$, respectively.

The Lie brackets in the Lie algebra $t(3) \triangleright so(3)$ have the following properties:

$$\begin{aligned} [\mathbf{T}_a, \mathbf{T}_b] &= 0, & [\mathbf{T}_a, \mathbf{T}_A] &= \epsilon_{aAB}\mathbf{T}_B, \\ [\mathbf{T}_A, \mathbf{T}_b] &= \epsilon_{AbC}\mathbf{T}_C, & [\mathbf{T}_A, \mathbf{T}_B] &= \epsilon_{ABC}\mathbf{T}_C \end{aligned} \tag{3.6}$$

with the structural constants given by the completely antisymmetric tensor ϵ.

In place of the ordered pair $(u_a,\ \varphi_A)$ in the Abelian theory, we consider a motor as an element of the non-Abelian group $T(3) \triangleright SO(3)$

$$\mathbf{M}(x^i) = u^a(x^i)\mathbf{T}_a + \exp\left[\varphi^A(x^i)\mathbf{T}_A\right], \tag{3.7}$$

where the tensor exponential function realizes the full matrix of a finite rotation $\mathbf{R}$.

An initial reper $\overset{\circ}{\mathbf{R}}$ containing the position vector $\overset{\circ}{\mathbf{r}}$ and the triad $\overset{\circ}{\mathbf{E}}_a$, $a = 1,2,3$, is defined as

$$\overset{\circ}{\mathbf{R}} = \left(\overset{\circ}{\mathbf{r}}, \overset{\circ}{\mathbf{E}}_1, \overset{\circ}{\mathbf{E}}_2, \overset{\circ}{\mathbf{E}}_3\right). \tag{3.8}$$

Under the action of the motor $\mathbf{M}$, the initial reper $\overset{\circ}{\mathbf{R}}$ transforms into the actual reper $\mathbf{R}$

$$\mathbf{R} = (\mathbf{r}, \mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3) \tag{3.9}$$

according to

$$\mathbf{R} = \mathbf{M}\overset{\circ}{\mathbf{R}}. \tag{3.10}$$

Differentiation of $\overset{\circ}{\mathbf{R}}$ with respect to x^i gives

$$\partial_i \overset{\circ}{\mathbf{R}} = \overset{\circ}{\mathbf{A}}_i \overset{\circ}{\mathbf{R}} \tag{3.11}$$

with the six values in the matrix algebra.

The covariant derivative with respect to the undeformed base is

$$\overset{\circ}{\mathbf{D}}_i = \partial_i - \overset{\circ}{\mathbf{A}}_i. \tag{3.12}$$

Thus, the gradient of the motor $\mathbf{M}$ with respect to x^i has the form

$$\operatorname{Grad}\mathbf{M} \equiv \mathbf{A} = \overset{\circ}{\mathbf{g}}{}^i \mathbf{A}_i = \overset{\circ}{\mathbf{g}}{}^i \left[(\partial_i \mathbf{M})\mathbf{M}^{-1} + \mathbf{M}\overset{\circ}{\mathbf{A}}_i \mathbf{M}^{-1} - \overset{\circ}{\mathbf{A}}_i\right]. \tag{3.13}$$

In a Cartesian coordinate system, by linearization of the rotation with $\mathbf{R} = \mathbf{1} + \boldsymbol{\varphi} \times \mathbf{1}$ we obtain

$$\mathbf{D}_i \mathbf{M} = \begin{bmatrix} 0 & \partial_i \mathbf{u} - \boldsymbol{\varphi} \times \mathbf{1} \\ \mathbf{0} & \partial_i \boldsymbol{\varphi} \end{bmatrix} \tag{3.14}$$

which corresponds to the definition (2.3).

Let us define $\mathbf{F}_{ij}$ as a result of the following operation:

$$\mathbf{F}_{ij} = \mathbf{D}_i \mathbf{D}_j - \mathbf{D}_j \mathbf{D}_i \equiv [\mathbf{D}_i, \mathbf{D}_j] \tag{3.15}$$

or

$$\mathbf{F}_{ij} = \overset{\circ}{\mathbf{D}}_j \mathbf{A}_i - \overset{\circ}{\mathbf{D}}_i \mathbf{A}_j + [\mathbf{A}_i, \mathbf{A}_j]. \tag{3.16}$$

Then

$$\mathbf{B} = \frac{1}{2}\epsilon^{kij}\mathbf{F}_{ij}\,\overset{\circ}{\mathbf{g}}_k \equiv \operatorname{rot}\mathbf{A} + \frac{1}{2}[(\mathbf{A}\times), \mathbf{A}], \tag{3.17}$$

and we can realize the non-Abelian extension of the rotor operator

$$\operatorname{Rot}\mathbf{M} = \operatorname{rot}\mathbf{M} + \frac{1}{2}[(\mathbf{A}\times), \mathbf{M}], \tag{3.18}$$

and its linearization coincides with (2.4).

4. The Cosserat bundle

Fiber bundles are the very concise tools for description of the Cosserat continuum. First, we shall very briefly reinterprete some results of [8] in terms of a vector fiber bundle with a four-dimensional base and a three-dimensional fiber.

The one-form of fiber connection is written as

$$\mathbf{A} = \boldsymbol{\gamma}\, dt + \boldsymbol{\Gamma}_1\, dx^1 + \boldsymbol{\Gamma}_2\, dx^2 + \boldsymbol{\Gamma}_3\, dx^3. \tag{4.1}$$

The two-form of bundle curvature

$$F_{\mu\nu p}{}^{k}_{\cdot} = \partial_\mu A^k_{\nu p} - \partial_\nu A^k_{\mu p} + A^k_{\mu q} A^q_{\nu p} - A^k_{\nu q} A^q_{\mu p} \tag{4.2}$$

can be split into two parts

$$R_{rsp}{}^{k}_{\cdot} = F_{rsp}{}^{k}_{\cdot} \tag{4.3}$$

and

$$P_{sp}{}^{k}_{\cdot} \equiv F_{0sp}{}^{k}_{\cdot} = \frac{\partial \Gamma^k_{sp}}{\partial t} - \nabla_s \gamma_p{}^{k}_{\cdot}\,, \tag{4.4}$$

where Roman indices are running over 1, 2, 3, Greek indices over 0, 1, 2, 3.

Equation (4.4) leads to the evolution equation for the torsion tensor

$$\frac{\partial S_{sp}{}^{k}_{\cdot}}{\partial t} = P_{[sp]}{}^{k}_{\cdot} + \nabla_{[s} \gamma_{p]}{}^{k}_{\cdot}\,. \tag{4.5}$$

From the Jacobi identity for three derivative operators

$$[\nabla_0, [\nabla_s, \nabla_r]] + [\nabla_s, [\nabla_r, \nabla_0]] + [\nabla_r, [\nabla_0, \nabla_s]] = 0, \tag{4.6}$$

we immediately obtain the evolution equation for the curvature tensor

$$\frac{\partial R_{ijk}{}^{m}_{\cdot}}{\partial t} = 2(\nabla_{[i} P_{j]k}{}^{m}_{\cdot} + S_{ij}{}^{p}_{\cdot} P_{pk}{}^{m}_{\cdot} + R_{ij[p}{}^{m}_{\cdot} \gamma_{k]}{}^{m}_{\cdot}). \tag{4.7}$$

As usually, the torsion tensor and the curvature tensor are interpreted in terms of dislocation and disclination densities, respectively, while the time connection $\boldsymbol{\gamma}$ and the tensor $\mathbf{P}$ are related with the dislocation current tensor

$$J_m{}^{n}_{\cdot} = \nabla_m v^n - \gamma_m{}^{n}_{\cdot}, \tag{4.8}$$

where $\mathbf{v}$ is the velocity vector, and the disclination current tensor

$$I_m{}^{n}_{\cdot} = -\frac{1}{2} \epsilon^{npk} P_{mpk}. \tag{4.9}$$

Being interpreted in such a way, Eqs. (4.5) and (4.7) provide nonlinear generalization of Eqs. (2.12).

Let us next consider a bundle $\mathcal{P}$ with four-dimensional or three-dimensional base $\mathcal{M}$ and the semi-simple group $G = T(3) \triangleright SO(3)$ as a fiber. It is a natural choice of the base $\mathcal{J}_a$, $a = 1, 2, ..., 6$ of algebra G to be the fundamental vector fields defining a vertical tangent to $\mathcal{P}$. The base $\mathcal{M}$ is parametrized by the Gaussian coordinates θ^α, ($\alpha = 0, 1, 2, 3$ or $\alpha = 0, 1, 2$, where index 0 corresponds to a time t) and its holonomic base vectors ∇_α. A pair $\partial_M = \{\nabla_\alpha, \mathcal{J}_a\}$, $M = \alpha, a$ spans the base of the tangent space to $\mathcal{P}$, the Greek indices α, β indicate pure geometry and the Latin indices a, b indicate pure physics.

The fundamental operation for both the gauge and the fiber construction is the horizontal lift

$$\partial_M \longrightarrow \ell_M \equiv \{\mathcal{D}_\alpha, \mathcal{J}_a\}. \tag{4.10}$$

This operation is synonymous with the Utiyama compensating fields or the non-inertial frame of reference in Poisson rigid-body mechanics.

The field

$$\mathcal{A}(\theta^\alpha, \theta^a) = \mathcal{A}^a_\alpha \mathcal{J}_a \mathrm{d}\theta^\alpha \tag{4.11}$$

is the one-form of fiber connection or the compensating gauge potential. Note also that the vector product

$$[\mathcal{D}_\alpha, \mathcal{D}_\beta] = \mathcal{F}^a_{\alpha\beta} \mathcal{J}_a \tag{4.12}$$

is purely vertical and can be expanded along $\mathcal{J}_a$ with θ^M-dependend coefficients

$$\mathcal{F}^a_{\alpha\beta} = -\nabla_\alpha \mathcal{A}^a_\beta + \nabla_\beta \mathcal{A}^a_\alpha + \mathrm{C}^a_{bc} \mathcal{A}^b_\alpha \mathcal{A}^c_\beta \tag{4.13}$$

called the two-form of bundle curvature

$$\mathcal{F} = \mathcal{F}^a_{\alpha\beta} \mathcal{J}_a \, d\theta^\alpha \wedge d\theta^\beta, \tag{4.14}$$

or the gauge strength tensor.

Within $\mathcal{P}$ such objects as the metric g_{MN} connection Γ^K_{MN}, torsion $\mathcal{S}_{MN}{}^L_{.}$, curvature $\mathcal{R}_{MN}{}^L$, etc. can be prescribed in a natural way:

$$\Gamma^K_{MN} = \frac{1}{2} g^{KL} (\partial_M g_{NL} + \partial_N g_{ML} - \partial_L g_{MN} + C_{LMN} + C_{LNM} - C_{MNL}), \tag{4.15}$$

$$\mathcal{S}_{MN}{}^L_{.} = \Gamma_{MN}{}^L_{.} - \Gamma_{MN}{}^L_{.} - C_{MN}{}^L_{.}, \tag{4.16}$$

$$\mathcal{R}_{MNK}{}^L_{.} = \ell_M \Gamma_{NK}{}^L_{.} - \ell_N \Gamma_{MK}{}^L_{.} - \Gamma_{MK}{}^P_{.} \Gamma_{NP}{}^L_{.} + \Gamma_{NK}{}^P_{.} \Gamma_{MP}{}^L_{.} - C_{MN}{}^P_{.} \mathcal{S}_{PK}{}^L_{.}, \tag{4.17}$$

where $\overset{\circ}{g}_{\alpha\beta} = \nabla_\alpha \cdot \nabla_\beta$ and $\overset{\circ}{g}_{ab} = C^c_{ad} C^d_{cb}$ are the metric of a base and the Killing–Cartan metric on a fiber, respectively; $[\ell_M, \ell_N] = C_{MN}{}^L_{.} \ell_L$.

The one-form of fiber connection $\mathcal{A} = \mathcal{A}^a_\alpha \mathcal{J}_a d\theta^\alpha$ can be interpreted as the measures of deformation of the three-dimensional Cosserat continuum or two-dimensional Cosserat surface, while the two-form of bundle curvature $\mathcal{F} = \mathcal{F}^a_{\alpha\beta} \mathcal{J}_a d\theta^\alpha \wedge d\theta^\beta$ can be regarded as the compatibility of these measures (see also [19]).

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POLISH ACADEMY OF SCIENCES
INSTITUTE OF FLUID FLOW-MACHINERY

and

UKRAINIAN ACADEMY OF SCIENCES
PIDSTRYHACH INSTITUTE FOR APPLIED PROBLEMS
OF MECHANICS AND MATHEMATICS;

and

PEDAGOGICAL UNIVERSITY OF CZĘSTOCHOWA.

Received October 13, 1997.

Arch. Mech., **50**, 3, pp. 377–388, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

Fractional calculus and stable probability distributions

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

R. GORENFLO (BERLIN) and F. MAINARDI (BOLOGNA)

FRACTIONAL calculus allows one to generalize the linear (one-dimensional) diffusion equation by replacing either the first time-derivative or the second space-derivative by a derivative of a fractional order. The fundamental solutions of these generalized diffusion equations are shown to provide certain probability density functions, in space or time, which are related to the relevant class of stable distributions. For the space fractional diffusion, a random-walk model is also proposed.

1. Introduction

THE PURPOSE of this note is to outline the role of fractional calculus in generating stable probability distributions through generalized diffusion equations of fractional order.

For the standard diffusion equation it is well known that the fundamental solution of the Cauchy problem provides the spatial *probability density function* (*pdf*) for the Gaussian or normal distribution, whose variance is proportional to time. For convenience, let us derive this result, using standard notation and leaving out the regularity requirements. The Cauchy problem for the diffusion equation reads

$$\frac{\partial}{\partial t}\,u(x,t) = D\,\frac{\partial^2}{\partial x^2}\,u(x,t)\,, \qquad -\infty < x < \infty\,, \qquad t \geq 0 \quad \text{with} \quad u(x,0) = g(x)\,, \tag{1.1}$$

and can be easily solved making use of the Fourier transform. Adopting the notation $g(x) \div \hat{g}(\kappa)$ with $\kappa \in \mathbb{R}$ and

$$\hat{g}(\kappa) = \mathcal{F}\,[g(x)] = \int_{-\infty}^{\infty} e^{+i\kappa x}\, g(x)\, dx\,,$$

$$g(x) = \mathcal{F}^{-1}\,[\hat{g}(\kappa)] = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\kappa x}\, \hat{g}(\kappa)\, d\kappa\,,$$

the transformed solution reads

$$\hat{u}(\kappa,t) = \hat{g}(\kappa)\, e^{-Dt\kappa^2}\,. \tag{1.2}$$

Then, introducing

$$\mathcal{G}_c^d(x,t) \div e^{-Dt\kappa^2}, \tag{1.3}$$

the required solution is provided by inversion in terms of the space convolution

$$u(x,t) = \int_{-\infty}^{\infty} \mathcal{G}_c^d(\xi,t)\, g(x-\xi)\, d\xi\,, \qquad \mathcal{G}_c^d(x,t) = \frac{1}{2\sqrt{\pi D}}\, t^{-1/2}\, e^{-x^2/(4Dt)}. \tag{1.4}$$

Here $\mathcal{G}_c^d(x,t)$ represents the fundamental solution (or Green function) of the Cauchy problem, since it corresponds to $g(x) = \delta(x)$.

The interpretation of such Green function in probability theory is straightforward since we easily recognize

$$\mathcal{G}_c^d(x,t) = p_G(x;\sigma) := \frac{1}{\sqrt{2\pi}\,\sigma}\, e^{-x^2/(2\sigma^2)}, \qquad -\infty < x < \infty, \quad \sigma^2 = 2Dt, \tag{1.5}$$

where $p_G(x;\sigma)$ denotes the well-known *Gauss* or *normal pdf* whose moment of the second order, the *variance*, is σ^2. The associated cumulative distribution function (*cdf*) is known to be

$$\mathcal{P}_G(x;\sigma) := \int_{-\infty}^{x} p_G(x';\sigma)\, dx' = \frac{1}{2}\left[1 + \operatorname{erf}\left(\frac{x}{\sqrt{2}\,\sigma}\right)\right] = \frac{1}{2}\left[1 + \operatorname{erf}\left(\frac{x}{2\sqrt{D\,t}}\right)\right], \tag{1.6}$$

where $\operatorname{erf}(z) := (2/\sqrt{\pi}) \int_0^z \exp(-u^2)\, du$ denotes the error function. Furthermore, the moments of even order of the *Gauss pdf* turn out to be

$$\int_{-\infty}^{\infty} x^{2n}\, p_G(x;\sigma)\, dx = \frac{(2n)!}{2^n\, n!}\, \sigma^{2n} = (2n-1)!!\, \sigma^{2n} = (2n-1)!!\, (2Dt)^n\,, \quad n \in \mathbb{N}, \tag{1.7}$$

where $\mathbb{N}$ denotes the set of the positive integers.

Let us show how the fundamental solution of the *signalling* problem in the semi-infinite line provides a time *pdf* related to the unilateral Lévy distribution, a property not so well-known as that for the Cauchy problem. Under fairly general conditions, the *signalling* problem

$$\frac{\partial}{\partial t}\, u(x,t) = D\, \frac{\partial^2}{\partial x^2}\, u(x,t)\,, \qquad x \geq 0, \quad t \geq 0 \quad \text{with} \quad u(0,t) = \phi(t)\,, \tag{1.8}$$

can be easily solved by making use of the Laplace transform. Adopting the notation $\phi(t) \div \tilde{\phi}(s)$ with $s \in \mathbb{C}$ and

$$\tilde{\phi}(s) = \mathcal{L}[\phi(t)] = \int_0^\infty e^{-st}\,\phi(t)\,dt\,, \qquad \phi(t) = \mathcal{L}^{-1}\left[\tilde{\phi}(t)\right] = \frac{1}{2\pi i}\int_{\mathrm{Br}} e^{st}\,\tilde{\phi}(s)\,ds,$$

where Br denotes the Bromwich path, the transformed solution reads

$$\tilde{u}(x,s) = \tilde{\phi}(s)\,e^{-(x/\sqrt{D})\,s^{1/2}}. \tag{1.9}$$

Then introducing

$$\mathcal{G}_s^d(x,t) \div e^{-(x/\sqrt{D})\,s^{1/2}}, \tag{1.10}$$

the required solution is provided by inversion in terms of the time convolution,

$$u(x,t) = \int_0^t \mathcal{G}_s^d(x,\tau)\,\phi(t-\tau)\,d\tau, \qquad \mathcal{G}_s^d(x,t) = \frac{x}{2\sqrt{\pi D}}\,t^{-3/2}\,e^{-x^2/(4\,D\,t)}. \tag{1.11}$$

Here $\mathcal{G}_s^d(x,t)$ represents the fundamental solution (or Green function) of the *signalling* problem, since it corresponds to $\phi(t) = \delta(t)$. We note that

$$\mathcal{G}_s^d(x,t) = p_L(t;\mu) := \frac{\sqrt{\mu}}{\sqrt{2\pi}\,t^{3/2}}\,e^{-\mu/(2t)}, \qquad t \geq 0\,, \quad \mu = \frac{x^2}{2\,D}\,, \tag{1.12}$$

where $p_L(t;\mu)$ denotes the *unilateral Lévy pdf*, with *cdf*

$$\mathcal{P}_L(t;\mu) := \int_0^t p_L(t';\mu)\,dt' = \operatorname{erfc}\left(\sqrt{\frac{\mu}{2t}}\right) = \operatorname{erfc}\left(\frac{x}{2\sqrt{D\,t}}\right), \tag{1.13}$$

see e.g. FELLER [1]. The *Lévy pdf* has all moments of integral order infinite, since it decays at infinity as $t^{-3/2}$. However, we note that the absolute moments of real order δ are finite only if $0 \leq \delta < 1/2$. In particular, for this *pdf* the mean (expectation) is infinite, but the *median* is finite. In fact, from $\mathcal{P}_L(t_{\mathrm{med}};\mu) = 1/2$, it turns out that $t_{\mathrm{med}} \approx 2\mu$, since the complementary error function gets the value $1/2$ as its argument is approximatively $1/2$ (a better estimate of the argument is $1/2.1$).

Both the *Gauss* and *Lévy* laws belong to the important class of *stable* probability distributions, which are mainly characterized by an index α $(0 < \alpha \leq 2)$, called index of stability or characteristic exponent. In particular, the index of the Gauss law is 2, whereas that of the Lévy law is $1/2$. A special case of stable distribution with $\alpha = 1$ is provided by the Cauchy law with *pdf* $p_C(x;\lambda) = \lambda/[\pi(x^2+\lambda^2)]$, $\lambda > 0$.

For the theory of *stable distributions* we refer to some classical treatises of probability theory as [1–4], to the monographs by ZOLOTAREV [5], JANICKI and WERON [6], SAMORODNITSKY and TAQQU [7] and to the article by SCHNEIDER [8]. Here we limit ourselves to recall the main properties essential for the present analysis.

All the stable *pdf* are *unimodal* and indeed *bell-shaped*, i.e. their n-th derivative has exactly n zeros, see GAWRONSKI [9]. However, while the Gaussian distribution has a finite variance and is symmetric around its mean, for $0 < \alpha < 2$ all the stable distributions have infinite variance and can have an arbitrary degree of skewness. The skewness parameter is varying around zero (*symmetric pdf*) between two extremal symmetrical values (*extremal pdf*); for $0 < \alpha < 1$ the *extremal pdf* turn out to be *unilateral*, i.e. restricted to a semi-infinite real line. For $0 < \alpha < 2$ all the stable distributions exhibit at least one long tail, which decays with the power $(\alpha + 1)$, so their absolute moments of order δ are finite only if $\delta < \alpha$. Note that for asymmetric distributions, the faster tail may decay exponentially.

For our present purposes it is sufficient to draw the attention to the Fourier transform of the *symmetric* stable distributions acting for $x \in \mathbb{R}$, i.e.

$$p_S(x;\alpha,a) \div \widehat{p}(\kappa;\alpha,a) = e^{-a|\kappa|^\alpha}, \qquad a > 0, \quad 0 < \alpha \leq 2 \tag{1.14}$$

and to the Laplace transform of the *unilateral* stable distributions acting for $t \in \mathbb{R}^+$, i.e.

$$p_U(t;\beta,b) \div \widetilde{p}(s;\beta,b) = e^{-b\,s^\beta}, \qquad b > 0, \quad 0 < \beta < 1. \tag{1.15}$$

In (1.14) – (1.15) the parameters α, β denote the characteristic exponent of the corresponding stable distribution whereas a, b are scaling factors. The singularity of the Fourier and Laplace transforms in the origin corresponds to the power-type long tails of the distribution.

As a matter of fact we note that for the standard diffusion equation, the Green function for the Cauchy problem yields (1.14) with $\alpha = 2$ and $a = Dt$, whereas the Green function for the *signalling* problem yields (1.15) with $\beta = 1/2$ and $b = x/\sqrt{D}$.

In order to reproduce both the classes of stable distributions (1.14) – (1.15), we need to consider separately the Cauchy problem and the *signalling* problem for two different diffusion equations in which the space or time derivatives of integral order are substituted by special pseudo-differential operators, which are shown to be expressed in terms of suitable "fractional derivatives". For the Cauchy problem we consider the so-called space fractional diffusion equation

$$\frac{\partial u}{\partial t} = D(\alpha)\frac{\partial^\alpha u}{\partial |x|^\alpha}, \qquad -\infty < x < \infty, \quad t \geq 0 \quad \text{with} \quad u(x,0) = \delta(x), \tag{1.16}$$

where $0 < \alpha \leq 2$ and $D(\alpha)$ is a suitable diffusion coefficient depending on α. Here the pseudo-differential operator of space fractional derivative (symmetric in x) is defined by its Fourier representation,

$$\frac{\partial^\alpha}{\partial |x|^\alpha} u(x,t) \div -|\kappa|^\alpha \, \widehat{u}(\kappa,t). \tag{1.17}$$

Correspondingly, for the *signalling* problem we consider the so-called time fractional diffusion equation

$$\frac{\partial^{2\beta} u}{\partial t^{2\beta}} = D(\beta) \frac{\partial^2 u}{\partial x^2}, \qquad x \geq 0, \quad t \geq 0 \quad \text{with} \quad u(0,t) = \delta(t), \tag{1.18}$$

where $0 < \beta < 1$ and $D(\beta)$ is a suitable diffusion coefficient depending on β. Here the pseudo-differential operator of time fractional derivative is defined by its Laplace representation,

$$\frac{\partial^{2\beta} u}{\partial t^{2\beta}} \div \begin{cases} s^{2\beta} \widetilde{u}(x,s) - s^{2\beta-1} u(x,0^+), & \text{if } 0 < \beta \leq 1/2, \\ s^{2\beta} \widetilde{u}(x,s) - s^{2\beta-1} u(x,0^+) - s^{2\beta-2} u_t(x,0^+), & \text{if } 1/2 < \beta \leq 1. \end{cases} \tag{1.19}$$

We easily recognize from (1.17) and (1.19) that the pseudo-differential operators reduce to the space and time derivatives of integral order entering the standard diffusion equation when $\alpha = 2$ and $\beta = 1/2$, respectively.

In the following sections we shall discuss the two fractional diffusion equations, providing an interpretation of the pseudo-differential operators (1.17) and (1.19) in the framework of some established theories of the fractional calculus.

We begin in Sec. 2 with the time fractional diffusion equation that in recent years has been extensively treated by MAINARDI [10–14]. Other significant treatments of this equation have been given by a number of authors including WYSS [15], SCHNEIDER and WYSS [16], SCHNEIDER [17], FUJITA [18], KOCHUBEI [19], EL-SAYED [20], and ENGLER [21]. In this case the fractional derivative can be interpreted recurring to the Riemann–Liouville approach to the fractional calculus.

For the space fractional diffusion equation, the literature on extensive and clear treatments appears poor, in that the topic is mostly treated only briefly from the mathematical point of view, as in SESHADRI and WEST [22], TAKAYASU [23], ZASLAVSKY [24], COMPTE [25]. In this case, the fractional derivative can be interpreted as recurring to the Riesz approach to the fractional calculus. In Sec. 3 we present a new and interesting analysis of the space fractional diffusion equation, originally started by GORENFLO and MAINARDI [26], which leads to an interpretation through a random-walk model. This analysis has been inspired by a classical (but almost ignored) contribution by FELLER [27] and by a recent paper by SAICHEV and ZASLAVSKY [28].

2. The time fractional diffusion equation

In the time fractional diffusion equation (1.18), the pseudo-differential operator of fractional derivative (1.19) is acting for $t \in \mathbb{R}^+$ and hence we must consider the Riemann - Liouville fractional calculus, which is suitable for causal functions $f(t)$, vanishing for $t < 0$. For details on this calculus the reader is referred to the standard treatises of fractional calculus, which include OLDHAM and SPANIER [29], SAMKO, KILBAS and MARICHEV [30], MILLER and ROSS [31], and to our recent CISM lecture notes [32 - 33].

Here, for our purposes, we adopt the following definition for the fractional derivative of order α of a causal function $f(t)$,

$$\frac{d^\alpha}{dt^\alpha} f(t) := \frac{1}{\Gamma(m-\alpha)} \int_0^t \frac{f^{(m)}(\tau)}{(t-\tau)^{\alpha+1-m}}\, d\tau \qquad \text{with} \quad m-1 < \alpha < m, \quad m \in \mathbb{N}, \tag{2.1}$$

where Γ is the Gamma function and $f^{(m)}(t)$ denotes the derivative of order m, which is assumed to be Laplace transformable. This definition has been originally introduced by CAPUTO [34, 35] in the late sixties, and extensively applied by CAPUTO & MAINARDI [36] for modelling dissipation effects in *Linear Viscoelasticity*. This derivative, that we refer to as the Caputo derivative, represents a sort of regularization in the time origin for the Riemann - Liouville fractional derivative by incorporating the relevant initial conditions. It has been extensively investigated in [32] in view of its major utility in treating physical and engineering problems with standard initial conditions, but has been ignored in the mathematical treatises [29–31]. The Caputo derivative satisfies the relevant properties: in particular, the derivative of any order of a constant is still zero and the Laplace transform of a derivative of non-integral order still requires the initial data for integral derivatives, according to the rule

$$\frac{d^\alpha}{dt^\alpha} f(t) \div s^\alpha \widetilde{f}(s) - \sum_{k=0}^{m-1} f^{(k)}(0^+)\, s^{\alpha-1-k}, \qquad m-1 < \alpha \le m. \tag{2.2}$$

Since the above property is consistent with (1.19) for $\alpha = 2\beta$, and $m = 1, 2$, the Caputo derivative is just the pseudo-differential operator suitable for the time fractional diffusion equation.

The application of the Laplace transform to the *signalling* problem (1.18) allows us to find the corresponding Green function, that we denote by $\mathcal{G}_s(x,t;\beta)$. In fact, after standard manipulations, we obtain the transformed solution

$$\widetilde{\mathcal{G}_s}(x,s;\beta) = e^{-(x/\sqrt{D(\beta)})\, s^\beta}, \qquad x \ge 0. \tag{2.3}$$

Introducing the similarity variable $r = x/(\sqrt{D(\beta)}t^{\beta})$ and the auxiliary function

$$F(r;\beta) := \frac{1}{2\pi i}\int_{\mathrm{Br}} e^{\sigma - r\sigma^{\beta}}\, d\sigma\,, \tag{2.4}$$

we find

$$\mathcal{G}_s(x,t;\beta) = \frac{1}{t}F(r;\beta) \sim c(x)\, t^{-(1+\beta)}\,, \qquad t \to \infty, \tag{2.5}$$

where $c(x)$ is a certain positive function. The definition of $F(r;\beta)$ can be analytically continued from $r > 0$ to any $z \in \mathbb{C}$, by deforming the Bromwich path into the Hankel path. The auxiliary function $F(z)$ turns out as an entire function of order $1/(1-\beta)$, which can be identified with a special function, known as Wright function [37].

In conclusion, the Green function for the *signalling* problem of the time fractional diffusion equation turns out to be a *unilateral* stable distribution in time, with characteristic exponent β and scale factor $b = x/\sqrt{D(\beta)}$, that is expressed in terms a Wright function in the similarity variable. For more details we refer the reader to [10–14], where also the Cauchy problem has been treated.

It is noteworthy to recall here that for the Cauchy problem, the corresponding Green function, obtained by the techniques of the Laplace or Fourier transform, turns out to be a *symmetric pdf* in space, provided by

$$\mathcal{G}_c(|x|,t;\beta) = \frac{1}{2\beta|x|}F(|r|;\beta) \sim a(t)\,|x|^{(\beta-1/2)/(1-\beta)}\, e^{-b(t)|x|^{1/(1-\beta)}}, \tag{2.6}$$

as $|x| \to \infty$, where $a(t)$, $b(t)$ are positive functions. Therefore the *pdf* exhibits two branches, for $x > 0$ and $x < 0$, obtained one from the other by reflection. The exponential decay of such *pdf* allows the existence of all the moments; we obtain

$$\int_{-\infty}^{\infty} x^{2n}\, \mathcal{G}_c(x,t;\beta)\, dx = \frac{\Gamma(2n+1)}{\Gamma(2\beta n+1)}\left[D(\beta)\, t^{2\beta}\right]^n, \qquad n = 0,\, 1,\, 2,\, \ldots\,. \tag{2.7}$$

We recognize that the variance is now proportional to $D\,t^{2\beta}$, which implies a phenomenon of *slow diffusion* (or *sub-diffusion*) if $0 < \beta < 1/2$, *fast diffusion* (or *hyper-diffusion*) if $1/2 < \beta < 1$, and, of course, *normal diffusion* if $\beta = 1/2$. Furthermore, we recognize that for $1/2 < \beta < 1$, any branch of the *pdf* is proportional to the exponential branch of an *extremal* stable distribution of index $1/\beta$.

3. The space fractional diffusion equation

In the space-fractional diffusion equation (1.16) the pseudo-differential operator of fractional derivative (1.16) is acting for $x \in \mathbb{R}$ in a symmetric way. Here we must consider the fractional calculus in the framework of Riesz potentials and define properly the fractional derivative (1.17) as inverse of the Riesz fractional integral. We recall that for $0 < \alpha \leq 2$, with $\alpha \neq 1$ and for a sufficiently well-behaved function $\phi(x)$, $x \in \mathbb{R}$, the Riesz integral operator or Riesz potential I^α and its image in the Fourier domain read

$$I^\alpha \phi(x) := \frac{1}{2\,\Gamma(\alpha)\,\cos(\pi\alpha/2)} \int_{-\infty}^{\infty} |x-\xi|^{\alpha-1}\,\phi(\xi)\,d\xi \;\div\; \frac{\hat{\phi}(\kappa)}{|\kappa|^\alpha}\,. \tag{3.1}$$

On its turn the Riesz potential can be written in terms of two Weyl integrals $I^\alpha_\pm$ according to

$$I^\alpha \phi(x) = \frac{1}{2\,\cos(\pi\alpha/2)}\,\left[I^\alpha_+\phi(x) + I^\alpha_-\phi(x)\right], \tag{3.2}$$

where

$$\begin{aligned} I^\alpha_+ \phi(x) &:= \frac{1}{\Gamma(\alpha)} \int_{-\infty}^{x} (x-\xi)^{\alpha-1}\,\phi(\xi)\,d\xi, \\ I^\alpha_- \phi(x) &:= \frac{1}{\Gamma(\alpha)} \int_{x}^{+\infty} (\xi-x)^{\alpha-1}\,\phi(\xi)\,d\xi. \end{aligned} \tag{3.3}$$

Then, at least in a formal way, the fractional derivative (1.17) turns out to be

$$\frac{d^\alpha}{d|x|^\alpha}\,\phi(x) := -I^{-\alpha}\,\phi(x) = -\frac{1}{2\,\cos(\pi\alpha/2)}\,\left[I^{-\alpha}_+\phi(x) + I^{-\alpha}_-\phi(x)\right]. \tag{3.4}$$

Notice that (3.4) becomes meaningless if $\alpha = 1$. Here we resist the temptation to dive into the delicate details of the analytical inversion of the Riesz potential but rather refer the interested reader to the specialized treatises by SAMKO, KILBAS and MARICHEV [30] and RUBIN [38], and to the paper by SAICHEV and ZASLAVSKI [28].

Here, for $0 < \alpha \leq 2$, $\alpha \neq 1$, we propose a numerical approach for such inversion, approximating the evolution of the solution $u(x,t)$ of (1.16), interpreted as a probability density, by a (symmetric) *random walk* model, discrete in space and time. We shall see how things become highly transparent, in that we properly generalize the classical random-walk argument of the common diffusion equation to our spatial fractional equation (1.16). So doing we are in a position to

provide in the future a numerical simulation of the related (symmetric) stable distributions in a way analogous to the standard one for the Gaussian law.

The *essential idea* is to approximate the inverse operators $I_{\pm}^{-\alpha}$ by the Grünwald–Letnikov scheme, on which the reader can be informed in the treatises on fractional calculus [29–31] and in [33]. If h denotes a "small" positive step-length, these approximate operators read

$$(3.5) \qquad {}_hI_{\pm}^{-\alpha}\,\phi(x) := \frac{1}{h^{\alpha}} \sum_{k=0}^{\infty} (-1)^k \binom{\alpha}{k} \phi(x \mp kh)\,.$$

Assume, for simplicity, $D(\alpha) = 1$, and introduce grid points $x_j = j\,h$ with $h > 0$, $j \in \mathbf{Z}$, and time instances $t_n = n\,\tau$ with $\tau > 0$, $n \in \mathbb{N}_0$. Let there be given the probabilities $p_{j,k} \geq 0$ of jumping from point x_j at instant t_n to point x_k at instant t_{n+1}, and define the probabilities $y_j(t_n)$ of the walker being at point x_j at instant t_n. Then, by

$$(3.6) \qquad y_k(t_{n+1}) = \sum_{j=-\infty}^{\infty} p_{j,k}\, y_j(t_n), \qquad p_{j,k} = p_{k,j}\,, \qquad \sum_{k=-\infty}^{\infty} p_{j,k} = \sum_{j=-\infty}^{\infty} p_{j,k} = 1,$$

a symmetric random walk (more precisely a symmetric random jump) model is described. With the approximation $y_j(t_n) \approx \int_{(x_j-h/2)}^{(x_j+h/2)} u(x,t_n)\,dx \approx h\,u(x_j,t_n)$, and introducing the "scaling parameter" $\mu = \tau/[h^{\alpha} 2|\cos(\alpha\pi/2)|]$, we have solved

$$(3.7) \qquad \frac{y_j(t_{n+1}) - y_j(t_n)}{\tau} = -\,{}_hI^{-\alpha}\, y_j(t_n)\,,$$

for $y_j(t_{n+1})$. So we have proved to have a consistent (for $h \to 0$) symmetric random walk approximation to (1.16) by taking

i) for $0 < \alpha < 1$,

$$(3.8) \qquad \begin{aligned} &{}_hI^{-\alpha}\, y_j(t_n) = \mu\,\frac{h^{\alpha}}{\tau}\left[{}_hI_{+}^{-\alpha}\, y_j(t_n) + {}_hI_{-}^{-\alpha}\, y_j(t_n)\right], \\ &0 < \mu \leq 1/2\,, \\ &p_{j,j} = 1 - 2\mu\,, \quad p_{j,j\pm k} = \mu \left|\binom{\alpha}{k}\right|, \quad k \geq 1\,; \end{aligned}$$

ii) for $1 < \alpha \leq 2$,

$$(3.9) \qquad \begin{aligned} &{}_hI^{-\alpha}\, y_j(t_n) = \mu\,\frac{h^{\alpha}}{\tau}\left[{}_hI_{+}^{-\alpha}\, y_{j+1}(t_n) + {}_hI_{-}^{-\alpha}\, y_{j-1}(t_n)\right], \\ &0 < \mu \leq 1/(2\alpha)\,, \\ &p_{j,j} = 1 - 2\mu\alpha, \;\; p_{j,j\pm 1} = \mu\left[1 + \binom{\alpha}{2}\right], \;\; p_{j,j\pm k} = \mu\left|\binom{\alpha}{k+1}\right|, \;\; k \geq 2. \end{aligned}$$

In the special case $\alpha = 2$ we recover the well-known three-point approximation of the heat equation, because $p_{j,j\pm k} = 0$ for $k \geq 2$. This means that for approximation of common diffusion, only jumps of one step to the right or one to the left or jumps of width zero occur, whereas, for all other values of α, i.e. $0 < \alpha < 2$ with $\alpha \neq 1$, arbitrary large jumps occur with power-like decaying probability, as it turns out from the asymptotic analysis for the probability coefficients. In fact, using the reflection and Stirling formulas for the Gamma functions entering the binomial coefficients, one finds

$$p_{j,j+k} \sim \frac{\mu}{\pi} \Gamma(\alpha+1) \, |\sin(\pi\alpha)| \, k^{-(\alpha+1)}, \qquad k \to \infty. \tag{3.10}$$

This result thus provides the discrete counterpart of the expected asymptotic behavior for the long power-law tails of the (symmetric) stable distributions when $0 < \alpha < 2$.

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DEPARTMENT OF MATHEMATICS AND COMPUTER SCIENCE,
FREE UNIVERSITY OF BERLIN

Arnimallee 2-6, D-14195 Berlin, Germany
e-mail: gorenflo@math.fu-berlin.de

DEPARTMENT OF PHYSICS,
UNIVERSITY OF BOLOGNA
Via Irnerio 46, I-40126 Bologna, Italy
e-mail: mainardi@bo.infn.it

Received November 13, 1997.

Arch. Mech., 50, 3, pp. 389–404, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

Canonical forms and conservation laws in linear elastostatics

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

G. HATFIELD (ST. PETER) and P.J. OLVER (MINNEAPOLIS)

IN THIS PAPER, we shall review earlier work on canonical forms in linear elasticity, and applications to the classification of conservation laws (path-independent integrals).

1. Introduction

THE DETAILED investigation of complex mathematical objects can often be simplified through the use of specially adapted coordinate systems in which the object takes a simple "canonical form". Elementary examples include the Jordan canonical form of a square matrix, Sylvester's Theorem on the representation of a quadratic form as a sum of squares, and Darboux' Theorem on the canonical form of Hamiltonian structures. In elasticity, the determination of canonical forms for elastic materials, either linear or nonlinear, is more recent. LEKHNITSKII [14], and TING [33], discuss canonical forms and invariants for elastic moduli under the physically based class of rotations. In [22] canonical forms for two-dimensional materials under general linear transformations were found. These were extended to planar displacements of three-dimensional materials in [25] with further refinements in [9]. The classification of canonical forms in fully three-dimensional materials is, however, not known. Applications of these results to the classification of conservation laws or path-independent integrals appear in [8, 9, 10, 20, 23]. Using a remarkable mathematical correspondence between planar elastic and dielectric media, MILTON and MOVCHAN [16], have applied the planar canonical forms to study waves in an anisotropic dielectric medium.

2. The equations of elasticity

The equations of hyper-elasticity constitute a self-adjoint, quasi-linear system of second-order partial differential equations for the deformation (or, in the linear case, displacement) $\mathbf{u} = \mathbf{f}(\mathbf{x})$. Here $\mathbf{u} = (u^1, \dots, u^q) \in \mathbb{R}^q$, and $\mathbf{x} = (x_1, \dots, x_p)$ are the material coordinates in the elastic body $\Omega \subset \mathbb{R}^p$. For planar elasticity, $p = q = 2$, while $p = q = 3$ for fully three-dimensional elastic media. The Stroh formalism discussed below applies to a hybrid case, that of planar displacements

of three-dimensional bodies, where $p = 2$, while $q = 3$. When $p = 2$, we will sometimes use the notation $\mathbf{x} = (x_1, x_2) = (x, y)$ and $\mathbf{u} = (u^1, u^2, u^3) = (u, v, w)$. The equilibrium equations are the Euler-Lagrange equations for the stored energy functional

$$\mathcal{W}[u] = \int_{\Omega} W(\mathbf{x}, \nabla \mathbf{u})\, d\mathbf{x}. \tag{2.1}$$

The physical conditions of frame indifference, strong ellipticity, etc., will restrict stored energy functions which are of relevance to elasticity, although our initial remarks apply to quite general variational problems. The stored energy is not uniquely determined by its Euler-Lagrange equations, since we can add any divergence, replacing W by $W + \operatorname{Div} \mathbf{P}$, although this will, in general, alter the natural boundary conditions associated with the problem.

At a fixed material point $\mathbf{x} = \mathbf{b}$ and a fixed value of deformation gradient $\mathbf{u} = F$, we define the *symbol* of the variational problem (2.1) to be the "biquadratic" polynomial

$$Q_{\mathbf{b},F}(\mathbf{x}, \mathbf{u}) = \sum_{i,j,k,l} \frac{\partial^2 W}{\partial u^i_j \partial u^k_l}(\mathbf{b}, F)\, u^i u^k x_j x_l, \qquad \mathbf{x} \in \mathbb{R}^p, \quad \mathbf{u} \in \mathbb{R}^q. \tag{2.2}$$

The symbol is unaffected by the addition of a null Lagrangian to W. The Legendre–Hadamard condition requires that the symbol Q be *positive definite* in the sense that

$$Q_{\mathbf{b},F}(\mathbf{x}, \mathbf{u}) > 0 \qquad \text{whenever} \qquad \mathbf{x} \neq 0, \quad \mathbf{u} \neq 0, \tag{2.3}$$

for all $\mathbf{b} \in \Omega$, and F such that $\det F > 0$. For simplicity, we will restrict our considerations to homogeneous materials, whereby the stored energy function $W(\nabla \mathbf{u})$ depends only on the deformation gradient.

In linear elasticity, the stored energy is a symmetric quadratic function of the displacement gradient

$$\mathcal{W}[\mathbf{u}] = \int_{\Omega} \sum_{i,j,k,l} a_{ijkl} \frac{\partial u^j}{\partial x_i} \frac{\partial u^k}{\partial x_l}\, d\mathbf{x}. \tag{2.4}$$

The equilibrium equations are the associated Euler-Lagrange equations:

$$\sum_{j,k,l} a_{ijkl} \frac{\partial^2 u^k}{\partial x_i \partial x_l} = 0, \qquad i = 1, \dots, q. \tag{2.5}$$

The values a_{ijkl} are the *variational moduli*. For a general quadratic variational problem (2.4), the symbol Q is independent of the value of the displacement gradient F, and also the material point $\mathbf{b}$ provided the body is homogeneous. It can be found directly by replacing $\nabla \mathbf{u}$ in W by the rank one tensor $\mathbf{x} \otimes \mathbf{u} = \mathbf{u} \cdot \mathbf{x}^T$:

$$Q(\mathbf{x}, \mathbf{u}) = W(\mathbf{x} \otimes \mathbf{u}) = \sum_{i,j,k,l} a_{ijkl}\, u^i u^k x_j x_l\,. \tag{2.6}$$

Since every quadratic divergence is a linear combination of the 2×2 Jacobian determinants $\partial(u^i, u^k)/\partial(x_j, x_l)$, a homogeneous quadratic stored energy function is uniquely determined by its symbol up to a divergence.

In the case $p = q$, the assumption of frame indifference requires that the stored energy (2.4) depends only on the strain tensor $\varepsilon = \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$, so

$$\mathcal{W}[\mathbf{u}] = \int_\Omega \sum_{i,j} \sigma_{ij}\, \varepsilon_{ij}\, d\mathbf{x} = \int_\Omega \sum_{i,j,k,l} c_{ijkl}\, \varepsilon_{ij} \varepsilon_{kl}\, d\mathbf{x}, \tag{2.7}$$

where $\sigma = \mathbf{C}(\varepsilon)$ is the associated stress tensor. In this case, the equilibrium equations (2.5) take the form

$$\operatorname{Div} \sigma = 0. \tag{2.8}$$

The fourth rank tensor $\mathbf{C} = (c_{ijkl})$ is the *elasticity tensor*. The components of $\mathbf{C}$ are called the *elastic moduli* or *elasticities* of the material, and have the following symmetries

$$c_{ijkl} = c_{jikl} = c_{ijlk} = c_{klij}\,. \tag{2.9}$$

There are 21 independent elasticities in three-dimensional problems and 6 independent moduli in two-dimensional problems. The symmetry restrictions (2.9) imply that the symbol is *symmetric*, i.e. $Q(\mathbf{x}, \mathbf{u}) = Q(\mathbf{u}, \mathbf{x})$.

3. The Stroh formalism

The Stroh formalism [5, 31, 32, 33] deals with the hybrid case of planar displacements, $p = 2$, of a three-dimensional body, $q = 3$. For any displacement $\mathbf{u}$ that satisfies (2.8), there exist three *stress potentials* $\Phi = (\phi^1(\mathbf{x}), \phi^2(\mathbf{x}), \phi^3(\mathbf{x}))$ such that

$$\sigma_{i1} = -\frac{\partial \phi^i}{\partial y}\,, \qquad \sigma_{i2} = \frac{\partial \phi^i}{\partial x}\,, \qquad i = 1, 2, 3. \tag{3.1}$$

We define the following 3×3 matrices:

$$Q = Q_{ij} = c_{i1j1}\,, \qquad T = T_{ij} = c_{i2j2}\,, \qquad R = R_{ij} = c_{i1j2}\,. \tag{3.2}$$

We note that Q and T are symmetric and positive definite. We then construct the following 6×6 matrices:

$$M_1 = \begin{bmatrix} -R^T & I \\ -Q & 0 \end{bmatrix}, \qquad M_2 = \begin{bmatrix} T & 0 \\ R & I \end{bmatrix}. \tag{3.3}$$

The relations (2.8), (3.1), can be rewritten as

$$M_1 \frac{\partial \mathbf{Y}}{\partial x} = M_2 \frac{\partial \mathbf{Y}}{\partial y}\,, \qquad \text{where} \qquad \mathbf{Y} = \begin{bmatrix} \mathbf{u} \\ \Phi \end{bmatrix} \in \mathbb{R}^6. \tag{3.4}$$

The 6×6 matrix

$$N = M_2^{-1} M_1 = \begin{bmatrix} -T^{-1}R^T & T^{-1} \\ RT^{-1}R^T - Q & -RT^{-1} \end{bmatrix} \tag{3.5}$$

is called the *fundamental elasticity matrix*.

The characteristic polynomial $s(\lambda)$ of N is a sixth-degree polynomial known as the "Stroh sextic". Since the strain energy is positive definite, so is $s(\lambda)$, [5], and hence its roots come in three complex conjugate pairs. If the matrix N is diagonalizable, the material is called *nondegenerate*. Let p_1, p_2, p_3 be the eigenvalues with positive imaginary part, and $\mathbf{V}_\alpha \in \mathbb{C}^6$ the corresponding complex eigenvectors. In the nondegenerate case, the general solution to (3.4) has the form

$$\mathbf{Y} = \sum_{\alpha=1}^{3} \Big[\mathbf{V}_\alpha \cdot f_\alpha(z_\alpha) + \overline{\mathbf{V}_\alpha} \cdot \overline{f_\alpha(z_\alpha)} \Big]. \tag{3.6}$$

Here the *Stroh functions* f_α are arbitrary complex-analytic functions of their respective argument $z_\alpha = x + p_\alpha y$; see [33] for details. If we write $\mathbf{V}_\alpha = \begin{bmatrix} \mathbf{A}_\alpha \\ \mathbf{B}_\alpha \end{bmatrix}$ with $\mathbf{A}_\alpha, \mathbf{B}_\alpha \in \mathbb{C}^3$, the vectors $\mathbf{A}_\alpha$ are called the *Stroh eigenvectors*. It is easy to show that they satisfy (no sum):

$$\begin{aligned} &\big(Q + p_\alpha(R + R^T) + p_\alpha^2 T\big)\, \mathbf{A}_\alpha = 0, \\ &\mathbf{B}_\alpha = \big(R^T + p_\alpha T\big)\, \mathbf{A}_\alpha = -\frac{1}{p_\alpha}\,(Q + p_\alpha R)\, \mathbf{A}_\alpha\,, \end{aligned} \tag{3.7}$$

where p_α is the corresponding root of the Stroh sextic. The solution for degenerate materials, which includes the isotropic case, is similar, but more complicated; see [33] or [9] for explicit formulations.

The Stroh formalism reduces to the well-known MUSKHELISHVILI [17] approach in the planar case. The Stroh sextic now reduces to a quartic polynomial with two complex-conjugate pairs of roots. The solution (3.6) is similar, but the sum only goes from 1 to 2. The Airy stress function is $U(x,y) = 2\,\mathrm{Re}\,[U_1(z_1) + U_2(z_2)]$ where U_α are arbitrary analytic functions of z_α, with $f_\alpha(z_\alpha) = U_\alpha'(z_\alpha)$ giving the solution (3.6).

4. Changes of variables

In the calculus of variations, the basic equivalence problem is to determine when two variational problems can be transformed into each other by a suitable change of variables. For nonlinear variational problems in several independent and dependent variables, there is as yet no solution, although preliminary analysis based on the powerful Cartan equivalence method, [27, 28], has been done. The first of the invariants arising from the Cartan method is the symbol (2.2),

and so we must understand canonical forms for linear variational problems before further progress in the general nonlinear problem is possible.

In the case of linear elasticity, we may restrict our attention to linear changes of variables:

$$\mathbf{x} \longmapsto A\,\mathbf{x}, \qquad \mathbf{u} \longmapsto B\,\mathbf{u}. \tag{4.1}$$

In the elastic case, we choose B to be a scalar multiple of A^{-T} to preserve the symmetry constraints. Under the change of variables (4.1), the stored energy is transformed according to

$$W(\nabla \mathbf{u}) \longmapsto \widetilde{W}(\nabla \mathbf{u}) = W(B\,\nabla \mathbf{u} A^{-1})\,|\det A|.$$

Our fundamental problem, then, is to determine matrices A and B which will simplify the elastic moduli c_{ijkl} (or variational moduli a_{ijkl} in the general case) as much as possible. Stated in this form, the question appears to be quite natural from the mathematical point of view, even though it may not have an immediate physical motivation. Indeed, the linear maps determined by the matrices A and B will not in general have any direct physical interpretation, except in the special case of orthogonal transformations (rotations), when they represent a physical change of frame, [14, 33].

The linear change of variables (4.1) acts on the symbol via $Q(\mathbf{x}, \mathbf{u}) \longmapsto Q(A\mathbf{x}, B\mathbf{u})$. (Actually, one should replace A by a multiple of A^{-T}, but this does not affect the discussion.) Thus we are led to the purely algebraic problem of determining canonical forms for biquadratic polynomials under the change of variables.

We now discuss the relevant algebraic properties of biquadratic symbols, concentrating on the cases $p = q = 2$ and $p = 2$, $q = 3$. (Note that if either $p = 1$ or $q = 1$, the symbol is an ordinary quadratic polynomial, whose canonical forms, determined by Sylvester's law of inertia, are well known. In particular, only the rank and signature are invariants, and there are no canonical moduli in these special cases.) Let us write the symbol in the matrix form

$$Q(\mathbf{x}, \mathbf{u}) = \mathbf{u}^T R(\mathbf{x})\mathbf{u}, \tag{4.2}$$

where, assuming strong ellipticity, $R(\mathbf{x})$ is a real $q \times q$ symmetric, positive-definite matrix of homogeneous quadratic polynomials of the variables $\mathbf{x}$. Just as the analysis of ordinary real polynomials requires an understanding of their complex roots, and so we may regard $\mathbf{x}$ and $\mathbf{u}$ as complex vectors, and Q as a complex-valued biquadratic polynomial. By the strong ellipticity assumption, for generic vectors $\mathbf{x} \in \mathbb{C}^p$, the matrix $R(\mathbf{x})$ has full rank; it is important to distinguish the exceptional points where R has less than maximal rank. Define the *discriminant*

$$\Delta_{\mathbf{u}}(\mathbf{x}) = \det R(\mathbf{x}), \tag{4.3}$$

which is a homogeneous polynomial of degree $2q$. A *root* of $\Delta_{\mathbf{u}}(\mathbf{x})$ is a nonzero vector $0 \neq \mathbf{x} \in \mathbb{C}^p$ satisfying $\Delta_{\mathbf{u}}(\mathbf{x}) = 0$. Homogeneity of the symbol polynomial implies that we should identify roots that are complex scalar multiples of each other. The roots of the discriminant play a crucial role in the classification of these biquadratic polynomials, and hence of quadratic variational problems. Strong ellipticity implies that the roots always appear in complex conjugate pairs. Interestingly, in cases covered by the Stroh formalism, the discriminant is the *same* as the Stroh quartic or sextic: $s(\lambda) = \Delta_{\mathbf{u}}(\lambda, 1)$.

Clearly, one can interchange the roles of $\mathbf{x}$ and $\mathbf{u}$ in the above discussion, producing a corresponding discriminant $\Delta_{\mathbf{x}}(\mathbf{u})$. Except in the symmetric elastic case with $p = q$, these two polynomials are not the same (indeed, if $p \neq q$, they do not even depend on the same number of variables), nor are their roots easily compared. Nevertheless, there are subtle and remarkable relations between the roots of the two discriminants. For example, in the planar case $p = q = 2$, the discriminant $\Delta_{\mathbf{u}}(\mathbf{x})$ has simple roots if and only if $\Delta_{\mathbf{x}}(\mathbf{u})$ does. However, it is not true that if $\Delta_{\mathbf{u}}(\mathbf{x})$ has a double root then $\Delta_{\mathbf{x}}(\mathbf{u})$ has a double root, although it does have a root of multiplicity at least two; see [24].

5. Canonical elastic moduli

The number of canonical moduli can be determined directly by a simple dimension count. A general biquadratic polynomial or symbol $Q(\mathbf{x}, \mathbf{u})$ depending on $\mathbf{x} \in \mathbb{R}^p$, and $\mathbf{u} \in \mathbb{R}^q$ has a total of $\frac{1}{4}p(p+1)q(q+1)$ independent variational moduli. The possible changes of variables (4.1) will involve $p^2 + q^2$ arbitrary parameters, but the transformation just rescaling $\mathbf{x}$ (where A is a multiple of the identity) has the same effect as that rescaling $\mathbf{u}$, so there are $p^2 + q^2 - 1$ independent parameters at our disposal. Thus, in general, we expect the canonical quadratic variational problem to depend on

$$\frac{p(p+1)q(q+1)}{4} - p^2 - q^2 + 1$$

canonical moduli. For planar elasticity, $p = q = 2$, so we will find just 2 canonical elastic moduli. In three dimensions, we should obtain 19 canonical elastic moduli; however, imposing the symmetry conditions (2.9) reduces the count to 12. In the case $p = 2$, $q = 3$ covered by the Stroh formalism, we expect 6 independent canonical elastic moduli.

5.1. The planar case

In the case of planar elasticity, $p = q = 2$, the discriminant $\Delta_{\mathbf{u}}(\mathbf{x})$ is a homogeneous quartic polynomial of the two variables $\mathbf{x} = (x, y)$, which has either two complex conjugate pairs of simple roots, or a complex conjugate pair of

double roots. In the former case, we can find a real linear change of variables which moves the roots onto the imaginary axis, to $(1, \pm\tau i), (1, \pm\tau^{-1} i)$, for some $\tau > 1$. (The constant τ is an invariant associated with the roots of the quartic.) In the latter case, we move the roots to $(1, \pm i)$. Performing the same change of variables on the other discriminant $\Delta_{\mathbf{x}}(\mathbf{u})$ (where, according to theory, the value of τ is necessarily the same), it can be proved, [22], that the symbol thereby reduces to one of "strongly orthotropic" form

$$x^2u^2 + y^2v^2 + \alpha(y^2u^2 + x^2v^2) + 2\beta xyuv, \tag{5.1}$$

where the canonical moduli α, β satisfy the inequalities

$$\alpha > 0, \qquad \beta \geq 0, \qquad |\alpha - 1| > \beta, \tag{5.2}$$

in the case when the discriminant has simple roots, or

$$0 < \alpha \leq 1, \qquad \beta = 1 - \alpha, \tag{5.3}$$

in the case of double roots. The corresponding stored energy function is given by the *orthotropic Lagrangian*

$$u_x^2 + \alpha u_y^2 + 2\beta u_x v_y + \alpha v_x^2 + v_y^2. \tag{5.4}$$

In fact, the Lagrangian (5.4) is, modulo a null Lagrangian, just a rescaled version of the standard stored energy of a linear, planar orthotropic elastic material

$$c_{1111}u_x^2 + c_{1212}(u_y + v_x)^2 + 2c_{1122}u_x v_y + c_{2222}v_y^2. \tag{5.5}$$

Indeed, after adding the null Lagrangian $c_{1212}(u_x v_y - u_y v_x)$, a simple rescaling will place this stored energy into the form (5.4), where

$$\alpha = \frac{c_{1212}}{\sqrt{c_{1111}c_{2222}}}, \qquad \beta = \frac{c_{1122}}{\sqrt{c_{1111}c_{2222}}}. \tag{5.6}$$

The discriminant has a complex conjugate pair of double roots if and only if the material is equivalent to an isotropic material, with $\alpha = \mu/(2\mu+\lambda)$, $\beta = (\mu+\lambda)/(2\mu+\lambda)$, where λ and μ are the classical Lamé moduli. Moreover, the isotropic stored energies are distinguished by the presence of a one-parameter symmetry group corresponding to the rotational invariance of (5.4) when $\alpha + \beta = 1$. Two isotropic Lagrangians determine the same orthotropic Lagrangian if and only if they have the same value for Poisson's ratio. The cases when the discriminant has simple roots, and the Lagrangian has at most discrete symmetries, correspond to "truly" anisotropic materials.

THEOREM 1. *Let $W(\nabla \mathbf{u})$ be a homogeneous first order planar quadratic Lagrangian which satisfies the Legendre–Hadamard strong ellipticity condition.*

Then W is equivalent to an orthotropic Lagrangian (5.4), *where the canonical elastic moduli α and β satisfy the strong ellipticity inequalities $\alpha > 0$, $|\beta| < \alpha + 1$. The corresponding Euler–Lagrange equations are thus equivalent to the "orthotropic Navier equations"*

$$u_{xx} + \alpha u_{yy} + \beta v_{xy} = 0, \qquad \beta u_{xy} + \alpha v_{xx} + v_{yy} = 0. \tag{5.7}$$

The six components of the elastic tensor $\mathbf{C}$ can be summarized in matrix form by

$$\mathbf{C} = \begin{bmatrix} c_{11} & c_{12} & c_{16} \\ & c_{22} & c_{26} \\ & & c_{66} \end{bmatrix},$$

where c_{ij} represents the standard contracted notation, [7]. In this version, the canonical form is found to be

$$\mathbf{C} = \begin{bmatrix} c_{11} & c_{12} & 0 \\ & c_{11} & 0 \\ & & c_{66} \end{bmatrix}.$$

Note that it is possible to rescale so that $c_{11} = 1$.

See [22] for the explicit formulas for the change of variables taking a given stored energy function into its canonical orthotropic form. One can reduce a general strongly elliptic orthotropic stored energy (5.4) to a unique strongly orthotropic Lagrangian satisfying the more restrictive inequalities (5.2) or (5.3), using one or more of the three basic discrete equivalences taking the moduli (α, β) to either

$$(\alpha, -\beta), \qquad \text{or} \qquad \left(\frac{1}{\alpha}, \frac{1}{\beta}\right), \qquad \text{or} \qquad \left(\frac{1+\alpha-\beta}{1+\alpha+\beta}, \frac{2-2\alpha}{1+\alpha+\beta}\right). \tag{5.8}$$

Therefore, except in a few "exceptional" cases, each orthotropic Lagrangian is equivalent to seven different orthotropic Lagrangians.

REMARK. A complete set of canonical forms for general quadratic variational problems in the case $p = q = 2$ is known; see [24] for details.

5.2. The Stroh case

Turning to the case of planar deformations of a three-dimensional material, i.e. $p = 2$, $q = 3$, we must determine canonical forms for a positive definite "bi-ternary quadratic"

$$Q(x, y; u, v, w) > 0, \qquad (x, y) \neq 0, \quad (u, v, w) \neq 0. \tag{5.9}$$

Such a symbol will be the planar restriction of a three-dimensional elastic stored energy function W provided it satisfies

$$Q(x, y; u, v, 0) = Q(u, v; x, y, 0). \tag{5.10}$$

The discriminant $\Delta_{\mathbf{u}}(\mathbf{x})$ is a homogeneous sextic polynomial in $\mathbf{x} = (x, y)$, which, according to the strong ellipticity assumption, has three complex conjugate pairs of roots.

A stored energy function is called *separable* if there exist coordinates $\mathbf{x}$, $\mathbf{u}$ such that its symbol takes the form

$$Q(x, y; u, v, w) = R(x, y; u, v) + s(x, y)w^2. \tag{5.11}$$

Note that in this case, the Euler–Lagrange equations separate into a linear system for u, v, and a single separate second order elliptic equation for w, so that the problem essentially reduces to a problem for purely planar elasticity (with a separate anti-planar problem). If R is isotropic, then the rotational symmetry group can be used to diagonalize the quadratic polynomial $s(\mathbf{x})$, but, in general, we are left with the 4 parameter class of separable canonical forms

$$u_x^2 + \alpha u_y^2 + 2\beta u_x v_y + \alpha v_x^2 + v_y^2 + \gamma w_x^2 + 2\delta w_x w_y + \varepsilon w_y^2. \tag{5.12}$$

(One of the parameters $\gamma, \delta, \varepsilon$ can be eliminated by rescaling w.) Thus, the equilibrium equations reduce to the orthotropic Navier equations (5.7) together with a second order elliptic equation for w, which can be easily transformed into Laplace's equation, although not without changing the orthotropic form of the planar part.

In the Stroh formalism, the essential elasticities can be summarized with the three symmetric matrices Q, $R + R^T$, and T, given by

$$\begin{bmatrix} c_{11} & c_{16} & c_{15} \\ & c_{66} & c_{65} \\ & & c_{55} \end{bmatrix} \begin{bmatrix} 2c_{16} & c_{12}+c_{66} & c_{14}+c_{56} \\ & 2c_{26} & c_{46}+c_{25} \\ & & 2c_{45} \end{bmatrix} \begin{bmatrix} c_{66} & c_{26} & c_{46} \\ & c_{22} & c_{24} \\ & & c_{44} \end{bmatrix}.$$

One can see that there are 15 independent moduli. The material is separable when the third columns of these matrices are of the form $[0\ 0\ *]^T$. In [9] it was shown that a material is separable if and only if one of the Stroh eigenvectors is a real vector.

If the material if not separable, we have the canonical form [25],

$$\begin{bmatrix} c_{11} & 0 & c_{15} \\ & c_{66} & c_{65} \\ & & c_{55} \end{bmatrix} \begin{bmatrix} 0 & c_{12}+c_{66} & 0 \\ & 0 & 0 \\ & & 0 \end{bmatrix} \begin{bmatrix} c_{66} & 0 & c_{46} \\ & c_{11} & c_{24} \\ & & c_{44} \end{bmatrix}.$$

Note again that we may scale so that $c_{11} = 1$. These can further be refined if the material is degenerate. It turns out that there are two inequivalent classes of degenerate materials [8, 9],

$$\begin{bmatrix} c_{11} & 0 & c_{15} \\ & \dfrac{c_{11}-c_{12}}{2} & c_{56} \\ & & c_{44}+2c_{11} \end{bmatrix} \begin{bmatrix} 0 & \dfrac{c_{11}+c_{12}}{2} & 0 \\ & 0 & 0 \\ & & 0 \end{bmatrix} \begin{bmatrix} \dfrac{c_{11}-c_{12}}{2} & 0 & c_{15} \\ & c_{11} & c_{56} \\ & & c_{44} \end{bmatrix}, \tag{5.13}$$

$$(5.14)\qquad \begin{bmatrix} c_{11} & 0 & c_{46}+\dfrac{1}{\sqrt{c_{11}}} \\ & c_{11} & 0 \\ & & (c_{12}+c_{11})^{-2} \end{bmatrix} \begin{bmatrix} 0 & c_{12}+c_{11} & 0 \\ & 0 & 0 \\ & & 0 \end{bmatrix} \begin{bmatrix} c_{11} & 0 & c_{46} \\ & c_{11} & 0 \\ & & (c_{12}+c_{11})^{-2} \end{bmatrix}.$$

If, in addition, there is only one Stroh eigenvalue, so N is "extraordinarily degenerate", then the canonical forms are either (5.13) with $c_{15} = 0$ and $c_{12} = [c_{11}(2c_{11}^2 - c_{56}^2)]/(2c_{11}^2 + c_{56}^2)$, or (5.14) with $c_{46} = -1/2\sqrt{c_{11}}$. For a discussion of inseparable, degenerate materials, see [34].

5.3. Three-dimensional case

Complete canonical forms for the fully three-dimensional elastic tensor under the action of the general linear group remains an open problem. LODGE [15] has provided a set of necessary and sufficient conditions on the elasticities that guarantee that the tensor can be transformed into an isotropic form. The general problem is difficult due to the complexity of the expressions involved. A promising approach seems to lie in constructing the invariants under the action of the general linear group. However, this also is an open problem. For the corresponding work with respect to the action of the orthogonal group, see [11, 36] and the references therein.

6. Conservation laws

By a *conservation law* for a system of partial differential equations, we mean a divergence expression $\operatorname{Div} \mathbf{P} = 0$ which vanishes on all solutions. The conservation law is called *trivial* if either $\mathbf{P} = 0$ vanishes on all solutions, or $\operatorname{Div} \mathbf{P} \equiv 0$ vanishes for *all* $\mathbf{u}$. Two conservation laws are *equivalent* if and only if they differ by a trivial conservation law. So far, only first order conservation laws, meaning that $\mathbf{P}(\mathbf{x}, \mathbf{u}, \nabla\mathbf{u})$ depends on at most first order derivatives, have been classified up to equivalence.

The most well-known example of a conservation law or path-independent integral in elasticity is the celebrated Eshelby energy-momentum tensor [4, 29], which governs the energy release rate at a singularity [1]. In general, Noether's Theorem [18, 26], provides a one-to-one correspondence between conservation laws and symmetries of the variational problem. Surprisingly, this fundamental result was not systematically applied in elasticity until the work of GÜNTHER [6], and KNOWLES and STERNBERG [13]. The latter claimed to have a complete classification of all possible elastic conservation laws, but they failed to take into account more general types of symmetries as well as particular constitutive relations which can increase the number of laws. This prompted EDELEN [3], to propose that "... a detailed cataloging of *all* invariance transformations and conservation laws in linear elasticity would seem a worthy task". This served to

motivate us to initiate a systematic classification program for conservation laws [19, 20, 23, 9]. In this section we review what is known to date.

6.1. Betti reciprocity

Any self-adjoint linear system admits a special class of conservation laws that arise from Betti's reciprocal theorem [7, Sec. 30]. A Betti-reciprocity law takes the explicit form

$$\text{Div}\, P = 0, \qquad \text{where} \qquad P_i = \sigma_{ij} \cdot \tilde{u}^j - \tilde{\sigma}_{ij} \cdot u^j. \tag{6.1}$$

Here $\mathbf{u}, \tilde{\mathbf{u}}$ are any two solutions of the equilibrium equations, with corresponding stress tensors $\sigma, \tilde{\sigma}$.

In the linear case, each symmetry provides a recursion operator that produces symmetries and conservation laws of arbitrarily high order. We conjecture that, like the Laplace equation, [30], every higher order symmetry and conservation law is generated by the first order ones. The higher order conservation laws have not been investigated so far.

6.2. Two independent variables

The approaches and results for the planar case and the Stroh formalism are similar and we will present them together. We consider first order conservation laws $\text{Div}\, \mathbf{P} = D_x P_1 + D_y P_2 = 0$. The conditions can be presented in the convenient matrix form

$$\nabla P_1 = M\, \nabla P_2, \qquad \text{where} \qquad M = \begin{bmatrix} 0 & QT^{-1} \\ -I & (R + R^T)T^{-1} \end{bmatrix}, \tag{6.2}$$

and ∇ denotes the gradient with respect to to the derivative variables $u^i_j = \partial u^i / \partial x_j$. The matrix in (6.2) is similar to $-N$, cf. (3.5), and hence its characteristic polynomial is essentially the same as the Stroh polynomial. The general solution to Eq. (6.2) depends on the Jordan structure of the matrix M and can be found in [12]. For each complex conjugate pair of eigenvalues, we define the complex variables

$$\eta_\alpha = \mathbf{b}_\alpha^T \cdot \nabla \mathbf{u}, \qquad \text{where} \qquad \mathbf{b}_\alpha = \begin{bmatrix} -\dfrac{1}{p_\alpha} Q \mathbf{A}_\alpha \\ T \mathbf{A}_\alpha \end{bmatrix}$$

is the corresponding eigenvector of M, and $\mathbf{A}_\alpha$ is the corresponding Stroh eigenvector. The index α ranges from 1 to either 2 in the planar case, or 3 in the Stroh case. If the matrix is not semisimple, we use the generalized eigenvectors to similarly define variables ξ (and ζ if there are two generalized eigenvectors). The first result appears in [9, 23, 37]; see also [35].

THEOREM 2. *Every nontrivial first order conservation law for a nondegenerate material is a linear combination of the Betti reciprocal laws and the laws* $\mathbf{P}^\alpha$ *corresponding to the eigenvalues* p_α *of the elasticity matrix, where* $F_\alpha(z_\alpha, \eta_\alpha) = P_1^\alpha + \overline{p_\alpha} P_2^\alpha$ *are complex analytic functions of their arguments* $z_\alpha = x + p_\alpha y$, $\eta_\alpha = \eta_{\alpha 1} + i\eta_{\alpha 2} = f'_\alpha(z_\alpha)$.

If the material is degenerate (i.e. the matrix in (6.2) is irreducible), there are several different cases.

6.3. Planar, irreducible

In the planar case, the material is equivalent to an isotropic material. If the material is isotropic, one can solve for the eigenvectors explicitly. The explicit form of the conservation laws in isotropic materials was first given in [20].

THEOREM 3. *Every degenerate planar material is equivalent to an isotropic material. Every nontrivial conservation law is a combination of Betti reciprocity and the laws given by*

$$P_1 + \bar{p} P_2 = F(z, \eta) - \frac{i}{2\operatorname{Im} p} \left(\bar{z} \frac{\partial G}{\partial z} + \overline{G(z, \eta)} \right) + \xi \frac{\partial G}{\partial \eta} + c\bar{z} \cdot \eta^2 + \omega \cdot \eta. \tag{6.3}$$

Here F *and* G *are analytic functions of* $\eta = \eta_1 + i\eta_2$, *and* $z = x + py$, c *is a complex scalar,* ω *is a certain linear combination of the displacements* u, v.

6.4. Stroh, irreducible

In the Stroh formalism, if the matrix is irreducible, one can have either two distinct pairs (one pair doubled) or one tripled pairs of roots. The following results appear in [9].

THEOREM 4. *Suppose* M *is irreducible with two real Jordan blocks. Let* p_1 *be the double root and* p_2 *the simple root with positive imaginary parts. Then every nontrivial conservation law is a combination of Betti reciprocity and the laws* $\mathbf{P}, \widetilde{\mathbf{P}}$, *where*

$$P_1 + \bar{p}_1 P_2 = F_1(z_1, \eta_1) - \frac{i}{2\operatorname{Im} p_1} \left(\bar{z}_1 \frac{\partial G}{\partial z_1} + \overline{G(z_1, \eta_1)} \right) + \xi \frac{\partial G}{\partial \eta_1} + c\bar{z}_1 \cdot \eta_1^2 + \omega \cdot \eta_1 ,$$
$$\widetilde{P}_1 + \overline{p_2} \widetilde{P}_2 = F_2(z_2, \eta_2).$$

Here F_i *and* G *are analytic in* $\eta_\alpha = \mathbf{b}_\alpha^T \cdot \nabla \mathbf{u}$ *and* $z_\alpha = x + p_\alpha y$, c *is a complex scalar, and* ω *is a certain linear combination of the displacements* $\mathbf{u}$. *The terms* $c\bar{z}_1 \cdot \eta_1^2 + \omega \cdot \eta_1$ *are nontrivial if and only if the material is separable.*

THEOREM 5. *Suppose that* M *is irreducible with one real Jordan block, and let* $p = p_1 + ip_2$ *be the corresponding triple root with positive imaginary part.*

Every nontrivial conservation law is a combination of Betti reciprocity and the laws **P** *with components*

$$P_1 + \overline{p}P_2 = F + \xi\frac{\partial G}{\partial \eta} - \frac{i}{2p_2}\bar{G} + \xi^2\frac{\partial^2 H}{\partial \eta^2} + 2\zeta\frac{\partial H}{\partial \eta} - \frac{i}{p_2}\cdot\xi\overline{\frac{\partial H}{\partial \eta}} + \frac{1}{2p_2^2}\bar{H},$$

where

$$\begin{aligned} F &= F_0(z,\eta) - \frac{i}{2p_2}\overline{z}\frac{\partial G_0}{\partial z} - \frac{1}{2p_2^2}\left(\frac{\overline{z}^2}{2}\frac{\partial^2 H}{\partial z^2} + \overline{z}\frac{\partial H}{\partial z}\right) - c_1\overline{z}\cdot\eta^2 + \omega\cdot\eta, \\ G &= G_0(z,\eta) - \frac{i}{p_2}\overline{z}\frac{\partial H}{\partial z} - \frac{1}{2}c_2\overline{z}\cdot\eta^2, \\ H &= H(z,\eta). \end{aligned}$$

The functions F_0, G_0 and H are complex analytic in their arguments, the c_i are complex scalars, and ω is a certain linear combination of the displacements u^i.

There is some subtlety between repeated roots and irreducible matrices. In general, distinct eigenvalues implies that a given matrix is semisimple but not the other way around. If the Stroh sextic has one tripled pair of complex conjugate roots, then the matrix N will have one real Jordan block if and only if the material is inseparable. If the material is separable, there are exactly two real Jordan blocks. On the other hand, if the Stroh sextic has one doubled pair of roots and a second distinct pair, then the matrix N is semisimple if and only if the material is separable and the two root pairs corresponding to the planar part are distinct. See [9] for details.

6.5. Three independent variables

Finally, let us consider the full three-dimensional case. In general, the number of conservation laws a material may have, depends whether or not the elasticities satisfy certain nondegeneracy conditions; these are closely related to the symmetry class of the elastic tensor. In particular, certain materials have more conservation laws than a generic material. We first state all the conservation laws which exist in all three-dimensional materials, regardless of its symmetry, [2].

THEOREM 6. *Every nontrivial conservation law which exists for all three-dimensional materials is a linear combination of the following laws:*

i) *the stress* $\sigma_{ij} = C_{ijkl}\cdot u^k_l$,

ii) *the Eshelby energy-momentum tensor* $P^i_m = C_{jkli}\cdot u^j_k\cdot u^l_m - \frac{1}{2}\delta^i_m C_{jkrs}\cdot u^j_k\cdot u^r_s$, *where* δ^i_m *is the Kronecker* δ,

iii) *the "scaling" density* $Y^i = x^j P^i_j + \frac{1}{2}u^j\sigma_{ij}$, *and*

iv) *the Betti reciprocal relations.*

THEOREM 7. *All conservation laws of a three-dimensional isotropic material are linear combinations of those listed in Theorem* 6 *along with the densities*

$$
\begin{aligned}
R_j^i &= \varepsilon_{jkl}\left(x^k P_l^i - u^k \sigma_{ik}\right), \\
Q_j^i &= c_{11}c_{66}u_i^j u_k^k + c_{66}^2 u_l^j\left(u_i^l - u_l^i\right) + \frac{1}{2}\left(c_{66}+c_{12}\right)c_{11}\delta_j^i u_k^k u_l^l, \\
T_j^i &= \varepsilon_{jkl}\left(\left(c_{66}+c_{12}\right)x^k Q_l^i + c_{66}(c_{11}+c_{66})u^k\sigma_{il}\right) \\
&\qquad + \frac{1}{2}c_{66}^2\left(c_{66}+c_{12}\right)\left(\varepsilon_{jkl}u^k u_j^l + \delta_j^i \varepsilon_{klm}u^l u_m^k\right),
\end{aligned}
$$

where ε_{jkl} *is the alternating tensor.*

The isotropic classification appears in [20]. If the material is transversely isotropic, the most general conservation laws are those listed in Theorem 6, and R_3^i and a generalization of Q_3^i in 7; see [10]. In this reference, it is also shown that under certain degeneracy conditions, a transversely isotropic material may have generalizations of Q_1^i and Q_2^i as well. There are no more laws unless the material is equivalent to an isotropic material. An open problem consists in determining precisely when an anisotropic material has conservation laws beyond those of Theorem 6. This problem is closely related to the canonical forms problem mentioned earlier.

Acknowledgments

The research of the second author was supported in part by NSF Grant DMS 95–00931. This work was presented at the Fourth Meeting on Current Ideas in Mechanics and Related Fields, in Kraków, Poland, August 1997. We would also like to thank the organizers, particularly Marek Elzanowski, for a most productive conference.

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DEPARTMENT OF MATHEMATICS AND COMPUTER SCIENCE
GUSTAVUS ADOLPHUS COLLEGE
St. Peter, MN 56082

and

DEPARTMENT OF MATHEMATICS
UNIVERSITY OF MINNESOTA
Minneapolis, MN 55455
e-mail: olver@ima.umn.edu

Received October 3, 1997.

Arch. Mech., 50, 3, pp. 405–413, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

Nambu – Poisson dynamics

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

R. IBÁÑEZ (BILBAO), M. de LEÓN (MADRID),
J.C. MARRERO (LA LAGUNA) and D.M. de DIEGO (MADRID)

SEVERAL PHYSICAL systems can be described by using multibrackets instead of the usual Poisson or Jacobi brackets. Starting with the original construction of Nambu we give a brief review on recent results on multibrackets on manifolds.

1. Classical Hamiltonian mechanics

THE PHASE-SPACE in classical Hamiltonian mechanics [1, 2, 3, 4] is the cotangent bundle T^*M of the configuration space M which is provided with a canonical symplectic structure ω. If we consider local coordinates $(q^1, \cdots, q^n, p_1, \cdots, p_n)$ on T^*M (q^i are the position coordinates of M and p_i the momentum coordinates), we have

$$\omega = \sum_{i=1}^{n} dq^i \wedge dp_i \,,$$

and the associated *canonical Poisson bracket* (which is non-degenerate) is given by

$$\{f, g\} = \sum_{i=1}^{n} \left(\frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q^i} - \frac{\partial f}{\partial q^i} \frac{\partial g}{\partial p_i} \right).$$

Hamilton's equations of motion are the first order differential equations

$$\frac{dq^i}{dt} = \{H, q^i\} = \frac{\partial H}{\partial p_i} \,, \qquad \frac{dp_i}{dt} = \{H, p_i\} = -\frac{\partial H}{\partial q^i} \,, \tag{1.1}$$

where H is the Hamiltonian energy of the mechanical system. The Hamilton equations of motion can be expressed in a global way as

$$\frac{df}{dt} = \{H, f\}. \tag{1.2}$$

However, the study of some mechanical systems, particularly systems with symmetries or constraints, may lead to more general Poisson brackets (degenerate brackets).

A *Poisson bracket* [19, 5, 6, 7] on a smooth manifold M is a bilinear operation $\{\ ,\ \}$ on $C^\infty(M,\mathbb{R})$ satisfying the following properties:

i) $\{f,g\} = -\{g,f\}$ (skew-symmetry),

ii) $\{f,gh\} = \{f,g\}h + g\{f,h\}$ (Leibniz rule),

iii) $\{\{f,g\},h\} + \{\{h,f\},g\} + \{\{g,h\},f\} = 0$ (Jacobi's identity),

for all $f,g,h \in C^\infty(M,\mathbb{R})$.

Given a function $H \in C^\infty(M,\mathbb{R})$, we associate a vector field X_H (called the Hamiltonian vector field) defined by

$$X_H(g) = \{H,g\}.$$

Thus, the solutions of the Hamilton's equations of motion (1.2) are just the integral curves of the Hamiltonian vector field X_H.

EXAMPLE 1. Newton's second law

The Newton's second law states that a particle of mass $m > 0$ moving under the influence of a potential $V(q)$, $q = (q^1,q^2,q^3) \in \mathbb{R}^3$, moves along a curve $q(t)$ in $\mathbb{R}^3$ in such a way that

$$F = ma, \tag{1.3}$$

where $a = d^2q/dt^2$ is the acceleration and $F(q) = -\operatorname{grad} V(q)$ is the force acting on the particle (the force field is conservative).

If we introduce the momemtum coordinates $p_i = m(dq^i/dt)$, then the phase-space is $\mathbb{R}^6$ with coordinates $(q^1,q^2,q^3,p_1,p_2,p_3)$ and canonical Poisson bracket. Therefore the Newton second law (1.3) is equivalent to the Hamilton equations (1.1) with respect to the total energy of the system $H(q,p) = K(p)+V(q)$, where $K(p) = \left(\dfrac{1}{2m}\right)\|p\|^2$ is the kinetic energy.

EXAMPLE 2. Rigid body

We will consider the motion of a free rigid body around a fixed point [3]. The Euler equations of rigid body dynamics in the absence of external forces are usually written as follows:

$$\begin{aligned} I_1\frac{d\Omega_1}{dt} &= (I_2 - I_3)\Omega_2\Omega_3\,, \\ I_2\frac{d\Omega_2}{dt} &= (I_3 - I_1)\Omega_3\Omega_1\,, \\ I_3\frac{d\Omega_3}{dt} &= (I_1 - I_2)\Omega_1\Omega_2\,, \end{aligned} \tag{1.4}$$

where $\Omega = (\Omega_1,\Omega_2,\Omega_3)$ is the body angular velocity vector and I_1, I_2, I_3 are the moments of inertia.

To see the Hamiltonian structure of the rigid body equations, one can use the description in terms of the Euler angles θ,ψ,ϕ and their conjugate momenta p_θ, p_ψ, p_ϕ (the configuration space is $SO(3)$ and the phase-space is $T^*(SO(3))$),

relative to which the equations are in canonical Hamiltonian form (1.1). However, this procedure requires using six equations instead of the three equations (1.4).

We introduce the angular momenta $\Pi = I\Omega \in so(3)^* \cong \mathbb{R}^3$, that is, $\Pi_i = I_i\Omega_i$ $(i = 1, 2, 3)$, so that Eqs. (1.4) become

$$\begin{aligned} \frac{d\Pi_1}{dt} &= \frac{I_2 - I_3}{I_2 I_3}\Pi_2\Pi_3\,, \\ \frac{d\Pi_2}{dt} &= \frac{I_3 - I_1}{I_3 I_1}\Pi_3\Pi_1\,, \\ \frac{d\Pi_3}{dt} &= \frac{I_1 - I_2}{I_1 I_2}\Pi_1\Pi_2\,, \end{aligned} \tag{1.5}$$

that is, $d\Pi/dt = \Pi \times \Omega$.

Introduce the following Poisson bracket on functions of the Π:

$$\{F, G\}(\Pi) = \Pi \cdot (\nabla F(\Pi) \times \nabla G(\Pi)),$$

where ∇f is the gradient of the function f. Notice that this bracket is the Lie-Poisson bracket of the dual $so(3)^*$ of the Lie algebra $so(3)$. If the Hamiltonian H is

$$H(\Pi) = \frac{1}{2}\left(\frac{\Pi_1^2}{I_1} + \frac{\Pi_2^2}{I_2} + \frac{\Pi_3^2}{I_3}\right),$$

then Eqs. (1.5) are the Lie – Poisson equations. Finally, we notice that the kinetic energy and the total angular momentum

$$C(\Pi) = \frac{1}{2}(\Pi_1^2 + \Pi_2^2 + \Pi_3^2), \tag{1.6}$$

are integrals of motion of the Hamiltonian vector field X_H.

2. Nambu mechanics

In 1973 Y. NAMBU [8] proposed a generalization of classical Hamiltonian mechanics to a Hamiltonian system defined on a 3-dimensional phase-space with respect to a ternary Poisson bracket and two Hamiltonian functions.

Nambu considered the 3-dimensional phase-space $\mathbb{R}^3$ with coordinates x_1, x_2, x_3 and the canonical Nambu bracket defined for three arbitrary functions f_1, f_2, f_3 by

$$\{f_1, f_2, f_3\} = \frac{\partial(f_1, f_2, f_3)}{\partial(x_1, x_2, x_3)}.$$

Then the *Nambu equations* of motion are given by

$$\frac{dx_1}{dt} = \frac{\partial(H_1, H_2)}{\partial(x_2, x_3)}, \qquad \frac{dx_2}{dt} = \frac{\partial(H_1, H_2)}{\partial(x_3, x_1)}, \qquad \frac{dx_3}{dt} = \frac{\partial(H_1, H_2)}{\partial(x_1, x_2)}, \tag{2.1}$$

or in a more general way

$$\frac{df}{dt} = \{H_1, H_2, f\}, \tag{2.2}$$

where H_1, H_2 are two Hamiltonian functions on $\mathbb{R}^3$.

Now, the solutions of Eqs. (2.2) are the integral curves of the Hamiltonian vector field $X_{H_1H_2}$, where $X_{H_1H_2}(g) = \{H_1, H_2, g\}$ for $g \in C^\infty(\mathbb{R}^3, \mathbb{R})$.

Nambu posed the following question: Are there real physical systems which may be described in this way?

The example considered by himself was the following.

EXAMPLE 3. Rigid body II

Nambu observed [8] that Eqs. (1.5) are nothing else but the Nambu equations (2.2) with respect to the canonical Nambu bracket for the coordinates Π_1, Π_2, Π_3 and the two Hamiltonians

$$H_1 = \frac{1}{2}(\Pi_1^2 + \Pi_2^2 + \Pi_3^2),$$
$$H_2 = \frac{1}{2}\left(\frac{\Pi_1^2}{I_1} + \frac{\Pi_2^2}{I_2} + \frac{\Pi_3^2}{I_3}\right),$$

that is, total angular momemtum and the kinetic energy.

EXAMPLE 4. Static $SU(2)$-monopoles

The Nahm's system in the theory of static $SU(2)$-monopoles [9, 10] is given by the following equations of motion:

$$\frac{dx_1}{dt} = x_2x_3, \qquad \frac{dx_2}{dt} = x_1x_3, \qquad \frac{dx_3}{dt} = x_1x_2\,.$$

The above equations can be written in Nambu form (2.1), where

$$H_1 = \frac{1}{2}(x_1^2 - x_2^2), \qquad H_2 = \frac{1}{2}(x_1^2 - x_3^2).$$

Other examples of Nambu dynamical systems are the $SU(n)$-isotropic harmonic oscillator and the $SO(4)$-Kepler problem studied in [11] or the rigid body with a single torque about a major axis [12], among others.

3. Nambu – Poisson and generalized Poisson manifolds

After the publication of NAMBU'S paper [8], Nambu mechanics has been discussed by many authors, but it was almost forgotten for many years. A recent paper by TAKHTAJAN [10] gave a new interest to this subject by introducing a geometrical setting for Nambu brackets. He considered brackets of n functions satisfying a generalization of the Jacobi identity, the so-called fundamental identity. More recently, DE AZCÁRRAGA, PEREMOLOV and PÉREZ BUENO [13, 14, 15]

have introduced an alternative generalization of the Jacobi identity, the so-called generalized Jacobi identity. Both kinds of multibrackets are natural generalizations of the ordinary Poisson brackets, and the fundamental and generalized Jacobi identities are the corresponding integrability conditions which extend the Jacobi identity.

In order to give a unified setting, we have introduced in [16, 17, 18] the following definition.

A *generalized almost Poisson bracket* of order n on a smooth manifold M is an n-linear mapping $\{\,,\ldots,\,\} : C^\infty(M,\mathbb{R}) \times \cdots \times C^\infty(M,\mathbb{R}) \longrightarrow C^\infty(M,\mathbb{R})$ satisfying the following properties:

1) $\{f_1,\ldots,f_n\} = (-1)^{\epsilon(\sigma)}\{f_{\sigma(1)},\ldots,f_{\sigma(n)}\}$, (*skew-symmetry*)

2) $\{f_1 g_1,\ldots,f_n\} = f_1\{g_1,\ldots,f_n\} + g_1\{f_1,\ldots,f_n\}$, (*Leibniz rule*)

for all $f_1,\ldots,f_n,g_1 \in C^\infty(M,\mathbb{R})$ and $\sigma \in \mathrm{Symm}\,(n)$, where $\mathrm{Symm}\,(n)$ is a symmetric group of n elements and $\epsilon(\sigma)$ is the parity of σ.

An alternative way to define an n-bracket of functions is to consider the skew-symmetric tensor Λ of type $(n,0)$ given by

$$\Lambda_x(df_1(x),\ldots,df_n(x)) = \{f_1,\ldots,f_n\}(x)\,,$$

for all $f_1,\ldots,f_n \in C^\infty(M,\mathbb{R})$ and $x \in M$. A manifold M with such a structure is called *generalized almost Poisson manifold* of order n [16].

In local coordinates $(x_1,\cdots,x_m)$ on M, the tensor Λ can be written as follows:

$$\Lambda = \frac{1}{n!}\sum_{i_1,\cdots,i_n=1}^{m} c_{i_1\cdots i_n}\frac{\partial}{\partial x_{i_1}}\wedge\cdots\wedge\frac{\partial}{\partial x_{i_n}}, \tag{3.1}$$

where the functions $c_{i_1\cdots i_n} = \{x_{i_1},\cdots,x_{i_n}\} = \Lambda(x_{i_1},\cdots,x_{i_n})$ are skew-symmetric.

With $n-1$ functions $H_1,\cdots,H_{n-1} \in C^\infty(M,\mathbb{R})$, we associate a vector field $X_{H_1\cdots H_{n-1}}$ called the *Hamiltonian vector field* and defined by

$$X_{H_1\cdots H_{n-1}}(g) = \{H_1,\cdots,H_{n-1},g\}, \qquad \text{for all} \quad g \in C^\infty(M,\mathbb{R}).$$

In addition, we can consider an integrability condition. A generalized almost Poisson manifold (M,Λ) of order n is said to be

- *Nambu–Poisson* [10, 16] if it satisfies the *fundamental identity*

$$\{f_1,\ldots,f_{n-1},\{g_1,\ldots,g_n\}\} = \sum_{i=1}^{n}\{g_1,\ldots,\{f_1,\ldots,f_{n-1},g_i\},\ldots,g_n\}, \tag{3.2}$$

for all $f_1,\ldots,f_{n-1},g_1,\ldots,g_n$ on M;

- *generalized Poisson manifold* [13, 16] if n is even and it satisfies the *generalized Jacobi identity*

$$\mathrm{Alt}\,(\{f_1,\ldots,f_{n-1},\{g_1,\ldots,g_n\}\}) = 0, \tag{3.3}$$

for all $f_1,\ldots,f_{n-1},g_1,\ldots,g_n$ on M.

We notice that the generalized Jacobi identity is equivalent to the condition $[\Lambda, \Lambda] = 0$, where $[\,,\,]$ is the Schouten-Nijenhuis bracket [5].

REMARK. If in the definition of a Poisson bracket we only assume that the bilinear operator $\{\,,\,\}$ is of local nature, we obtain a Jacobi bracket (see [20, 21]). The corresponding generalizations to multibrackets have been recently discussed in [22, 23, 24].

EXAMPLE 5. Volume form

Let M be an oriented n-dimensional manifold and v_M a volume form. Given n functions $f_1, \ldots, f_n$ on M, we define a Nambu-Poisson bracket by the formula [25]

$$df_1 \wedge \cdots \wedge df_n = \{f_1, \ldots, f_n\} v_M \,.$$

Notice that the associated Nambu-Poisson tensor Λ is non-zero everywhere: $\Lambda(x) \neq 0$, for all $x \in M$.

Conversely, each Nambu-Poisson tensor $\Lambda \neq 0$ of order n on a smooth manifold M of dimension n follows from a volume form [16]. If we take $M = \mathbb{R}^n$, and v_M is the standard volume form $v_M = dx_1 \wedge \cdots \wedge dx_n$, we recover the example originally discussed by Nambu [8].

The Nambu-Poisson structure associated with a volume form (for $n \geq 3$) can be considered as the analogue of the symplectic structure in Poisson geometry (see [16]).

EXAMPLE 6. Constant Nambu–Poisson structures

A generalized almost Poisson structure of order n on $\mathbb{R}^m$ is given by the expression (3.1) and this structure is constant if the coefficients $c_{i_1 \cdots i_n} \in \mathbb{R}$. GAUTHERON proved in [25] that the constant Nambu-Poisson structures of order n on $\mathbb{R}^m$ are just the decomposable n-vectors. Notice that, in contrast, all the constant generalized almost Poisson structures are trivially generalized Poisson structures.

4. Foliation of Nambu–Poisson manifolds

As is well known, a Poisson manifold possesses a symplectic foliation [6, 5]. Given a Nambu-Poisson manifold (M, Λ) of order $n \geq 3$, if for each point $x \in M$ we consider the subspace D_x of $T_x M$ spanned by the Hamiltonian vector fields $X_{f_1 \cdots f_{n-1}}$ evaluated at x, then we obtain a generalized distribution D on M (called *characteristic distribution*). By using the results in [25] we have proved in [16] that the characteristic distribution D is completely integrable and therefore, it defines a foliation on M such that the restriction of Λ to each leaf defines an induced Nambu-Poisson structure. There are two kinds of leaves:

i) for $x \in M$ such that $\Lambda(x) \neq 0$, the leaf passing through x has dimension n, and the induced Nambu-Poisson structure on it comes from a volume form;

ii) for $x \in M$ such that $\Lambda(x) = 0$, the leaf passing through x reduces to the point x, and the induced Nambu-Poisson structure is trivial.

5. Local structure of Nambu–Poisson manifolds

The local structure of a Poisson manifold was elucidated in [6]. For a Nambu – Poisson manifold was proved a sort of Darboux theorem (see [25, 16]):

Let (M, Λ) be a Nambu – Poisson manifold of order $n \geq 3$. Then around each point $x \in M$ such that $\Lambda(x) \neq 0$, there exist local coordinates $(x_1, \cdots, x_n, x_{n+1}, \cdots, x_m)$ such that

$$\Lambda = \frac{\partial}{\partial x_1} \wedge \cdots \wedge \frac{\partial}{\partial x_n}.$$

This result shows that the Nambu – Poisson manifolds are extremely rigid.

A consequence of this result is that every Nambu – Poisson manifold of even order is generalized Poisson, but the converse does not hold, as we have observed in Example 6.

6. Other properties of Nambu – Poisson manifolds

Let (M, Λ) be a Nambu – Poisson manifold of order n, then:

i. A function $f \in C^\infty(M, \mathbb{R})$ is an *integral of motion* of a Nambu system with Hamiltonians $H_1, \cdots, H_{n-1}$ if $\{H_1, \cdots, H_{n-1}, f\} = 0$. By using the fundamental identity, one can prove that the Nambu – Poisson bracket of n integrals of motion is again an integral of motion.

ii. If $f \in C^\infty(M, \mathbb{R})$ then the tensor $\Lambda_f = i(df)\Lambda$ is also a Nambu – Poisson tensor of order $n - 1$ on M. In general, $\Lambda_{f_1 \cdots f_r}$ is a Nambu – Poisson tensor of order $n - r$, for r functions $f_1, \cdots, f_r \in C^\infty(M, \mathbb{R})$.

iii. Every Hamiltonian vector field $X_{F_1 \cdots F_{n-1}}$ is an infinitesimal automorphism of Λ, that is,

$$\mathcal{L}_{X_{F_1 \cdots F_{n-1}}} \Lambda = 0.$$

Then its flow consists of Nambu – Poisson morphisms (see [16]).

EXAMPLE 7. Completely integrable systems

Let (M, ω, H) be a completely integrable Hamiltonian system, that is, M is a $2n$-dimensional symplectic manifold with symplectic form ω such that there exist $f_1, \ldots, f_n$ independent functions pairwise in involution, i.e., $\{f_i, f_j\} = 0$ for $i, j = 1, \ldots, n$. Then the associated Hamiltonian vector fields X_{f_i} commute, that is, $[X_{f_i}, X_{f_j}] = 0$. Thus, $\Lambda = X_{f_1} \wedge \ldots \wedge X_{f_n}$ is a Nambu – Poisson tensor on M of order n (see [17]).

Since the system is completely integrable, there exists (at least, locally) a family of independent conjugate functions $g_1, \ldots, g_n$, that is, we have

$$\{f_i, g_j\} = \delta_{ij}\,, \ \{g_i, g_j\} = 0.$$

A direct computation shows that

$$X_{g_1 \ldots g_{n-1}} = X_{f_n}\,.$$

Therefore, if the symplectic dynamical system is given by a Hamiltonian function $H = f_n$, then it is also a Nambu – Poisson dynamical system for the Hamiltonians $g_1, \cdots, g_{n-1}$.

EXAMPLE 8. Compatible Poisson structures

Let M be a differentiable manifold and Λ_1, Λ_2 two compatible Poisson structures, that is, $[\Lambda_1, \Lambda_2] = 0$; then $\Lambda_1 \wedge \Lambda_2$ is a generalized Poisson structure of order 4 (see [17]).

Acknowledgments

This work has been partially supported through grants DGICYT (Spain) Projects PB94-0106, PB94-0633-C02-02, Consejería de Educación y Cultura de la Comunidad de Madrid, Universidad de La Laguna, and UNED (Spain).

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DEPARTAMENTO DE MATEMÁTICAS,
FACULTAD DE CIENCIAS, UNIVERSIDAD DEL PAIS VASCO,
Apartado 644, 48080 Bilbao, SPAIN,
e-mail: mtpibtor@lg.ehu.es

INSTITUTO DE MATEMÁTICAS Y FÍSICA FUNDAMENTAL,
CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS,
Serrano 123, 28006 Madrid, SPAIN,
e-mail: mdeleon@fresno.csic.es

DEPARTAMENTO DE MATEMÁTICA FUNDAMENTAL,
FACULTAD DE MATEMÁTICAS, UNIVERSIDAD DE LA LAGUNA,
La Laguna, Tenerife, Canary Islands, SPAIN,
e-mail: jcmarrer@ull.es

DEPARTAMENTO DE ECONOMÍA APLICADA
CUANTITATIVA, FACULTAD DE CIENCIAS ECONÓMICAS Y EMPRESARIALES,
UNED, 28040 Madrid, SPAIN,
e-mail: dmartin@sr.uned.es

Received October 7, 1997.

Arch. Mech., 50, 3, pp. 415–421, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

On generalized parallelisms

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

I. KOLÁŘ (BRNO)

M. EPSTEIN AND M. DE LEÓN defined the second order non-holonomic parallelism on a manifold and applied it to a geometric description of generalized Cosserat continua. We explain that the underlying geometric idea is the concept of generalized parallelism on an arbitrary principal fiber bundle. Some properties of generalized parallelisms are characterized in terms of induced connections or from the viewpoint of the theory of generalized G-structures.

1. Introduction

THE STARTING POINT of the present paper were some recent results by M. Epstein and M. de León [3, 4], which describe geometrically generalized Cosserat continua in terms of the second order non-holonomic frame bundle $\tilde{P}^2M$ of a manifold M. In particular, they introduced a second order non-holonomic parallelism on M as a section $M \to \tilde{P}^2M$ and deduced several geometric properties of this parallelism. Taking into account that $\tilde{P}^2M$ is the first principal prolongation of the first order frame bundle P^1M of M, [5], we demonstrate that an interesting geometric situation appears even if one replaces the first order frame bundle by an arbitrary principal fiber bundle P over M. That's why we introduce a generalized parallelism on P as a section $M \to W^1P$ of the first principal prolongation W^1P of P.

In Sec. 3 we show that the functoriality of W^1 makes possible a simple construction of a prolongation $p(s, B) : M \to W^1P$ of every section $s : M \to P$ and every classical parallelism $B : M \to P^1M$. In Sec. 4 we deduce that every generalized parallelism on P induces two connections on P and one connection on P^1M with analogous properties to the special case of second order non-holonomic parallelisms by Epstein and de León. Then we apply our theory of generalized G-structures, [5]. In Sec. 5 we describe the local flatness of generalized parallelisms from such a point of view. In the last section we prove that the generalized parallelism can be characterized in terms of its structure function similarly to the case of classical parallelisms. All manifolds and maps are assumed to be infinitely differentiable. A connection means always a principal (i.e. right-invariant) connection in the terminology of the book [6].

2. Prolongation of principal fiber bundles

Consider an arbitrary principal fiber bundle $P(M, G)$ with projection $\pi : P \to M$, $\dim M = m$. The first principal prolongation W^1P of P is the space of all 1-jets at $(0, e) \in \mathbb{R}^m \times G$ of local principal bundle isomorphisms $\varphi : \mathbb{R}^m \times G \to P$, where e is the unit of G, [6]. It follows that W^1P is a principal bundle over M, the structure group of which is $W^1_m G = W^1_0(\mathbb{R}^m \times G)$ (= the fiber of $W^1(\mathbb{R}^m \times G)$ over $0 \in \mathbb{R}^m$), where both the multiplication in $W^1_m G$ and the right action of $W^1_m G$ on W^1P are defined by jet composition. Since φ is a principal bundle morphism, it is determined by the restriction $\tilde{\varphi} = \varphi|\mathbb{R}^m \times \{e\} : \mathbb{R}^m \to P$. The composition $\varphi_0 = \pi \circ \tilde{\varphi} : \mathbb{R}^m \to M$ is a local diffeomorphism, so that we can construct locally the inverse map $(\varphi_0)^{-1}$. Then $\tilde{\varphi} \circ (\varphi_0)^{-1}$ is locally a section of P. Passing to 1-jets we find that W^1P coincides with the fiber product over M

$$W^1P = P^1M \times_M J^1P, \tag{2.1}$$

where P^1M is the first order (= linear) frame bundle of M and J^1P is the first jet prolongation of P, [6]. Every manifold M can be identified with a principal bundle $M(M, \{e\})$, whose projection is the identity of M and the structure group is the one-element group $\{e\}$. In this case we have $W^1M = P^1M$. Further, if P itself is the first order frame bundle of M, its first principal prolongation W^1P^1M coincides with the second order non-holonomic frame bundle $\tilde{P}^2M$ of M, [3, 4, 5].

Consider another principal fiber bundle $\bar{P}(\bar{M}, \bar{G})$ satisfying $\dim \bar{M} = \dim M$. Every principal bundle morphism $f : P \to \bar{P}$ such that its base map $f_0 : M \to \bar{M}$ is a local diffeomorphism is extended into a map $W^1f : W^1P \to W^1\bar{P}$ defined by

$$W^1f(j^1_0\tilde{\varphi}) = j^1_0(f \circ \tilde{\varphi}), \tag{2.2}$$

where $\tilde{\varphi} : \mathbb{R}^m \to P$ is the above map generating an element of W^1P. Clearly, W^1 is a functor. In particular, every section $s : M \to P$ can be interpreted as a principal bundle morphism $M(M, \{e\}) \to P(M, G)$. Hence we have the induced map $W^1s : W^1M = P^1M \to W^1P$.

The adjoint bundle of any principal bundle $P(M, G)$ is the associated bundle

$$LP = P[\mathfrak{g}, Ad], \tag{2.3}$$

whose standard fiber is the Lie algebra $\mathfrak{g}$ of G with the adjoint action. According to [6], p. 161, LP is identified with the vertical tangent bundle VP of P factorized by the induced action of G on VP, i.e.

$$LP = VP/G. \tag{2.4}$$

In general, the first jet prolongation J^1Y of any fibered manifold $Y \to M$ is an affine bundle over Y, whose associated vector bundle is $VY \otimes T^*M$ [6], p. 125.

Let $\pi_0^1 : J^1P \to P$ be the target jet prolongation. Using the identification (2.4), we obtain immediately

LEMMA 1. Let $s_1, s_2 : M \to J^1P$ be two sections satisfying $\pi_0^1 \circ s_1 = \pi_0^1 \circ s_2 : M \to P$. Then $s_1 - s_2$ is a section of $LP \otimes T^*M$. □

3. Generalized parallelisms

The classical parallelism on a manifold M means an m-tuple $(B_1, \dots, B_m)$ of vector fields on M, which are linearly independent at every point. Clearly, this parallelism can be interpreted as a section $B : M \to P^1M$. We recall that B is said to be locally flat, if for every $x \in M$ there exists a neighbourhood $U \subset M$ and a local coordinate system x^i on U such that the restrictions $B_i|U$ are the coordinate vector fields $\dfrac{\partial}{\partial x^i}$, $i = 1, \dots, m$.

As mentioned in the introduction, Epstein and de León defined a second order non-holonomic parallelism on M as a section $M \to \widetilde{P}^2M = W^1P^1M$. We are going to study the following general concept (the classical parallelism corresponds to the case $P = M(M, \{e\})$).

DEFINITION 1. *A generalized parallelism on a principal bundle $P(M, G)$ is a section $A : M \to W^1P$.*

Since $W^1P = P^1M \times_M J^1P$, generalized parallelisms on P are identified with pairs $A = (A_1, A_2)$ of sections $A_1 : M \to P^1M$ and $A_2 : M \to J^1P$. Applying the projection $\pi_0^1 : J^1P \to P$, we obtain an induced section $A_0 = \pi_0^1 \circ A_2 : M \to P$.

For every section $s : M \to P$, we have constructed $W^1s : P^1M \to W^1P$.

DEFINITION 2. *For every section $s : M \to P$ and every classical parallelism $B : M \to P^1M$, the generalized parallelism $p(s, B) := (W^1s) \circ B : M \to W^1P$ on P is called the prolongation of s with respect to B.*

This construction leads to the following important concept.

DEFINITION 3. *A generalized parallelism $A : M \to W^1P$ is said to be decomposable, if $A = p(A_0, A_1)$.*

By Lemma 1, the difference

$$D(A) = A - p(A_0, A_1) \tag{3.1}$$

is a section $M \to LP \otimes T^*M$. This is the obstruction for decomposability of A. We remark that in the case $P = P^1M$ we have $LP^1M = TM \otimes T^*M$.

PROPOSITION 1. Generalized parallelisms on P are in bijection with triples of sections $A_0 : M \to P$, $A_1 : M \to P^1M$ and $D : M \to LP \otimes T^*M$.

P r o o f. We set $(A_0, A_1, D) = p(A_0, A_1) + D$. □

Clearly, $A = (A_0, A_1, D)$ is decomposable, if and only if $D = D(A) = 0$.

We remark that a similar result for connections on W^1P was deduced in [8].

4. Induced connections

Every section of a principal bundle P induces an integrable connection Γ on P, which is determined by the tangent spaces of the right translations of the section. In the case of a classical parallelism $B : M \to P^1M$, a classical result reads that B is locally flat, if and only if the connection Γ is torsion-free [3, 4].

In the case of a generalized parallelism $A : M \to W^1P$, the underlying section $A_0 : M \to P$ or $A_1 : M \to P^1M$ induces an integrable connection Γ_0 on P or Γ_1 on P^1M, respectively. Another connection $\Gamma_2 : P \to J^1P$ on P is defined by prescribing its values along the section A_0 by

$$\Gamma_2(A_0(x)) = A_2(x) \tag{4.1}$$

and by using the right-invariance condition. The following assertion generalizes the results by Epstein and de León about the second order non-holonomic parallelism.

PROPOSITION 2. A generalized parallelism $A : M \to W^1P$ is decomposable, if and only if $\Gamma_0 = \Gamma_2$.

P r o o f. If we use the product formula (2.1), we have $p(A_0, A_1) = (A_1, j^1A_0)$, where $j^1A_0 : M \to J^1P$ is the first jet prolongation of A. Hence A is decomposable, if and only if $A_2 = j^1A_0$. By (4.1), $\Gamma_0 = \Gamma_2$ means $A_2(A_0(x)) = j^1A_0(x)$ for all $x \in M$. This is equivalent to $A_2 = j^1A_0$. □

5. Generalized G-structures

Let $G \subset GL(m, \mathbb{R})$ be a subgroup. We recall that a classical G-structure on a manifold M is a reduction Q of the frame bundle P^1M to G, [9]. For a classical parallelism $B : M \to P^1M$, $B(M)$ is an $\{e\}$-structure on M, where e is the unit of $GL(m, \mathbb{R})$. In [5] we introduced the following generalization (which was motivated by the theory of higher order G-structures). Let $H \subset W^1_mG$ be a subgroup.

DEFINITION 4. *An H-structure on principal bundle $P(M, G)$ is a reduction Q of W^1P to H.*

We also say that Q is a generalized G-structure.

We have $W^1(\mathbb{R}^m \times G) = \mathbb{R}^m \times W^1_mG$. The product $\mathbb{R}^m \times H$, which is an H-structure on $\mathbb{R}^m \times G$, is called the standard flat H-structure.

Write $P|U$ for the restriction of $P(M, G)$ over an open subset $U \subset M$.

DEFINITION 5. *An H-structure $Q \subset W^1P$ is said to be locally flat, if for every $x \in M$ there exists a neighbourhood $U \subset M$ and a principal bundle isomorphism $f : \mathbb{R}^m \times G \to P|U$ such that $W^1f(\mathbb{R}^m \times H) = Q|U$.*

For every generalized parallelism $A : M \to W^1P$, $A(M)$ is an $\{e\}$-structure on P, where e is the unit of W^1_mG.

DEFINITION 6. *A generalized parallelism is said to be locally flat, if it is locally flat as an $\{e\}$-structure.*

PROPOSITION 3. A generalized parallelism $A : M \to W^1P$ is locally flat, if and only if A is decomposable and the underlying classical parallelism A_1 on M is locally flat.

P r o o f. Assume that A is decomposable and A_1 is locally flat. Let $U \subset M$ be an open subset and $h : \mathbb{R}^m \to U$ be a diffeomorphism transforming the classical standard flat parallelism $\left(\frac{\partial}{\partial x^1}, \ldots, \frac{\partial}{\partial x^m}\right)$ on $\mathbb{R}^m$ into $A_1|U$. Define a map $f : \mathbb{R}^m \to P$ by $f(x) = A_0(h(x))$. Then $A|U = W^1 f(\mathbb{R}^m \times \{e\})$ follows directly from the proof of Proposition 2. The converse assertion can be proved by the same argument. □

Proposition 2 and 3 imply the following result, which compares our approach with the research by Epstein and M. de León [3, 4].

COROLLARY 1. A generalized parallelism is locally flat, if and only if $\Gamma_0 = \Gamma_2$ and Γ_1 is torsion-free.

6. Semiprolongable generalized G-structures

In [5] we have established that the most interesting generalized G-structures are the semiprolongable ones. Consider the jet projection $\pi_0^1 : W^1P \to P$. For every H-structure $Q \subset W^1P$, $H_0 := \pi_0^1(H)$ is a subgroup in G and $Q_0 := \pi_0^1(Q)$ is a reduction of P to H_0. By Sec. 2, the injection $i : Q \to P$ induces an injection $W^1 i : W^1Q_0 \to W^1P$. The following concept was introduced in [5], where the reader can find a justification of the terminology.

DEFINITION 7. *An H-structure $Q \subset W^1P$ is called semiprolongable, if $Q \subset W^1Q_0$.*

If we apply this concept to a generalized parallelism on P, we obtain, as a direct consequence of Proposition 2, the following assertion.

COROLLARY 2. A generalized parallelism $A : M \to W^1P$ is semiprolongable, if and only if A is decomposable.

7. The structure function

From the viewpoint of the theory of generalized G-structures, it is interesting that the local flatness of generalized parallelisms can be characterized in terms of the structure function, analogously to the case of a classical parallelism.

On the linear frame bundle P^1M, we have the canonical form $\psi : TP^1M \to \mathbb{R}^m$, [6, 9]. For a classical G-structure $Q \subset P^1M$, a horizontal tangent space means any m-dimensional linear subspace in TQ which is complementary to the

vertical tangent space. The structure function τ of Q is defined by restricting the exterior differential $d\psi$ to the horizontal tangent spaces of Q, [7, 9]. This is a map $\tau : Q \to H^{0,2}(\mathfrak{g})$, where $H^{0,2}(\mathfrak{g})$ denotes the Spencer cohomology class of bidegree $(0, 2)$ of the Lie algebra $\mathfrak{g}$ of G. In the case of a classical parallelism $B : M \to P^1M$, the structure function of $B(M)$ is a map $\tau : B(M) \to \mathbb{R}^m \otimes \Lambda^2\mathbb{R}^{m*}$. By the definition of ψ, the structure function of $B(M)$ coincides with the torsion of the integrable connection Γ determined by B. Hence B is locally flat if and only if its structure function vanishes.

On W^1P, we have a canonical form $\theta : TW^1P \to \mathbb{R}^m \oplus \mathfrak{g}$, [6]. Proposition 2 of [5] reads that an H-structure $Q \subset W^1P$ is semiprolongable if and only if the values of the restriction of θ to TQ lie in $\mathbb{R}^m \oplus \mathfrak{h}_0$, where $\mathfrak{h}_0$ is the Lie algebra of $H_0 = \pi_0^1(H) \subset G$. In particular, for a decomposable generalized parallelism $A : M \to W^1P$ the values of the restriction of θ to $T(A(M))$ lie in $\mathbb{R}^m \oplus \{0\}$. For a semiprolongable H-structure Q, we defined its structure function τ by restricting the exterior differential $d\theta$ to certain distinguished horizontal tangent subspaces of Q, [5]. By [5], τ is a map $\tau : Q \to H^{0,2}(\mathfrak{k})$, where $\mathfrak{k}$ is the Lie algebra of the kernel K of the jet homomorphism $\pi_0^1 : H \to H_0$. In particular, the structure function of a decomposable generalized parallelism has values in $\mathbb{R}^m \otimes \Lambda^2\mathbb{R}^{m*}$.

PROPOSITION 4. A decomposable generalized parallelism $A : M \to W^1P$ is locally flat, if and only if its structure function vanishes.

P r o o f. The bundle projection $W^1P \to M$ identifies $A(M)$ with M. This identifies $T(A(M))$ with TM. By definition, the restriction of θ to $T(A(M))$ corresponds to the restriction of the canonical form ψ of P^1M to $T(A_1(M))$. Then our assertion follows from the above mentioned classical result. □

Acknowledgment

The author was supported by a grant of the GA ČR No 201/96/0079.

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DEPARTMENT OF ALGEBRA AND GEOMETRY
FACULTY OF SCIENCE, MASARYK UNIVERSITY
Janáčkovo nám. 2a, 662 95 Brno, Czech Republic.

Received September 12, 1997.

Arch. Mech., 50, 3, pp. 423–450, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

Hyperbolic framework for thermoelastic materials

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

W. KOSIŃSKI (WARSZAWA)

A THERMODYNAMIC framework of a deformable continuum is developed in which the conservative state variable vector is enlarged by adding the spatial gradient of a scalar thermal internal state variable responsible for the description of thermal history effects. The theory leads to a modified model of thermoelasticity with internal state variables and with a wave-type heat conduction governed by a system of quasi-linear hyperbolic equations. In a general non-deformable case, the observed material properties such as specific heat, quasi-equilibrium thermal conductivity and speed of thermal (the so-called second sound) waves, all regarded as functions of ϑ, lead to a particular specification of all material functions and the evolution equation for the scalar internal state variable. The short review of the heat pulse experiment is made. Main assumptions of the present approach are formulated and some arguments referred to the rate-type description are presented. A set of remarks and comparisons with another modification of the Fourier law characterizes the model. An analysis of hyperbolicity of thermoelasticity by propagation conditions of weak discontinuity waves is performed.

1. Introduction

MANY physical experiments at low temperatures and technological situations at moderate and high temperatures show the necessity of taking into account the wave structure of the heat transport. Those experiments performed at low temperatures dealt with

- second sound in dielectrics, e.g. [29, 30, 52, 61, 63], and
- second sound in solid helium, e.g [2].

On the other hand, those technological situations at moderate and high temperatures are related to

- the distribution of temperature around propagating ([1]) cracks [68, 69, 73], and
- temperature distribution in solid materials due to laser pulse train of a very short duration (in the picosecond range), e.g. [26].

The aim of this paper is to build a modified framework of thermomechanical theory of heat conducting and deformable materials in which the structure of the set of governing equations is of hyperbolic type; it means that both disturbances:

([1]) For continuum damage mechanics bibliography and its trends, compare [10].

mechanical and thermal ones propagate with finite speeds. Moreover, our further aim is to model quantitatively the observed wave phenomena in solids and fluids.

The organization of the paper is as follows. In Sec. 2 a typical experiment performed at low temperature for solid crystals will be shortly presented together with its results. In Sec. 3 the rate-type approaches most often used in the literature of thermodynamic theories with hyperbolic-type heat conduction equation will be discussed. Then in Sec. 4 some arguments supporting the internal state variable approach in the case of a non-deformable continuum will be given. From them general forms of evolution equation for the scalar internal state variable and heat flux constitutive equation, both based on the thermal history effects, will be more evident. Some particular forms of the evolution equation are presented. Then the developed model is characterized by a set of remarks and comparison with the extended thermodynamic approach of Morro and Ruggeri. In Sec. 5 the thermomechanical framework will be outlined. Then in Sec. 6 the hyperbolicity of the thermoelasticity is analysed with the help of weak discontinuity wave. Propagation conditions are formulated together with the general form of the system of governing equations suitable for the analysis of strong discontinuity waves.

2. Heat pulse experiment

According to the authors of [18], the heat pulse experiment was first introduced into crystal physics by GUTFELD and NETHERCOT [25]. The experiment was intended to detect second sound. The possibility that under certain conditions, a temperature wave might propagate in a good thermal conductor was first considered in detail by WARD and WILKS [71], following an earlier suggestion by PESHKOV [64]. The authors of [25], however, failed to see the evidence of the second sound.

Finite speed thermal waves, known collectively as second sound, distinguishing them from generally faster propagating mechanical waves, were first detected in ^{3}He, ([2]), and then in high purity dielectric crystals of sodium fluoride, NaF, [29], and bismuth, Bi, [61].

For heat pulse experiments the NaF and Bi single crystals of high chemical and isotopic purity were used (cf. [30, 52, 61, 66]). Since both crystals have a particular symmetry, the authors performed experiments for several different samples geometries with path lengths varying between 3.6 and 13 mm, and for pulse propagation direction along $< 100 >$, $< 110 >$ and $< 111 >$.

The heat pulse experiments were performed in a simple metal cryostat [66]. The sample was mounted in a vacuum on stainless-steel post anchored to the helium bath which could be pumped to 1.8 K. A heater on the post allowed the sample temperature to be raised above the bath temperature, a carbon resistance thermometer mounted on the crystal provided a measure of its temperature.

Two opposite surfaces of the crystal were covered by an evaporation technique with thin metallic films, which serve as heater and bolometer, respectively. The distance between those surfaces varied from 3.5 to 13 mm.

Pure Pb was chosen for the bolometer film. The lead detector was biased with a constant current so that resistance changes gave rise to signal voltage across the film. The change of the resistance of the metallic film at the other side of the crystal was taken as a measure for the temperature. A current pulse generator supplied the impulse to the crystal heater; its duration varied between 0.2 and 0.5 μs. The signals from the lead detector were usually of a sufficient amplitude to allow their direct display on an oscilloscope after some wide-band preamplification. The temperature rise of the bolometer never exceeded 1 K [52]. Signals were recorded graphically. The arrival time of the leading edges of the pulses were measured. At low temperatures (i.e at 12 K for NaF and 1.38 K for Bi) the fastest peak, denoted by L, travelled with the speed of a longitudinal sound wave. The peak which arrives next, denoted by T, travelled with the speed of a transversal sound wave (cf. Fig. 1).

This behaviour is interpreted theoretically as the ballistic phonon effect: phonons ([2]) representing eigenvibrations of the atom of a crystal lattice, travel through the crystal without any interaction. On the other hand, in the framework of thermoelasticity this behaviour can be viewed as a thermomechanical coupling in acoustic wave propagation: due to the plane strain condition, two sound waves: longitudinal and transversal, may propagate under such condition. They were initiated by the temperature rise at one end (side) of the crystal, while the temperature measurement on the other end (side) reported the arrival signal of thermomechanical wave, propagating with those sound speeds. No mechanical variables, like strain, stress or particle velocity were measured in the heat pulse experiments.

The experiments were repeated at different bath temperatures, and no particular dependence of those sound speeds were reported. However, in some range of temperature, an extra peak following those two already observed peaks were detected (cf. Fig. 1). That third peak has been interpreted as partially developed second sound. It is interesting that the second sound peaks in Fig. 1 are followed by long tails; they could represent the diffusive part of the heat pulse ([18, 61]).

In the case of the NaF crystals it seen from the plots of heat-pulse arrival time *vs* temperature, that the so-called ballistic longitudinal and transverse pulses denoted by L and T, respectively, occur at the lowest temperatures, and that the second-sound pulse begins to appear at 10 K.

([2]) In the phonon model the actual crystal is replaced by a box containing a gas of phonons: i.e. a gas of quasi-particles bearing energy and momentum. Transport processes in the crystal are treated analogously to transport processes in the gas. Phonons may interact among themselves as well as with lattice imperfections and with boundaries of the crystal. In the so-called N(normal)-processes phonon momentum is conserved, in contrast to the so-called R(resistive)-processes, that do not conserve the momentum.

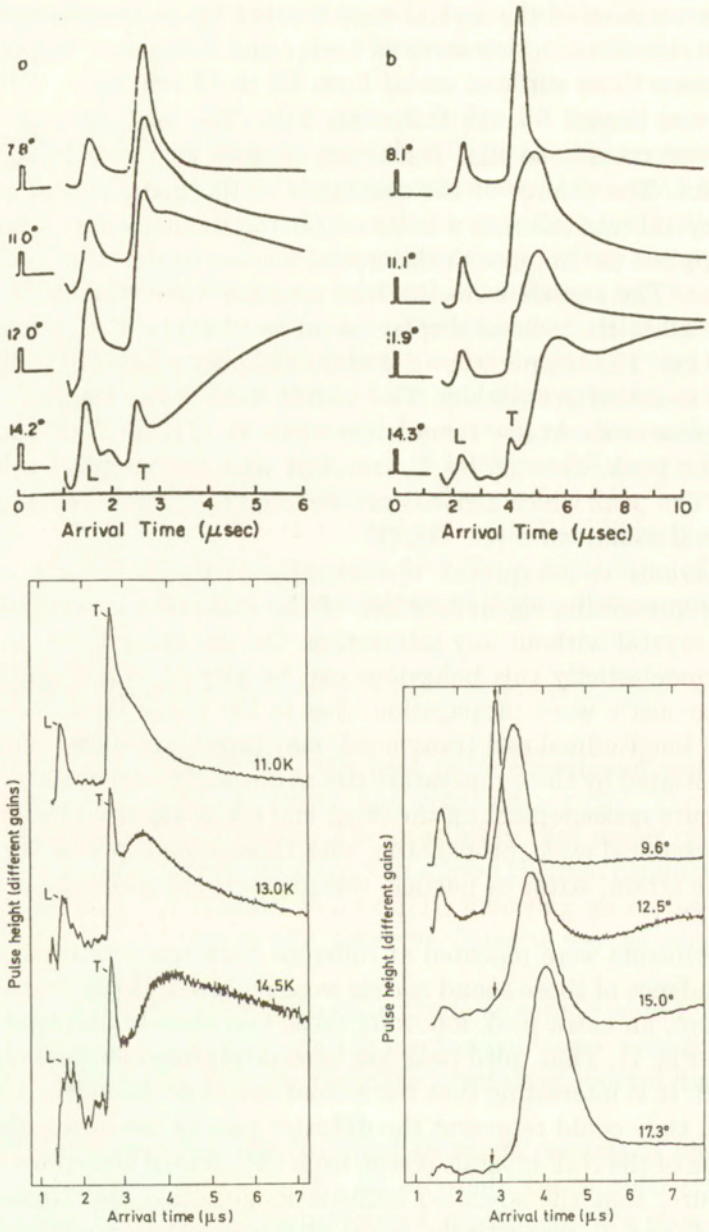

FIG. 1. Heat pulses in a pure NaF sample (a – $l = 7.9\,\text{mm}$, b – $l = 12.7\,\text{mm}$), after [29] and [52]. L and T mark the peaks of the longitudinal and transverse ballistic pulses, respectively. The third distinct pulse (second sound) appears at higher temperatures.

It was there observed (cf. Fig. 2, and figures from [16] and the review article [18]), that in the range of low temperature at which experiments have been performed, the time of arrival of the third heat pulse is approximately a linear

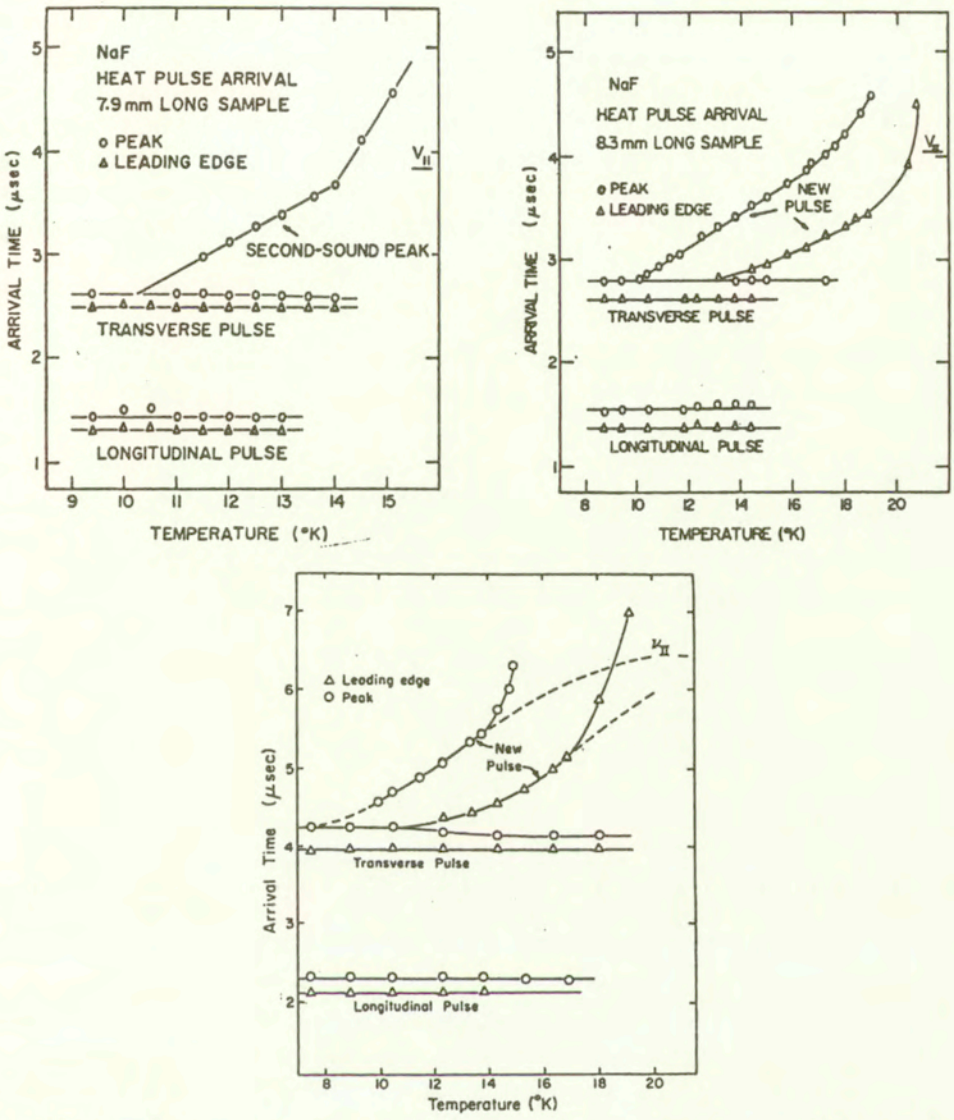

FIG. 2. Arrival times versus temperatures for leading edges and peaks of longitudinal ballistic pulse, the transverse ballistic pulse, and the second-sound pulse for the sample of Fig. 1, after [29] and [52] ($l = 12.7\,\mathrm{mm}$, $\nu_{II} = 2 \times 10^5\,\mathrm{cm\,s^{-1}}$).

function of the reference (bath) temperature. However, near the upper limit of the measured bath temperature values, the arrival time of the leading edge of heat pulses rises rapidly with increasing temperature. The latter corresponds to a very fast decay (with respect to temperature) of the second sound speed. We can repeat after the authors of [52]: "Eventually a temperature is reached at which this pulse disappears into the diffusive signals".

Experimental investigations with the second sound reported by the authors of [29, 30, 66] have been preceded with steady-state thermal-conductivity measurements. Figure 3 shows thermal conductivity versus temperature data for several samples of different purity. For the heat conductivity a very strong temperature dependence has been observed. Even more: for both crystals NaF and Bi, there is a particular temperature at which the conductivity of the material reaches a peak. The thermal conductivity is highest for purest NaF fourth-regrowth sample *A* (cf. Fig. 3.)

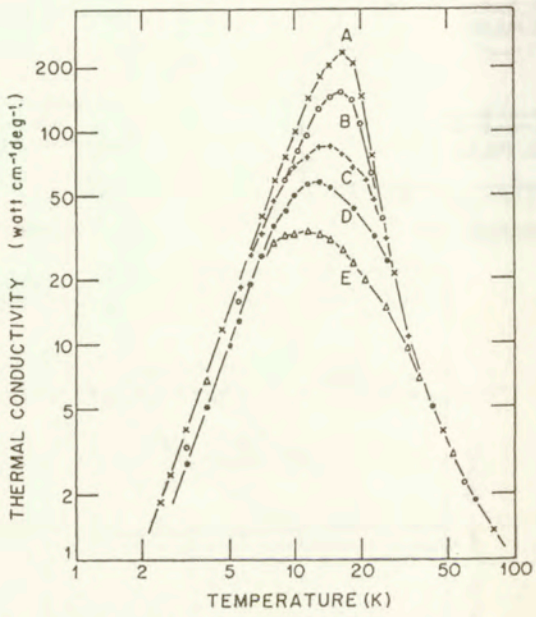

FIG. 3. Steady-state heat conductivity of NaF crystals of different purity, after [30].

Comparing those experimental results on the second sound and heat conductivity, one could derive a possible conclusion, that the second sound phenomenon appears more strongly close to a particular temperature at which the conductivity of the material reaches a peak [30]. In our model developed further in the paper, motivated by the experimental data, and trying to fit experiments for the second sound speed in NaF, we make in [43, 67] the hypothesis that the temperature of maximum heat conductivity coincides with that below which second sound appears. Above this temperature value the heat conduction becomes purely diffusive, obeying a general nonlinear Fourier law. We have called this *critical temperature* ϑ_λ.

There is an additional possible explanation why in the first range of low temperatures, the thermal pulse of the second sound were not observed. Namely, at that range of temperature, the speed of the second sound is very close to the speed of the transversal wave, and both the peaks are reported at the same

time as a rather big peak (cf. Figs. 2, 3 for NaF for temperature values 8.1 K, 11.1 K, 11.9 K).

3. Rate-type approach to thermal waves

The above cited experimental facts contradict the results of phenomenological approach to the heat transfer based on a proportionality law between the heat flux and the temperature gradient, called the Fourier law. That law incorporated with the balance of energy leads to a parabolic equation for the temperature field, in solutions of which heat pulses are transmitted with infinite speed. Even including mechanical fields leading to thermoelasticity, the final system of equations is hyperbolic only in a mechanical variable – the displacement vector, being still parabolic in terms of the temperature field. Consequently, only ballistic thermomechanical wave propagation could be described in such a model. No possibility exists for describing the second sound, i.e. thermal wave (i.e. the third peak in experimental results) then exists.

There are several phenomenological approaches aimed at the new heat conduction equation, that could describe that phenomena. Some of them are reviewed in the papers [31, 32].

In order to give more reasons for the present approach, we start with referring to the rate-type methods leading to a kind of telegraph equation for the temperature field, which is the second order hyperbolic equation.

Let us start our short presentation with the following

OBSERVATION.

Assume that a non-deformable material is characterized by its energy function e that depends on the thermodynamic temperature ϑ. If for the heat flux $\mathbf{q}$ one incorporates a classical *Fourier proportionality law*

$$\mathbf{q} = -k(\vartheta)\nabla\vartheta \tag{3.1}$$

then, as a consequence of the *balance of energy*

$$\varrho\dot{e}(\vartheta) + \operatorname{div}\mathbf{q} = \varrho r\,, \tag{3.2}$$

where ϱ represents the mass density and r – the body heat supply, per unit time, one gets a *parabolic* nonlinear *heat conduction equation*

$$\varrho c_v(\vartheta)\dot{\vartheta} = \operatorname{div}(k(\vartheta)\nabla\vartheta) + \varrho r \qquad \text{with} \quad c_v(\vartheta) = \frac{d\varepsilon(\vartheta)}{d\vartheta}\,, \tag{3.3}$$

which turns out to be a *diffusion equation*

$$\varrho c_v\dot{\vartheta} = k\triangle\vartheta + \varrho r, \tag{3.4}$$

for constant coefficients, i.e. thermal disturbances propagate with infinite speed. The same is true if additionally one introduces the dependence of the free energy function $\psi = \varepsilon - \vartheta\eta$, where η is the specific entropy, on ϑ and on its gradient $\nabla\vartheta$. This is due to the *second law of thermodynamics.*

Hence, to incorporate a *wavelike phenomenon* (hyperbolicity) in the heat transfer, one needs to enlarge the set of thermal state variables $(\vartheta, \nabla\vartheta)$ in the energy constitutive function by additional quantities. Such an enlargement will cause of course an additional source of dissipation.

There is the well-known method which can lead to a wavelike heat conduction, namely a rate-type approach, in which the Fourier law (3.1) is modified by adding to (3.1) a term in which the time derivative of the heat flux is multiplied by a coefficient τ; the latter is called a *thermal relaxation time.* Then the governing equation of this approach called the Maxwell - Cattaneo - Vernotte - Kaliski equation, is

$$\tau\dot{\mathbf{q}} + \mathbf{q} = -k(\vartheta)\nabla\vartheta, \tag{3.5}$$

where τ is a *thermal relaxation time.*

If τ is constant then the 2-nd order dissipative wave equation follows for the thermodynamic temperature

$$\tau\frac{\partial}{\partial t}(\varrho c_v(\vartheta)\dot{\vartheta}) + \varrho c_v(\vartheta)\dot{\vartheta} = \operatorname{div}(k(\vartheta)\nabla\vartheta), \tag{3.6}$$

which occurs to be a *telegraph equation*

$$\tau\varrho c_v\ddot{\vartheta} + \varrho c_v\dot{\vartheta} = k\triangle\vartheta, \tag{3.7}$$

for constant coefficients, and is *hyperbolic* if $\tau c_v\kappa$ is positive. The prototypes of this modification one can find in [1, 8, 9, 11, 33, 53, 70] for non-deformable (rigid) conductors (cf. also [54]). The thermoelastic developments of this modification in the earlier stages of development one can find in [5, 19, 51]. For more recent development we refer to the review paper of IGNACZAK [28].

Another method had been proposed by Bogy and Naghdi, and the McCarthy approach: a dependence of the specific entropy η on ϑ, $\nabla\vartheta$ and temperature rate $\dot{\vartheta}$:

$$\eta = \eta(\vartheta, \nabla\vartheta, \dot{\vartheta}). \tag{3.8}$$

They arrived at an equation similar to (3.7) with additional term $\nabla\dot{\vartheta}$. In [6] and [55] thermodynamic derivations of the heat conduction equations can be found with the temperature-rate dependence of free energy and entropy. Thermomechanical developments of that approaches in the earlier stages one can find in [19, 23, 51].

In both the above approaches based on the rate-type method, the final equation is a kind of telegraph equation for the temperature field, which is the second order hyperbolic equation. Such a formulation has the main drawback, namely

the order of the equation, for which the initial conditions in terms of the time derivative of the temperature field have to be given additionally to the temperature itself. Moreover, thermal shocks in the form of temperature pulses cannot be described. In the approach we are going to present, this inconvenience will be omitted.

Almost parallel to the rate-type methods, a history approach was developed by GURTIN and PIPKIN [24] and NUNZIATO [62]. In their papers the heat flux vector was assumed to depend on the summed history of the temperature gradient $\bar{\mathbf{g}}$

$$\mathbf{q}(t) = \int_0^\infty \frac{d}{ds}\mathbf{A}(s)\,\bar{\mathbf{g}}(t-s)\,ds, \tag{3.9}$$

where

$$\bar{\mathbf{g}}(t-s) = \int_0^s \operatorname{grad}\vartheta(t-\lambda)\,d\lambda, \qquad \text{with} \quad \mathbf{g} = \operatorname{grad}\vartheta.$$

NUNZIATO in [62] assumed a more general dependence on the actual value of the temperature gradient. That assumption changes drastically the type of the final heat conduction equation. Under the isotropy assumption concerning the tensor function $\mathbf{A}$, the derivative of which appears in (3.9), took the form $\mathbf{A}(s) = a(s)\mathbf{1}$, with a differentiable scalar-valued function $a(\cdot)$ defined on $[0,\infty)$ with $a(\infty) = 0$; the authors of [24] wrote the heat flux constitutive equation (3.9) in the form

$$\mathbf{q}(t) = -\int_0^\infty a(s)\,\mathbf{g}(t-s)\,ds. \tag{3.10}$$

It is interesting to notice that the Maxwell – Cattaneo – Vernotte – Kaliski equation (3.5) can be obtained from (3.10) under rather weak smoothness assumptions about the function $\mathbf{g}(t-s)$ and the following kernel representation $a(s) = \exp(-t/\tau)\,k/\tau$.

There are some drawbacks in applying the equation (3.5) to the thermodynamic theory of thermomechanics, especially because of the internal dissipation inequality. It was pointed out by MAZILU in [54], MORRO and RUGGERI in [58, 59], by the authors of review papers [18, 31, 32] (cf. also [7, 50, 56, 60]) and by others.

Due to the lack of space we only mention two other approaches which make use of the phonon gas for the wave phenomena in heat transport, namely those of LARECKI and PIEKARSKI [48], and the authors of [18] that make use of many-moments model of extended thermodynamics.

4. Internal variable as a thermal history of material

The present author with PERZYNA in [40] (and latter in [34] in a more general setup) calculated for the first time finite speeds of thermal (and thermomechan-

ical) waves in the framework of a thermodynamic theory with internal state variables. The results of those derivations were applied to 3D thermoelasticity in [57]. Further generalizations for more complex materials (cf. [47], and [72]) have been partially reported in the monograph [35]. Later on COLEMAN *et al.* [15] repeated the first results of KOSIŃSKI and PERZYNA from 1972 in a slightly different set-up, without referring to the internal state variable approach and to the original paper [40].

In [36], the material gradient of an internal, scalar state variable was introduced as a fundamental state variable in the response functions of thermoelastic materials. In the course of obtaining the consequences for the laws of thermodynamics, a modified Fourier-type law was found leading to finite speeds of propagation of thermal and thermomechanical waves. This model differed from an earlier one, ([40]), in the form of the evolution and constitutive equations.

In the model proposed by the author in [36], a different procedure for the derivation of a wavelike heat propagation equation was proposed. In that model a scalar internal state variable β has been introduced to represent at the same time a history of the thermodynamic temperature and the potential for its gradient. That gradient appears in the heat flux constitutive equation. The model has been mostly applied to heat conductors in 1D and 3D cases and to thermoelastic solids (cf. [3, 12, 13, 14, 17, 41, 42, 37, 38, 39, 43, 67]. Its numerical implementations are discussed in [4, 20, 21, 22].

In the present section we are going to give additional arguments for the model initiated in [36] and developed further in a dozen of publications.

Let us look once more at the Maxwell – Cattaneo – Vernotte – Kaliski equation (3.5). At each material point X this equation is regarded as an ODE for the heat flux vector $\mathbf{q}$. For any time instant $t \geq 0$ its solution under homogeneous initial conditions for $\mathbf{q}$ and $\nabla\vartheta$ at $t = 0$ will be

$$\mathbf{q}(t) = -\int_0^t \frac{k}{\tau}\exp\left(\frac{s-t}{\tau}\right)\nabla\vartheta(s)\,ds. \tag{4.1}$$

In the linear case one assumes that the heat conductivity coefficient k is constant as well as the relaxation time τ. Then one can write the gradient operator in front of the integral to get

$$\mathbf{q}(t) = -k\nabla\int_0^t \frac{1}{\tau}\exp\left(\frac{s-t}{\tau}\right)\vartheta(s)\,ds. \tag{4.2}$$

If we denote the whole integral by β

$$\beta(t) = \int_0^t \frac{1}{\tau}\exp\left(\frac{s-t}{\tau}\right)\vartheta(s)\,ds, \tag{4.3}$$

then the last equation can be written in the form

$$\mathbf{q}(t) = -k\nabla\beta(t). \tag{4.4}$$

On the other hand, let us notice that the variable β satisfies the following ODE

$$\dot{\beta} = \frac{1}{\tau}(\vartheta - \beta). \tag{4.5}$$

From this point it is not difficult to arrive at the more general *evolution equation*

$$\dot{\beta} = F(\vartheta, \beta), \tag{4.6}$$

which could be accompanied by the more general heat conduction constitutive equation

$$\mathbf{q} = -\alpha^*(\vartheta)\nabla\beta \tag{4.7}$$

in a particular quasi-linear case, instead of the previous (4.4).

Further on, this extra thermal variable β (called in [12] a new semi-empirical temperature) will be regarded in this *more general set-up* (instead of the previous way (4.3)), as a solution of the evolution equation (4.6) with a thermodynamic temperature nonlinear, in general, dependence on the right-hand side (RHS).

This short derivation has been performed to present the role of the variable β, and its interpretation as an internal state variable. The derivation shows that this variable has been introduced in order to represent a *thermal history* of the material. The fact that a scalar internal state variable can represent a history of the temperature (while its gradient can represent the history of the temperature gradient) and in this way, influence the response of the material at hand, is compatible with the general framework of the internal state variable approach. As it was shown in several publications (cf. for example [44]), the internal state variable approach and the theory using constitutive functionals with a past history dependence have some common points. Those two approaches are to some extent equivalent as far as the description of memory effects of the material is concerned. The difference appears in the very far past: in the internal state variable approach one has to give an initial value of the internal state variable at time t tending to minus infinity, on the other hand in the constitutive functional description one has to assume some value of the history at that far past.

Coming back to the main stream of the paper, we would like to point out that in some applications analyzing the propagation of weak discontinuity waves (cf. [41, 42]) we have used the linear evolution equation (4.5). However, in more advanced problems related to the temperature-dependence of the speed of thermal waves (i.e. the speed of the second sound), such linear equation is not suitable and we had to look for a nonlinear one. It was the case discussed in the recent papers [43, 67] where, based on low temperature experiment data in solid dielectric crystals NaF, the present author together with the Saxtons used in the

evolution equation (4.6) the function F of the form $F = F_1(\vartheta) + F_2(\beta)$, with

$$F_1(z) = a(|z|^{p-1}z)_-, \qquad 1 < p < 2, \tag{4.8}$$

where a is a positive constant, and the subscript "$_-$"means that when $z \geq 0$, F_1 is taken to be zero. For the second function F_2, they put

$$F_2(z) = -b|z|^{h-1}z, \qquad h \geq \frac{p}{2-p}, \tag{4.9}$$

where b is another positive constant. In the first case z represents $\vartheta - \vartheta_\lambda$ where ϑ_λ denotes the *critical* temperature at which the heat conductivity of the material reaches a peak. The model developed in [43, 67] based on the general framework developed in [45], is intended to admit wavelike propagation of heat below – and diffusive conduction above – a particular temperature value ϑ_λ. This is mainly due to the fact that the range of temperature for which the second sound (thermal waves) is detectable is in fact quite small, and normal diffusive propagation takes place above it.

5. Foundation of thermodynamics with modified Fourier law

The aim of this section is to list fundamental assumptions concerning the thermodynamics with modified Fourier law as well as its main features. The present consideration will be restricted, for simplicity of the presentation, to a non-deformable continuum, while in the next section a thermodynamics of deformable, elastic continuum will be shortly presented.

To this end we formulate an alternative, gradient model with internal state variables to describe thermal wave phenomena, with a possibility to pass to the Fourier model of heat conduction. Then we propose, in the next section, the full thermomechanical coupling with wave phenomenon.

Based on that as well as on other physical observations, the main assumption of the model developed by the author in [36] can be summarized in the following assumptions (cf. [13]):

ASSUMPTION 1

Memory effect is introduced by a scalar-valued function β that plays the role of a potential in the heat conduction law, i.e. β is a solution of an initial value problem

$$\dot{\beta} = F(\vartheta, \beta), \qquad \beta(t_0) = \beta_0\,. \tag{5.1}$$

In one of our previous papers [12] we have called β a *semi-empirical temperature*. However, this term is not essential for the development.

ASSUMPTION 2

Gradient $\nabla\beta$ appears in constitutive equations instead of the gradient of the thermodynamic (absolute) temperature ϑ,

$$\begin{aligned} \psi &= \psi^*(\vartheta, \nabla\beta), \\ \eta &= \eta^*(\vartheta, \nabla\beta), \\ \mathbf{q} &= \mathbf{q}^*(\vartheta, \nabla\beta). \end{aligned} \tag{5.2}$$

ASSUMPTION 3

Fourier law is necessary to obtain in the limit transition, called a quasi-equilibrated (or steady-state) case, when the left-hand side of (5.1) tends to zero. In other words, we suppose there exists an invertible *quasi-equilibrated* relation between ϑ and β, i.e. a differentiable homeomorphism $B(\vartheta)$ such that when the left-hand side of (5.1) vanishes then $F(\vartheta, \beta) = 0$, and under the assumption of the local monotonicity of F one gets β as a function of ϑ. Hence in terms of the function B, we get

$$\text{if } \dot{\beta} \to 0 \text{ then } \beta = B(\vartheta), \text{ with } F(\vartheta, B(\vartheta)) \equiv 0. \tag{5.3}$$

This function will appear in the representation of the steady-state thermal conductivity coefficient. Let us present this for the case of the quasi-linear proportionality constitutive law (4.7). Namely, admitting that in general dynamic case, the heat flux vector $\mathbf{q}$ is proportional to the gradient of β (cf. (4.7), then under the quasi-equilibrated condition (or steady-state) (5.3), the heat flux turns to be proportional to $\nabla\vartheta$ itself, as it is in the Fourier law (3.1), however, with another heat conduction coefficient $\mathbf{k}^*$, called now *steady-state thermal conductivity coefficient*, and given by

$$\mathbf{q} = -\mathbf{k}^* \nabla\vartheta \quad \text{with} \quad \mathbf{k}^* := \alpha^*(\vartheta) \frac{d\, B(\vartheta)}{d\vartheta}. \tag{5.4}$$

Now, let us make the derivation of the thermodynamic consequences for the general case of the constitutive equations (5.2) if we employ the 1-st and 2-nd laws of thermodynamics in the form:

$$\varrho\dot{e} + \operatorname{div} \mathbf{q} = \varrho r, \tag{5.5}$$

$$\varrho\dot{\eta} + \operatorname{div}(\mathbf{q}/\vartheta) \geq \varrho r/\vartheta, \tag{5.6}$$

where the specific internal energy $e = \psi + \eta\vartheta$. If we require that each Lipschitz continuous solution of (5.1), (5.2), (5.5) satisfies the thermodynamic inequality (5.6) then we get

REMARK 0

The necessary and sufficient conditions for satisfying the second law of thermodynamics by each Lipschitz continuous solution to (5.1), (5.2) and (5.5), are:

$$\begin{aligned} \mathbf{q} &= -\varrho\vartheta(\partial F/\partial\vartheta)(\partial\psi^*/\partial\nabla\beta), \\ \eta &= -\partial\psi^*/\partial\vartheta, \end{aligned} \tag{5.7}$$

and the residual internal dissipation inequality

$$(\partial F/\partial\beta)/(\vartheta\partial F/\partial\vartheta)\mathbf{q}\cdot\nabla\beta \geq 0. \tag{5.8}$$

Moreover, one gets the next consequence

$$F(\vartheta,\beta) = F_1(\vartheta) + F_2(\beta). \tag{5.9}$$

In the present paper we will follow the internal state variable approach based on the evolution equation (4.6). Now we list some most fundamental observations concerning the developed model.

REMARK 1

If Eq. (5.7) for $\mathbf{q}$ is linear in $\nabla\beta$, i.e.

$$\mathbf{q} = -\alpha^*(\vartheta)\nabla\beta, \tag{5.10}$$

then, two functions ψ_1^* and ψ_2^* should exist such that

$$\psi = \psi_1^*(\vartheta) + 0.5\psi_2^*(\vartheta)|\nabla\beta|^2, \tag{5.11}$$

where

$$\alpha^*(\vartheta) = \varrho\vartheta F_1'(\vartheta)\psi_2^*(\vartheta). \tag{5.12}$$

Notice that the assumption on the linearity in the heat flux constitutive equation $(5.7)_2$ is equivalent to the splitting of the free energy function ψ into two terms, with quadratic dependence on $\nabla\beta$. Moreover, the first term $\psi_1^*(\vartheta)$ is rather classical. In [37] 3D thermal weak discontinuity waves were investigated. It was shown there, for example, that in the rigid case with (4.7) and (5.11) the governing system of equations for determining β and ϑ is composed of (5.1) with F given by (5.9), and

$$\begin{aligned} \varrho c_v(\vartheta)\ddot{\beta} - \alpha^{*\prime}(\vartheta)\nabla\dot{\beta}\cdot\nabla\beta - \alpha^*(\vartheta)F_1'(\vartheta)\triangle\beta \\ - \varrho c_v(\vartheta)F_2'(\beta)\dot{\beta} + \alpha^{*\prime}(\vartheta)F_2'(\beta)\nabla\beta\cdot\nabla\beta = \varrho r F_1'(\vartheta). \end{aligned} \tag{5.13}$$

Since ϑ can be expressed in terms of β and $\dot{\beta}$ from (5.1), the equation (5.13) can be solved independently for β. The speed λ of a pure thermal wave is given by

$$\varrho c_v(\vartheta)\lambda^2 - \alpha^{*\prime}(\vartheta)\nabla\beta\cdot\mathbf{n}\lambda - \alpha^*(\vartheta)F_1'(\vartheta) = 0, \tag{5.14}$$

with $\mathbf{n}$ as a unit normal to the wave front. We can see that the wave propagation is not symmetric if $\nabla\beta$ differs from zero, and the hyperbolicity condition is

$$c_v(\vartheta)\alpha^*(\vartheta)F_1'(\vartheta) \geq 0 \qquad \text{or} \qquad c_v(\vartheta)\vartheta(F_1'(\vartheta))^2\psi_2^*(\vartheta) \geq 0, \tag{5.15}$$

where the second equivalent form is due to the representation (5.12).

Let us check the consequences of the residual dissipation inequality (5.8) in the present form of Eq. (5.10) for $\mathbf{q}$. Substituting it into (5.8) we get

$$-\varrho F_2'(\beta)\psi_2^*(\vartheta) \geq 0. \tag{5.16}$$

Let us make the additional requirement on the asymptotic stability of solutions β of the evolution equation

$$\dot{\beta} = F_1(\vartheta) + F_2(\beta). \tag{5.17}$$

Then due to the classical Lapunov stability result we can require

$$F_2'(\beta) \leq 0. \tag{5.18}$$

This implies

$$\psi_2^*(\vartheta) \geq 0.$$

Hence in view of the (5.15) we may formulate the proposition:

REMARK 2

Under the assumption of Remark 1 and the asymptotic stability requirements (5.18), the *hyperbolicity condition* (5.15) is satisfied if $c_v(\vartheta) \geq 0$.

REMARK 3

Under the assumption of Remark 1, if the internal energy $\varepsilon = \psi + \eta\vartheta$ is a function of ϑ only, then for the constitutive functions ψ_2^* and α^* we obtain

$$\psi_2^*(\vartheta) = \psi_{20}^*\vartheta \qquad \text{and} \qquad \alpha^*(\vartheta) = \varrho\psi_{20}^*\vartheta^2F_1'(\vartheta), \tag{5.19}$$

with a positive constant ψ_{20}^*, that could be written as

$$\psi_{20} = \frac{\tau_0 k_0}{\varrho\vartheta_0^2},$$

where the dimensions of material constants $k_0, \tau_0, \vartheta_0^2$ are obvious and follow from the dimensional analysis (cf. [36]). Then the specific free energy, entropy and heat flux are given by

$$\begin{aligned} \psi &= \psi_1^*(\vartheta) + 0.5\psi_{20}^*\vartheta|\nabla\beta|^2, \\ \eta^*(\vartheta, \nabla\beta) &= \eta_E(\vartheta) - 0.5\psi_{20}|\nabla\beta|^2, \qquad \text{with} \quad \eta_E(\vartheta) = -\psi_1^{*\prime}(\vartheta), \\ \mathbf{q} &= -\varrho\psi_{20}^*\vartheta^2F_1'(\vartheta)\nabla\beta, \end{aligned} \tag{5.20}$$

and the principle of maximum entropy at equilibrium ($\mathbf{q} = \mathbf{0}$) holds, for $\psi_{20} \geq 0$. Let us notice that the first term $\eta_E(\vartheta)$ is rather classical and can be called the equilibrium entropy.

REMARK 4

If in the thermodynamic inequality (5.6) one assumes a more general form of the entropy flux, namely

$$\frac{\mathbf{q}}{\vartheta} + \mathbf{h}$$

then in the derivation of the consequences one gets the potential relations (5.7) with the same residual dissipation inequality together with the requirement $\mathbf{h} = \mathbf{0}$.

REMARK 5

With the representations (4.8) and (4.9), it can be shown (cf. [67]) that in that model, an expression for the second sound speed, U_E, (the speed of temperature rate waves propagating in an undisturbed region) is given by

$$U_E^2 = \frac{\alpha^*(\vartheta) F_1'(\vartheta)}{\varrho c_v(\vartheta)} = \frac{\psi_{20}}{c_0 \vartheta} a^2 p^2 (\vartheta - \vartheta_\lambda)_-^{2(p-1)}. \tag{5.21}$$

At the same time, in the *steady state* case, for which $F_1(\vartheta) + F_2(\beta) = 0$, (i.e. β is a function of ϑ) the heat flux (4.7) now reduces to (cf. (5.4)) and

$$\mathbf{q} = -(c\psi_{20}\vartheta^2 |(\vartheta - \vartheta_\lambda)_-|^{p(1+1/h)-2}) \nabla\vartheta, \tag{5.22}$$

where c depends on a, b, p and h.

We note that the obtained expression for the second sound propagation speed in undisturbed region described very well the experimental results reported in Sec. 2. Moreover, the solid curve in Fig. 1 in [43] fits very well the experimental curve of Coleman and Newman. On the other hand, the expression (5.22) predicts a peak in heat conductivity as ϑ tends to ϑ_λ from below, followed by a sharp drop. At the same time, in particular if p is close to 1, Eq. (5.21) delivers a sudden drop to zero of the wave speed U_E, where it could be expected that we were entering the range of temperature of purely diffusive heat conductivity in which parabolic heat conduction equation holds.

If we look once more at the general expression (5.21) for the second sound speed $U_E(\vartheta)$, then using (5.12) we get

$$U_E^2(\vartheta) = \frac{(\vartheta F_1'(\vartheta))^2 \psi_2^*(\vartheta)}{c_v(\vartheta)}. \tag{5.23}$$

From this expression and the form (5.4) of the steady-state heat conductivity coefficient $\mathbf{k}^*$, we can get the following conclusion:

REMARK 6

The model is determined, i.e. all its constitutive functions can be determined, if the following quantities: specific heat $c_v(\vartheta)$, steady-state heat conductivity coefficient $\mathbf{k}^*$ and speed of propagation of thermal second sound wave U_E, all in terms of the absolute temperature ϑ, are known.

REMARK 7

One can get the model of extended thermodynamics developed by MORRO and RUGGERI [59] with the following evolution equation for the heat flux:

$$\frac{\partial}{\partial t}\left(\frac{\mathbf{q}}{\alpha(\vartheta)}\right) + \operatorname{grad}\nu(\vartheta) = -\frac{\nu'(\vartheta)}{k(\vartheta)}\mathbf{q}, \tag{5.24}$$

under the identities

$$\alpha(\vartheta)F_1'(\vartheta) \equiv 1/\alpha^*(\vartheta) \qquad \text{and} \qquad \nu \equiv F_1(\vartheta),$$

and $F_2(\beta)$ being linear in β. Similarly one can get a particular model with internal state variable developed by KOSIŃSKI and PERZYNA [40].

REMARK 8

There is a parabolic thermodynamic development [45, 46] of the present approach in which the additional dependence on the actual value of the temperature gradient is allowed. In a particular isotropic, linearized case one gets for the heat flux the equation (cf. [43, 67])

$$\mathbf{q} = -k(\vartheta)\nabla\vartheta - \alpha^*(\vartheta)\nabla\beta, \qquad \text{with} \quad \dot{\beta} = F(\vartheta,\beta). \tag{5.25}$$

That development can play two roles: the first role is a thermodynamically consistent parabolic regularization of the present hyperbolic model, the second one – a full model that can be used in order to describe the whole regime of the heat conduction: the wave-type and diffusive parts (cf. [43, 67]).

A new (non-hyperbolic) nonlinear model has been recently developed by HETNARSKI and IGNACZAK and used in [27] in the analysis of soliton-like waves in a non-deformable heat conductor. Their model could be regarded as a particular case of (5.25) in which they are not introducing (formally) the scalar internal state variable β, but its gradient, as a vector field $\boldsymbol{\beta}$. However, it could correspond to the present case with a scalar internal state case, however, the function F in the RHS of the evolution equation for β will not depend on β, having the form $F(\vartheta,\beta) = A \ln\vartheta$ with $A = \text{const}$ (cf. Eq. (11) in [27] and substitute their $\boldsymbol{\beta}$ with the present $\nabla\beta$).

In the recent papers of LARECKI [49] the analysis of the phenomenological model of a non-deformable conductor of heat with a vector-valued internal state variable has been performed. There its comparison with the present model as well as its relations to other models based on some generalizations of the Maxwell – Cattaneo – Vernotte – Kaliski equation have been broadly discussed.

6. Thermomechanics

To present shortly the case of thermomechanics we notice that at finite strains, the referential (Lagrangean) description is used. Then $\varrho_0(X)$ is the reference mass density, known for each X in the reference placement $\mathcal{B}$ and related to the actual mass density ϱ by the mass continuity law $\varrho_0 = J\varrho$, with $J = \det \mathbf{F}$ and $\mathbf{F}$ as the deformation gradient tensor. If $\mathbf{T}$ is the symmetric Cauchy stress tensor then it is related to the first Piola–Kirchhoff stress tensor $\mathbf{S}$ by the identity $\mathbf{S} = J\,\mathbf{T}\,\mathbf{F}^{-T}$. Here $\mathbf{v}$ is the particle velocity, $\mathbf{b}$ – the body force, $\mathbf{q}$ – the heat flux vector related to the reference heat flux $\mathbf{q}_\kappa$ by the identity $\mathbf{q}_\kappa = J\mathbf{q}\,\mathbf{F}^{-T}$, ε – the specific internal energy per unit mass, r – the body heat supply, η – the specific entropy, ϑ – the absolute temperature. By E we shall denote the sum of internal and kinetic energies. The dot $\cdot$ denotes the scalar product operation.

In the recent paper of the author with ARCISZ [3], two formulations of a thermomechanics with a vector-valued internal state variable at finite strains have been presented incorporating a wave-type heat transport. The authors have made the fundamental assumption concerning the dependence of the Helmholtz free energy and the heat flux vector on thermal variables and concerning the limiting quasi-equilibrated case. In the case of finite strains the classical Fourier proportionality law can be written in two non-equivalent forms. Those two forms are crucial for the isotropic case mainly. Hence the question appears: is the proportionality isotropic law between the actual heat flux vector $\mathbf{q}$ and the spatial gradient of temperature valid or rather the proportionality isotropic law between the referential heat flux vector $\mathbf{q}_\kappa$ and the Lagrangean gradient of temperature $\operatorname{Grad}\vartheta$? The authors of that paper answer "yes" to the first part of the question. For those and the present cases such an answer has implied that the free energy should depend on the spatial gradient of the scalar internal state variable β.

Now following [3, 38] we state the main assumption:

$$\psi = \psi^*(\mathbf{F}, \vartheta, \operatorname{grad}\vartheta, \mathbf{h}), \tag{6.1}$$

with

$$\mathbf{h} = \operatorname{grad}\beta, \tag{6.2}$$

where β is the solution of an initial value problem

$$\dot{\beta} = F(\vartheta, \beta), \qquad \beta(t_0) = \beta_0\,, \tag{6.3}$$

where t_0 is an initial instant and β_0 is an initial distribution of β, assumed to be given at t_0 for each X of $\mathcal{B}$.

Incorporating (6.2) into (6.1) we obtain, as it was required above, the spatial gradient $\operatorname{grad}\beta = \nabla\beta$ in the constitutive equation for the free energy

$$\psi = \psi^*(\mathbf{F}, \vartheta, \nabla\vartheta, \nabla\beta). \tag{6.4}$$

For the other constitutive quantities

$$\begin{aligned} \eta &= \eta^*(\mathbf{F}, \vartheta, \nabla\vartheta, \nabla\beta), \\ \mathbf{S} &= \mathbf{S}^*(\mathbf{F}, \vartheta, \nabla\vartheta, \nabla\beta), \\ \mathbf{q}_\kappa &= \mathbf{Q}^*(\mathbf{F}, \vartheta, \nabla\beta). \end{aligned} \tag{6.5}$$

Notice that the independence of the heat flux of the actual value of the temperature gradient is crucial for the development of the hyperbolic model.

Now the second law of thermodynamics

$$\varrho_0(\dot{\eta}\vartheta - \dot{\varepsilon}) + \mathbf{S}\cdot\dot{\mathbf{F}} - \vartheta^{-1}\mathbf{q}_\kappa\cdot\operatorname{Grad}\vartheta \geq \varrho_0 r/\vartheta, \tag{6.6}$$

will be in use. To derive its consequences let us put the form of ψ into (6.6). Then if we perform the (material) time differentiation in (6.4), use the chain rule property and insert the result of these operations in (6.6) then we get, after grouping the terms standing in front of the appropriate time derivatives of the components the state variable vector $\mathbf{F}, \vartheta, \nabla\vartheta, \nabla\beta$,

$$\begin{aligned} (\varrho_0\partial\psi^*/\partial\mathbf{F} - \mathbf{S})\cdot\dot{\mathbf{F}} + \varrho_0(\partial\psi^*/\partial\vartheta + \eta^*)\dot{\vartheta} + (\varrho_0\partial\psi^*/\partial\nabla\vartheta)\cdot\dot{\overline{\nabla\vartheta}} \\ + \varrho_0(\partial\psi^*/\partial\nabla\beta)\cdot\dot{\overline{\nabla\beta}} + \mathbf{q}_\kappa\cdot\operatorname{Grad}\vartheta/\vartheta \leq 0. \end{aligned} \tag{6.7}$$

Now, taking the gradient of (6.3) calculated in the actual configuration and observing that the material time derivative does not commute with grad, we get

$$\dot{\overline{\nabla\beta}} = \operatorname{grad} F(\vartheta, \beta) - \nabla\beta\dot{\mathbf{F}}\mathbf{F}^{-1}. \tag{6.8}$$

The latter enables us to express the product $\mathbf{q}_\kappa\cdot\operatorname{Grad}\vartheta$ in the last inequality (6.7) as

$$\mathbf{q}_\kappa\cdot\operatorname{Grad}\vartheta = (\partial F/\partial\vartheta)^{-1}\{\mathbf{q}_\kappa\mathbf{F}^T\cdot\dot{\overline{\nabla\beta}} - (\partial F/\partial\beta)\mathbf{q}_\kappa\mathbf{F}^T\cdot\nabla\beta + (\nabla\beta\otimes\mathbf{q}_\kappa)\cdot\dot{\mathbf{F}}\}.$$

Hence, owing to this, the last inequality can be represented as

$$\begin{aligned} \{\varrho_0\partial\psi^*/\partial\mathbf{F} - \mathbf{S} + (\vartheta\partial F/\partial\vartheta)^{-1}(\nabla\beta\otimes\mathbf{q}_\kappa\}\cdot\dot{\mathbf{F}} \\ + \varrho_0(\partial\psi^*/\partial\vartheta + \eta^*)\dot{\vartheta} + (\varrho_0\partial\psi^*/\partial\nabla\vartheta)\cdot\dot{\overline{\nabla\vartheta}} \\ + \{\varrho_0\partial\psi^*/\partial\nabla\beta + (\vartheta\partial F/\partial\vartheta)^{-1}\mathbf{q}_\kappa\mathbf{F}^T\}\cdot\dot{\overline{\nabla\beta}} \\ - (\vartheta\partial F/\partial\vartheta)^{-1}(\partial F/\partial\beta)\mathbf{q}_\kappa\mathbf{F}^T\cdot\nabla\beta \leq 0. \end{aligned} \tag{6.9}$$

Due to the independence of the time derivatives of the components of the (restricted) state variable vector $(\mathbf{F}, \vartheta, \nabla\vartheta, \nabla\beta)$, the inequality (6.9) leads to identities

$$\begin{aligned} \mathbf{0} &= \partial\psi^*/\partial\nabla\vartheta, \\ \eta &= -\partial\psi^*/\partial\vartheta, \\ \mathbf{S} &= \varrho_0\partial\psi^*/\partial\mathbf{F} + (\vartheta\partial F/\partial\vartheta)^{-1}(\nabla\beta\otimes\mathbf{q}_\kappa), \\ \mathbf{q}_\kappa &= -\varrho_0(\vartheta\partial F/\partial\vartheta)(\partial\psi^*/\partial\nabla\beta)\mathbf{F}^{-T}, \end{aligned} \tag{6.10}$$

and to a reduced inequality

$$(\vartheta\partial F/\partial\vartheta)^{-1}(\partial F/\partial\beta)\mathbf{q}_\kappa\mathbf{F}^T\cdot\nabla\beta\geq 0. \tag{6.11}$$

The independence and three other potential relations in (6.10) have particular meaning. The identities from the first three lines of (6.10) are well known, the last relation is rather not typical. The stress potential relation in $(6.10)_3$ contains two components: the first component is rather classical and appears in all stress potential relations, while the second one represents the direct coupling between mechanical and thermal fields in which extra stresses appear. The potential relation for the heat flux can be obtained in some models with internal state variables (cf. [34]). Eliminating $\mathbf{q}_\kappa$ from $(6.10)_3$, $(6.10)_4$ and (6.11) we get a new potential relation for the Piola-Kirchhoff stress and a residual inequality

$$\begin{aligned}\mathbf{S}=\varrho_0\partial\psi^*/\partial\mathbf{F}-\varrho_0(\nabla\beta\otimes\partial\psi^*/\partial\nabla\beta)\mathbf{F}^{-T},\\ \varrho_0(\partial F/\partial\beta)(\partial\psi^*/\partial\nabla\beta\cdot\nabla\beta\leq 0.\end{aligned} \tag{6.12}$$

Using (6.10) and (6.12) we can write the final form of the constitutive equations for the Cauchy stress and the actual heat flux vector in a general anisotropic case, as

$$\begin{aligned}\mathbf{T}&=\varrho\partial\psi^*/\partial\mathbf{F}\,\mathbf{F}^T-\varrho\nabla\beta\otimes\partial\psi^*/\partial\nabla\beta,\\ \mathbf{q}&=-\varrho\vartheta(\partial\psi^*/\partial\nabla\beta)(\partial F/\partial\vartheta),\end{aligned} \tag{6.13}$$

respectively.

The general constitutive equations (6.13) can be investigated for the particular case of a free energy with a general law between $\mathbf{q}$ and $(\mathbf{F},\vartheta,\nabla\beta)$

$$\mathbf{q}=-\boldsymbol{\alpha}^*(\mathbf{F},\vartheta,\nabla\beta), \tag{6.14}$$

with a material tensor function (in a general, anisotropic case) $\boldsymbol{\alpha}^*$ given by

$$\boldsymbol{\alpha}^*=\varrho\vartheta\frac{\partial F}{\partial\vartheta}\frac{\partial\psi^*}{\partial\nabla\beta}. \tag{6.15}$$

The linearity and the isotropy of (6.14) in $\nabla\beta$, on the other hand, will be reached iff the free energy function is of the form (cf. Remark 1)

$$\psi=\psi_1^*(\mathbf{B},\vartheta)+0.5\psi_2^*(\mathbf{B},\vartheta)\nabla\beta\cdot\nabla\beta, \tag{6.16}$$

where the factor 0.5 has been assumed for convenience only, and the tensor $\boldsymbol{\alpha}^*$ is spherical, i.e. $\boldsymbol{\alpha}^*=\alpha^*\mathbf{1}$, with

$$\mathbf{q}=-\alpha^*(\mathbf{B},\vartheta)\nabla\beta\qquad\text{with}\qquad\alpha^*(\mathbf{B},\vartheta)=\varrho\vartheta\partial F/\partial\vartheta\psi_2^*(\mathbf{B},\vartheta). \tag{6.17}$$

It is worthwhile to point out, that the above linearity assumption is compatible with the following observation. As discussed in [13], it becomes reasonable to make the following assumptions remaining consistent with classical thermostatics, at the same time making it straightforward to use experimental results to identify the material functions needed:

- the free energy is independent of β and quadratic in $|\nabla\beta|$,
- the coefficient α^* may depend on $\mathbf{B}$ and on ϑ.

REMARK 9

In the present thermomechanical case, the independence of the free energy function of β leads to splitting (compare (5.9) of the function $F(\vartheta,\beta)$ into two independent terms

$$F(\vartheta,\beta) = F_1(\vartheta) + F_2(\beta).$$

Moreover, in the linear and isotropic case of the heat flux constitutive relation (6.17) if the proportionality material coefficient α^* is independent of strain, i.e. $\alpha^*(\mathbf{B},\vartheta) = \alpha^*(\vartheta)$, then

$$\mathbf{q} = -\alpha^*(\vartheta)\,\nabla\beta, \tag{6.18}$$

and due to (6.17)

$$\psi_2^*(\mathbf{B},\vartheta) = \psi_{21}^*(\vartheta)J, \tag{6.19}$$

where, as before, $J = \det\mathbf{F} = \varrho_0/\varrho$, and ψ_{21}^* is a nonnegative material function ([3]). In this case the final form of the Cauchy stress constitutive law $(6.13)_1$ due to (6.16) expression will take the form

$$\mathbf{T} = 2\varrho(\partial\psi_1^*/\partial\mathbf{B})\mathbf{B} + \varrho\psi_{21}^*(\vartheta)J(0.5|\nabla\beta|^2\mathbf{I} - \nabla\beta\otimes\nabla\beta), \tag{6.20}$$

or equivalently, by using (6.18),

$$\mathbf{T} = 2\varrho(\partial\psi_1^*/\partial\mathbf{B})\mathbf{B} + \varrho\frac{\psi_{21}^*(\vartheta)J}{\alpha^*(\vartheta)^2}(0.5|\mathbf{q}|^2\mathbf{I} - \mathbf{q}\otimes\mathbf{q}). \tag{6.21}$$

Let us notice that even in this simplified case the stress-strain relation has an extra term due to the thermomechanical coupling; this term can be called an *extra thermal stress*. This extra contribution is similar to that already known in the Landau's superfluid model of liquid helium at low temperature [65]. It seems to us that this contribution can have a substantial meaning in describing the damage phenomena in deformable materials due thermomechanical coupling. The thermomechnanics with damage effects introduced by the internal state variables has been developed in the last paper [39].

([3]) If the internal energy ε^* is independent of $\nabla\beta$ then the function ψ_{21}^* is linear in ϑ, cf. (5.19).

7. Hyperbolicity of thermoelasticity

In order to check the hyperbolicity of the model, let us discuss shortly the propagation of weak discontinuity waves. On the surface of discontinuity ([4]) of the second derivatives of the displacement function $\mathbf{u}$ and the function β, we have at our disposal the classical kinematical and geometrical compatibility conditions. A jump discontinuity in the field is denoted by a bracket $[\![\cdot]\!]$. Here u_n is called its (intrinsic) *normal speed* of propagation and $\mathbf{n}$ is a *unit normal* to the wave front, regarded as a 2D surface in 3D Euclidean space ([35]). Hence for derivatives of the fields $\mathbf{v}, \mathbf{F}, \vartheta$ and β, we have the following relations:

$$
\begin{aligned}
[\![\operatorname{grad}\mathbf{v}]\!] &= -U\mathbf{s}\otimes\mathbf{n},\\
[\![\operatorname{grad}(\partial\beta/\partial t)]\!] &= -u_n v\mathbf{n},\\
[\![\operatorname{grad}\mathbf{F}]\!] &= \mathbf{s}\otimes\mathbf{F}^T\mathbf{n}\otimes\mathbf{n},\\
[\![\partial\mathbf{v}/\partial t + \operatorname{grad}\mathbf{v}\mathbf{v}]\!] &= [\![\dot{\mathbf{v}}]\!] = U^2\mathbf{s},
\end{aligned}
\tag{7.1}
$$

where we have used the following notations for the relative speed U and the amplitudes of jumps

$$
\begin{aligned}
U := u_n - \mathbf{v}\cdot\mathbf{n}, \qquad [\![\operatorname{grad}\mathbf{v}\,\mathbf{n}]\!] &= -U\mathbf{s},\\
[\![\operatorname{grad}\operatorname{grad}\beta\,\mathbf{n}]\!] &= v\mathbf{n},
\end{aligned}
\tag{7.2}
$$

together with the continuity of the first order derivatives of β. On the other hand, for the second derivatives of the thermal variable β, in view of (6.3), and its prolongation (6.8), we get

$$
[\![\operatorname{grad}\vartheta]\!] = -U\tau(\vartheta)(v + \nabla\beta\cdot\mathbf{s})\mathbf{n}, \qquad [\![\dot{\vartheta}]\!] = -U[\![\nabla\vartheta]\!]\cdot\mathbf{n},
\tag{7.3}
$$

where we use the following short denotation

$$
\tau(\vartheta) = 1/F_1'(\vartheta).
\tag{7.4}
$$

For further calculation we need the local form of the energy

$$
\partial\varrho(\varepsilon + 0.5\mathbf{v}\cdot\mathbf{v})/\partial t + \operatorname{div}(E\mathbf{v} + \mathbf{q} - \mathbf{v}\,\mathbf{T}) = \varrho r + \varrho\mathbf{v}\cdot\mathbf{b},
\tag{7.5}
$$

and the motion equation

$$
\partial\varrho\mathbf{v}/\partial t + \operatorname{div}(\varrho\mathbf{v}\otimes\mathbf{v} - \mathbf{T}) = \varrho\mathbf{b}
\tag{7.6}
$$

in the spatial description. Now performing the differentiation of the stress constitutive function $\mathbf{T}^*$ in the equation of motion (7.6), and of ε^* in the reduced energy equation, written below as the consequence of (7.6) and (7.5),

$$
\varrho\dot{\varepsilon} + \operatorname{div}\mathbf{q} - \mathbf{T}\cdot\operatorname{grad}\mathbf{v} = \varrho r,
\tag{7.7}
$$

([4]) Such a surface of discontinuity represents geometrically the thermo-acoustic wave front.

and taking the results across the wave front, we obtain

$$
\begin{aligned}
&(\varrho U^2\mathbf{I} - \mathbf{Q} + \tau U\mathbf{P}\mathbf{n}\otimes\nabla\beta)\mathbf{s} = (-\tau U\mathbf{P} + (\mathbf{G}\mathbf{n}))v\mathbf{n},\\
&(\varrho U^2 c_v\tau\nabla\beta + \tau U\alpha^{*\prime}(\vartheta)\nabla\beta\cdot\mathbf{n}\nabla\beta)\cdot\mathbf{s}\\
&\qquad = (-\varrho U^2 c_v\tau + U\mathbf{t}\cdot\mathbf{n} - \tau U\alpha^{*\prime}(\vartheta)\nabla\beta\cdot\mathbf{n} + \alpha^*)v,
\end{aligned}
\tag{7.8}
$$

where we have assumed the following abbreviations:

$$
\begin{aligned}
\mathbf{Q} &:= \underset{(3,5)}{\mathrm{tr}}\,\underset{(4,6)}{\mathrm{tr}}\,\frac{\partial\mathbf{T}^*(\mathbf{F},\vartheta,\nabla\beta)}{\partial\mathbf{F}}\otimes\mathbf{F}^T\mathbf{n}\otimes\mathbf{n},\\
\mathbf{P} &:= \partial\mathbf{T}^*(\mathbf{F},\vartheta,\nabla\beta)/\partial\vartheta,\\
\mathbf{G} &:= \partial\mathbf{T}^*(\mathbf{F},\vartheta,\nabla\beta)/\partial\nabla\beta,\\
\alpha^{*\prime} &:= \partial\alpha^*(\vartheta)/\partial\vartheta,\\
\mathbf{t} &:= \partial\varepsilon^*(\mathbf{F},\vartheta,\nabla\beta)/\partial\nabla\beta,\\
c_v &:= \partial\varepsilon^*(\mathbf{F},\vartheta,\nabla\beta)/\partial\vartheta.
\end{aligned}
\tag{7.9}
$$

Here the symbol $\underset{(3,5)}{\mathrm{tr}}$ denotes the operation of the simple saturation (composition) of the third index with the fifth one of the tensor following the symbol.

Let us notice that in 3D case we have a system of four homogeneous equations for two amplitudes: the vector-valued mechanical amplitude $\mathbf{s}$ and the scalar thermal one v. To get a nontrivial solution, the determinant of the system has to vanish. This gives us the so-called characteristic (or dispersion) relation for the speed U in terms of $\mathbf{n}$ and values of state variables at the wave front.

The hyperbolicity of the governing system of equations (6.3), (7.6), (7.7) will be guaranteed if for any normal vector $\mathbf{n}$ eight real solutions for U and four linear independent amplitude vectors $(\mathbf{s}, v)$ exist.

We are not going to write this relation, restricting ourselves to some particular cases. If the wave propagates in the state with the vanishing heat flux, i.e. $\nabla\beta = \mathbf{0}$, then the system (7.8) is simpler and the characteristic relation will take the form

$$
\det(\varrho U^2\mathbf{I} - \mathbf{Q})(\varrho U^2 c_v\tau - \alpha*) = 0,
\tag{7.10}
$$

giving three symmetric mechanical wave speeds, provided the acoustic tensor $\mathbf{Q}$ is positive definite, and also one symmetric thermal wave speed, provided the specific heat c_v is positive. In the general case, with nonvanishing $\nabla\beta$ we can have coupled thermomechanical wave speeds.

We will conclude this section with the governing system of equations of the modified model of thermoelasticity written in a 4D divergence form. Such a form is necessary in order to discuss strong discontinuity waves and weak solutions, that are piecewise continuous and Lipschitz continuous with jump discontinuities. The system should be written as a first order one for the following fields: $\mathbf{u}$ –

displacement vector, $\mathbf{F}$ – the deformation gradient tensor, β – internal state variable, $\mathbf{v}$ – particle velocity vector, η – the specific entropy, $\mathbf{p}$ – the spatial gradient of β, where for the E (total specific energy), the following relationship has been assumed: $E = \varepsilon^*(\mathbf{F}, \eta, \mathbf{p}) + 0.5\mathbf{v}\cdot\mathbf{v}$ with the thermodynamic (absolute) temperature ϑ, given by the potential relation $\vartheta = \partial\varepsilon^*/\partial\eta$.

$$
\begin{aligned}
\dot{\mathbf{u}} &= \mathbf{v}, \\
\dot{\mathbf{F}} - \operatorname{Div}(\mathbf{v}\otimes\mathbf{1}) &= \mathbf{0}, \\
\dot{\beta} &= F_1(\vartheta) + F_2(\beta), \\
\varrho_0\dot{\mathbf{v}} - \operatorname{Div}\mathbf{S} &= \varrho_0\mathbf{b}, \\
\varrho_0\dot{E} + \operatorname{Div}(\mathbf{q}_\kappa - \mathbf{v}\,\mathbf{S}) &= \varrho_0 r + \varrho_0\mathbf{v}\cdot\mathbf{b}, \\
\dot{\overline{\mathbf{pF}}} - \operatorname{Div}(F_1(\vartheta)\mathbf{1}) &= F_2'(\beta)\mathbf{pF}.
\end{aligned}
\tag{7.11}
$$

Let us notice that the last equation in this system is the differential consequence of the evolution equation (6.3) (compare also (6.8)). Moreover, from this equation the jump condition follows

$$
-\sigma[\![\mathbf{pF}]\!] = [\![F_1(\vartheta)]\!]\mathbf{N},
\tag{7.12}
$$

where σ denotes normal component of the strong discontinuity wave (shock speed) while the unit vector $\mathbf{N}$ is normal to the wave front in the reference placement (configuration). This jump condition is compatible with the condition following from the evolution equation (6.3), namely $[\![\dot{\beta}]\!] = [\![F_1(\vartheta)]\!]$ and the differential compatibility conditions for the first and second derivatives of β, namely $\operatorname{Grad}\beta = \mathbf{pF}$ and $\dot{\overline{\mathbf{pF}}} = \operatorname{Grad}\dot{\beta}$.

8. Conclusions

The extensive discussion of possible propagation conditions will be given in the next paper. Now we can refer to [41, 42], where some particular 1D cases were considered, while in [37] 3D thermal weak discontinuity waves were investigated. The reader is referred to the recent paper of FRISCHMUTH and CIMMELLI [22], where 1D thermomechanical case with linearized constitutive equations has been numerically treated. There two waves have been calculated: one corresponding to longitudinal ballistic phonon propagation and the other, the second sound wave. That paper is the first one in which the present model has been successfully applied in the linear case for numerical treatment of coupled thermomechanical and second sounds waves observed in the heat pulse experiments described shortly in Sec. 2 of the present paper. In the next paper we will be concerned with the numerical simulation in 1D nonlinear case.

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POLISH ACADEMY OF SCIENCES
INSTITUTE OF FUNDAMENTAL TECHNOLOGICAL RESEARCH
e-mail: wkos@ippt.gov.pl

Received February 2, 1998.

Arch. Mech., 50, 3, pp. 451–458, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

Random elastic media: Why zero mean stress does not imply zero mean strain

Dedicated to Prof. Henryk Zorski on the occasion of his 70-th birthday

E. KRÖNER (STUTTGART)

IN THIS NOTE we are concerned with (linearized) elastic media that are heterogeneous on the microscale and homogeneous on the macroscale. We assume the validity of an ergodic hypothesis so that we can form ensemble averages such as mean stress $\langle\sigma\rangle$ and mean strain $\langle\varepsilon\rangle$. We argue that $\langle\sigma\rangle = 0$ does not, in general, imply that also $\langle\varepsilon\rangle = 0$ (end of Sec. 2). This is the case, for instance, when the distribution of the stress sources (external forces or incompatibilities) are correlated with the spatial distribution of the local elastic moduli. It is shown how problems of this type can be treated.

1. Introduction

IN THIS WORK we are concerned with *linear elastic* media that are heterogeneous on the microscale and, at the same time, homogeneous on the macroscale. Many composite materials and also polycrystals can be, at least approximately, in such a state. Under certain conditions such a medium can be treated as a so-called *effective medium* whose material properties are described by a constant effective tensor C^{eff} of elastic moduli. The main interest here lies in the situation where such a description is *not* possible. Among others, we pay attention to the following problem: If the mean stress in the medium is zero, does it follow that also the mean strain vanishes? The answer is "No". I have treated this question previously [1, 2], but perhaps not convincingly enough, because I continue to receive remarks of this type: "Many people have claimed that since the average stress vanishes, the average strain also vanishes." In the following we show that this is not generally true. To make our investigations lucid we use a symbolic notation which is largely free of tensor indices. Various quantities are integral or differential operators with tensorial kernels. Integral operators are underlined by double line, such as $\underline{\underline{\Gamma}}$ or $\underline{\underline{\gamma}}$, differential operators are underlined by a single line, as $\underline{L}$. Instead of specifying positions in the medium by $r_1, r_2, r_3 \ldots$ or $r', r'', r''' \ldots$ we shall indicate them just by numbers, i.e. (1), (2), (3) ... Explanations are often somewhat short. For a more detailed representation the reader is referred to the review [3], even though this note goes beyond this review.

2. Averages of stress and strain

Assume that the medium characterized in Sec.1 be loaded by volume forces $f_k(1)$ and surface forces $t_k(1)$. Applying the method of Green's functions, the displacement (vector) field $u_i(1)$ can be represented as

$$u_i(1) = \int_V \gamma_{ik}(1,2)\, f_k(2)\, dV_2 + \int_S \gamma_{ik}(1,2)\, t_k(2)\, dS_2\,, \tag{2.1}$$

where the integrations extend over the volume V and the surface S of the medium. For convenience (1) is abbreviated in symbolic notation as

$$u = \underline{\underline{\gamma}} F, \tag{2.2}$$

where $\underline{\underline{\gamma}}$ is the *displacement Green's operator* and F comprises the volume and surface forces. (2.1), or (2.2), is the general solution of the traction boundary value problem of an arbitrary, in general heterogeneous or microheterogeneous medium. $u, \underline{\underline{\gamma}}$ and F are, in our investigation, random functions of position.

Since we are interested in macroscopic (ensemble) averages (symbol $\langle\cdot\rangle$) rather than in the local quantities, we take the ensemble average of (2.2):

$$\begin{aligned} &\langle u\rangle = \langle \underline{\underline{\gamma}} F\rangle = \langle \underline{\underline{\gamma}}\rangle\langle F\rangle + \langle \underline{\underline{\gamma}}' F'\rangle, \\ &F' \equiv F - \langle F\rangle, \qquad \underline{\underline{\gamma}}' \equiv \underline{\underline{\gamma}} - \langle \underline{\underline{\gamma}}\rangle, \qquad \langle F'\rangle = 0, \qquad \langle \underline{\underline{\gamma}}'\rangle = 0. \end{aligned} \tag{2.3}$$

Working with ensemble averages (rather than with volume averages) is convenient because ensemble averaging commutes with differentiating and integrating. This however requires the validity of an ergodic hypothesis, which essentially means that the situation is "sufficiently statistical". The statistics of $\underline{\underline{\gamma}}$ is determined by that of c, the (4-th rank) tensor of the microheterogeneous moduli.

From (2.3) it follows that

$$\langle u\rangle = \langle \underline{\underline{\gamma}}\rangle\langle F\rangle, \tag{2.4}$$

provided $\langle \underline{\underline{\gamma}}' F'\rangle$ vanishes, i.e. if, according to a well-known theorem of probability theory, the distribution of the forces is not correlated with that of the (microheterogeneous) elastic moduli. This "no-correlation" is the case in many applications (see below). In this note we shall admit correlations and give realizations below.

The strain tensor derived from (2.1) and from the equilibrium conditions $f = \nabla\sigma$, $t = n\sigma$ (n being the external unit vector normal to the surface) by a routine calculation is

$$\varepsilon_{ij}(1) = \int_V \Gamma_{ijkl}(1,2)\, \sigma_{kl}(2)\, dV_2\,, \qquad \Gamma_{ijkl}(1,2) \equiv \partial_j\, \partial_{l'}\, \gamma_{ik}(1,2)\,|_{(ij)(kl)} \tag{2.5}$$

which is abbreviated as

$$\varepsilon = \underline{\underline{\Gamma}}\,\sigma. \tag{2.6}$$

Here $\underline{\underline{\Gamma}}$ is the so-called *modified* or *strain Green's function*, a 2-point, 4-th rank tensor field, and (ij), (kl) denotes symmetrization in the subscripts concerned. Note that the abbreviation introduced in (2.2) involves vector and 2-nd rank tensor fields, whereas that of (2.6) concerns 2-nd and 4-th rank tensor fields.

Taking the average of (2.6) gives us the mean strain tensor

$$\langle\varepsilon\rangle = \langle\underline{\underline{\Gamma}}\,\sigma\rangle = \langle\underline{\underline{\Gamma}}\rangle\,\langle\sigma\rangle + \langle\underline{\underline{\Gamma}}'\,\sigma'\rangle, \tag{2.7}$$

where the primed quantities are again deviations from the mean. In (2.7) $\langle\underline{\underline{\Gamma}}\rangle\,\langle\sigma\rangle$ derives from $\langle\underline{\underline{\gamma}}\rangle\,\langle F\rangle$ and $\langle\underline{\underline{\Gamma}}'\sigma'\rangle$ vanishes when $\langle\underline{\underline{\gamma}}'F'\rangle$ does. In analogy to (2.4) we have

$$\langle\varepsilon\rangle = \langle\underline{\underline{\Gamma}}\rangle\,\langle\sigma\rangle, \tag{2.8}$$

provided that u and F, thus $\underline{\underline{\Gamma}}$ and σ are mutually uncorrelated. By comparison with (2.6) $\langle\underline{\underline{\Gamma}}\rangle$ is then the modified Green's function of a random elastic medium with an effective compliance tensor defined by

$$\langle\varepsilon\rangle = S^{\text{eff}}\langle\sigma\rangle, \qquad S^{\text{eff}} = (C^{\text{eff}})^{-1}. \tag{2.9}$$

Note that contrary to $\langle\underline{\underline{\Gamma}}\rangle$, S^{eff} is not an operator itself, but derives from the operator $\langle\underline{\underline{\Gamma}}\rangle$ according to

$$S^{\text{eff}}_{ijkl} = \int_V \langle\Gamma_{ijkl}(1,2)\rangle\, dV_2\,, \tag{2.10}$$

cf. [3], p. 265.

In the "no-correlation" case $\langle\sigma\rangle = 0$ leads to $\langle\varepsilon\rangle = 0$ and *vice versa*. Obviously this is not so in the more general case of (2.7), when $\langle\underline{\underline{\Gamma}}'\sigma'\rangle \neq 0$.

3. The general scheme

In the frame of linearized elasticity theory the equation

$$u = \underline{\underline{\gamma}}\,F \tag{3.1}$$

with the meaning of F as defined in Sec. 2 solves the deterministic problem of finding the displacement field from the knowledge of the external force distribution in the body. Our interest lies in situations with random distributions. That means that we have to extract the random information possibly contained in (3.1). This is usually done with reference to a homogeneous isotropic, but otherwise quite arbitrary *comparison medium* that has the same form and load as the real medium of interest. The named properties of the comparison medium allow us to calculate its Green's function, which therefore will be treated as known.

Let

$$\underline{L}\,u = F, \qquad \underline{L}^{\circ}\,u^{\circ} = F \tag{3.2}$$

be the (statical) field equations (in volume and on surface) of the real and the comparison medium, respectively. The displacement Green's operators are $\underline{\underline{\gamma}}$ and $\underline{\underline{\gamma}}^{\circ}$; they obey the conditions

$$\underline{L}\,\underline{\underline{\gamma}} = I, \qquad \underline{L}^{\circ}\,\underline{\underline{\gamma}}^{\circ} = I \tag{3.3}$$

(the Green's operators $\underline{\underline{\gamma}}$ are inverse to the field operators $\underline{L}$. This property *defines* the Green's functions.) In (3.3), set $\underline{L} = \underline{L}^{\circ} + \delta\,\underline{L}$ and multiply from the left by $\underline{\underline{\gamma}}^{\circ}$ to obtain, after solution for $\underline{\underline{\gamma}}$,

$$\begin{aligned}\underline{\underline{\gamma}} &= (I + \underline{\underline{\gamma}}^{\circ}\,\delta\,\underline{L})^{-1}\underline{\underline{\gamma}}^{\circ} \\ &= (I - \underline{\underline{\gamma}}^{\circ}\,\delta\,\underline{L} + \underline{\underline{\gamma}}^{\circ}\,\delta\,\underline{L}\,\underline{\underline{\gamma}}^{\circ}\,\delta\,\underline{L} - \underline{\underline{\gamma}}^{\circ}\,\delta\,\underline{L}\,\underline{\underline{\gamma}}^{\circ}\,\delta\,\underline{L}\,\underline{\underline{\gamma}}^{\circ}\,\delta\,\underline{L} + \cdots - \cdots)\underline{\underline{\gamma}}^{\circ}.\end{aligned} \tag{3.4}$$

Here

$$\delta\,\underline{L} = \nabla\delta c\nabla, \qquad \delta c \equiv c - C^{\circ}, \tag{3.5}$$

c denoting the tensor of local elastic moduli, C° – that of the comparison medium. δc and $\delta\,\underline{L}$ are random functions of position. All the quantities appearing in (3.4) have vector or tensor character. We have used a symbolic notation in which indices and their positions do not occur. They can easily be determined a *posteriori*. If so, then the positions of the $\underline{\underline{\gamma}}^{\circ}$ and $\delta\,\underline{L}$ in (3.4) are not important. In actual calculations one uses indices, their positions follow easily from (3.4). Thus (3.4) may also be written as

$$\underline{\underline{\gamma}} = (I - \underline{\underline{\gamma}}^{\circ}\,\delta\,\underline{L} + \underline{\underline{\gamma}}^{\circ}\,\underline{\underline{\gamma}}^{\circ}\,\delta\,\underline{L}\,\delta\,\underline{L} - \underline{\underline{\gamma}}^{\circ}\,\underline{\underline{\gamma}}^{\circ}\,\underline{\underline{\gamma}}^{\circ}\,\delta\,\underline{L}\,\delta\,\underline{L}\,\delta\,\underline{L} + \cdots - \cdots)\underline{\underline{\gamma}}^{\circ}. \tag{3.6}$$

This equation relates the Green's function $\underline{\underline{\gamma}}$ of the, in general, complicated real medium to the Green's function $\underline{\underline{\gamma}}^{\circ}$ of the simpler comparison medium. It is an implicit equation, because $\delta\underline{L}$ ($\equiv \underline{L} - \underline{L}^{\circ}$) contains $\underline{\underline{\gamma}}$ which is the inverse of $\underline{L}$.

If the elastic moduli (the components of c) of the real medium are randomly distributed, then the averaged Green's function $\langle\underline{\underline{\gamma}}\rangle$ follows from (3.6), since $\underline{\underline{\gamma}}^{\circ}$ is nonrandom, as

$$\langle\gamma\rangle = (I - \underline{\underline{\gamma}}^{\circ}\langle\delta L\rangle + \underline{\underline{\gamma}}^{\circ}\,\underline{\underline{\gamma}}^{\circ}\langle\delta\,\underline{L}\,\delta\,\underline{L}\rangle - \underline{\underline{\gamma}}^{\circ}\,\underline{\underline{\gamma}}^{\circ}\,\underline{\underline{\gamma}}^{\circ}\langle\delta\,\underline{L}\,\delta\,\underline{L}\,\delta\,\underline{L}\rangle + \cdots - \cdots)\underline{\underline{\gamma}}^{\circ}. \tag{3.7}$$

To calculate $\langle\underline{\underline{\gamma}}\rangle$ from this equation we need the statistical information in the form of n-point correlation functions of the elastic operator $\underline{L}$, namely $\langle\delta\,\underline{L}\rangle$, $\langle\delta\,\underline{L}\delta\,\underline{L}\rangle$, $\langle\delta\,\underline{L}\,\delta\,\underline{L}\,\delta\,\underline{L}\rangle$, i.e. $\langle\delta\,\underline{L}^{n}\rangle$, $n = 1, \ldots \infty$. Writing a bit more explicitly we have for instance $\langle\delta c^4\rangle = \langle\delta c(1)\delta c(2)\delta c(3)\delta c(4)\rangle$ and a corresponding expression for $\langle\delta L^4\rangle$.

The statistical information is only seldom given *a priori* in the form of correlation functions. Usually one has to calculate the correlation functions from some other information such as "spherical or ellipsoidal elastic inclusions are embedded in a matrix material of other elastic moduli" etc. This calculation is often a most difficult task, for which the science of mathematical morphology has been developed [4, 5]. The basic equation (3.6) is sometimes named after Lippmann and Schwinger, or Dyson (i.e. LSD), who introduced such an equation into quantum mechanical scattering theory. (3.6) can be transformed into a relationship between *modified* Green's functions:

$$\underline{\underline{\Gamma}} = (I - \underline{\underline{\Gamma}}^{\circ}\delta c + \underline{\underline{\Gamma}}^{\circ}\underline{\underline{\Gamma}}^{\circ}\delta c\delta c - \underline{\underline{\Gamma}}^{\circ}\underline{\underline{\Gamma}}^{\circ}\underline{\underline{\Gamma}}^{\circ}\delta c\delta c\delta c + \cdots - \cdots)\underline{\underline{\Gamma}}^{0}. \tag{3.8}$$

To calculate $\langle\underline{\underline{\Gamma}}\rangle$ from this equation we again need the statistical information on the correlation functions of the elastic moduli, $\langle\delta c^n\rangle$, $n = 1, \cdots, \infty$.

We have seen in Sec. 2, that $\langle\underline{\underline{\Gamma}}\rangle$ is the Green's function of a medium whose elasticity is described by a tensor C^{eff} of elastic moduli.

In such a medium the local elastic moduli c are uncorrelated with the distribution of the external forces F. If this is not true in some random elastic medium, then we have a more general statistical situation. In fact, to describe such a situation, we need not only to know correlations between elastic moduli at different positions, but also correlations between moduli and forces. We see this as follows: Combining (3.1) and (3.6) gives us

$$u = \underline{\underline{\gamma}}^{\circ}F - \underline{\underline{\gamma}}^{\circ}\underline{\underline{\gamma}}^{\circ}\,\delta\,\underline{L}\,F + \underline{\underline{\gamma}}^{\circ}\underline{\underline{\gamma}}^{\circ}\underline{\underline{\gamma}}^{\circ}\,\delta\,\underline{L}\,\delta\,\underline{L}F - \cdots + \cdots \tag{3.9}$$

and after averaging

$$\langle u\rangle = \underline{\underline{\gamma}}^{\circ}\langle F\rangle - \underline{\underline{\gamma}}^{\circ}\underline{\underline{\gamma}}^{\circ}\langle\delta\,\underline{L}\,F\rangle + \underline{\underline{\gamma}}^{\circ}\underline{\underline{\gamma}}^{\circ}\underline{\underline{\gamma}}^{\circ}\langle\delta\,\underline{L}\,\delta\,\underline{L}\,F\rangle - \cdots + \cdots\,. \tag{3.10}$$

Since we now treat a situation with $(\underline{L}-F)$-correlations (or $(u-F)$-correlations), $\langle u\rangle$ no longer equals $\underline{\underline{\gamma}}^{\circ}\langle F\rangle$. To calculate $\langle u\rangle$, we rather need the mixed correlations $\langle\delta\,\underline{L}^n\,F\rangle$, $n = 1, \cdots, \infty$, where for instance $\langle\delta\,\underline{L}^3F\rangle = \langle\delta\,L(1)\,\delta\,L(2)\,\delta\,L(3)\,F(4)\rangle$. If we are interested in correlation functions of u such as $\langle u(1)\,u(2)\rangle$, or $\langle u(1)\,u(2)\,u(3)\rangle$, then we need to know the set of correlation functions of the form $\langle\delta\,\underline{L}^m F^n\rangle$, $m, n = 0, \ldots, \infty$, where e.g. $\langle\delta\,\underline{L}^2F^3\rangle = \langle\delta\,\underline{L}(1)\,\delta\,\underline{L}(2)\,F(3)\,F(4)\,F(5)\rangle$. Here we have included the correlation functions with $m = 0$ (functions among F alone) and those with $n = 0$ (functions among $\delta\,\underline{L}$ alone).

A further case: Thanks to the ergodic hypothesis, differentiation and integration commute with ensemble averaging. This means for instance, that the average of the strain tensor ε is

$$\langle\varepsilon\rangle = \frac{1}{2}(\langle u\rangle\nabla + \nabla\langle u\rangle), \tag{3.11}$$

so that for the calculation of $\langle\varepsilon\rangle$ we need the same correlation functions like for $\langle u\rangle$, namely $\langle\delta c^n\rangle = \langle\delta c(1)\,\delta c(2)\ldots\delta c(n)\rangle$. Of course, similar statements can be made for higher derivatives of u and ε.

Summing up, we have found that for the general situation (but always linearized elasticity theory!) we need to know the full set of correlation functions among $\delta \underline{L}$ and F, or δc and F (including the correlation functions among δL (or δc) and F alone). Having this information, we can calculate, in principle, the whole statistical information about the system, again in the form of correlation functions, namely now the functions $\langle u^l \delta \underline{L}^m F^n \rangle$ (or $\langle \varepsilon^l \delta \underline{L}^m F^n \rangle$) where for instance $\langle u^2 \delta \underline{L}^3 F^2 \rangle = \langle u(1)\, u(2) \delta \underline{L}(3)\, \delta \underline{L}(4)\, \delta \underline{L}(5)\, F(6)\, F(7) \rangle$.

Its is known in the probability theory, the information about the full set of correlation functions is equivalent to that of the probability density functional. That means, given this functional, all correlation functions can be derived by well-known methods. Therefore we can formulate our general problem as follows:

Given the probability density functional $P[\delta c, F]$ in terms of δc and F, the probability density functional $P[u, \delta c, F]$ or $P[\varepsilon, \delta c, F]$ is sought for in terms of u (or ε), δc and F [1]. We think, that this formulation holds even in nonlinear elasticity.

4. Examples of applications

a. In microheterogeneous matter, the constituents which possess different elastic moduli usually are of different mass density (this is not true for 1-phase polycrystals). Different mass densities imply different gravitational forces between the various constituents. The gravitational forces are clearly correlated to the distribution of the masses, i.e. also of the elastic moduli. To calculate for instance the macroscopic stress state of such a medium, we need information about the (c-f)-correlations.

b. Inertia forces, like gravitational forces, are volume forces. In the case of wave propagation they are correlated with the mass distribution, hence also with the elastic moduli. To calculate problems of wave propagation, one needs again information about the (c-f)-correlations, where f are now the inertia forces. Strongly fluctuating elastic moduli cause a considerable energy flux into the *correlation waves*. E.g. correlations like $\langle uc^n \rangle$ participate in the wave motion. Here $\langle uc^3 \rangle$, for instance, stands for $\langle u(1)\, c(2)\, c(3)\, c(4) \rangle$.

c. To judge the importance of stress and strain fluctuations, their size must be known. Particularly important for this are the 2-point correlations $\langle \varepsilon(1)\, \varepsilon(2) \rangle$ and $\langle \sigma(1)\, \sigma(2) \rangle$.

d. Internal stresses (eigenstresses) appear when the incompatibility tensor does not vanish. After plastic deformation this tensor, say η, occurs as a new random function. To calculate the macroscopic eigenstress after unloading, one needs to have information about the $(\sigma - \eta)$-correlations. Since, according to a theorem of ALBENGA [6], the volume average of the eigenstresses always vanishes, one is inclined to assume that also the average strain, $\langle \varepsilon \rangle = \langle s\sigma \rangle$ vanishes. This however is not true thanks the occurrence of the $(\sigma - \eta)$-correlations.

e. A great number of further applications have to do with conditional averages. For instance, it might be of interest to know the average stress in all grains of a polycrystal, that have the same lattice orientation or grain shape. Also this problem can be solved, at least in principle, with the tools discussed in this note. We renounce further examples since those given already show the power of the method of correlation functions for the solution of statistical problems in the (linearized) elasticity theory.

5. Conclusion

For materials which are materially uniform even on the microscale, elasticity theory has proven to be a tool of extraordinary success. A large part of materials in practical use, however, are not at all materially uniform but rather heterogeneous, often on a microscale. Speaking of microscale we have in mind something that is very small compared with the scale of our perceptions – the macroscale – but distinctly larger than the atomic scale whose unit is the atomic distance. Including the atomic scale into our considerations would mean to discuss the question, to what degree can the atomic discreteness be neglected in the theory of the mechanical behaviour of micro- and macro-continuous matter. However, this topic, which is not at all scientifically exhausted, is beyond the ambition of the present note. So is also the question of nonlocality in the elastic interaction. The corresponding theory is in a rather good state, but its inclusion would enlarge this note too much.

The equations of the theory of local and linear elastic media are, of course, also valid, when the elastic parameters vary on the macro- and microscale. But the solution of these equations becomes extremely involved when the distribution of elastic parameter is partially or completely random, the case to which we now restrict ourselves.

In fact, except in very special situations, it is even impossible to write down explicitly the elastic field equations, that we had abbreviated as $\underline{\underline{L}}\, u = F$. Even less possible is then to calculate the Green's function which solves the problem in the form $u = \underline{\underline{\gamma}} F$. All the quantities appearing in these two equations are so complex that we would need an infinity of sheets of papers to write them down. For this reason there is not even a desire to know these quantities in all detail.

It is in the spirit of probability theory and statistical mechanics, to replace the functions of the microscale by probability density functionals. These contain much less information than the original fluctuating functions. In doing this, we move from the field of continuum mechanics into the field of statistical continuum mechanics (see e.g. [7]) whose most important tool are the correlation functions. These relate to one or more random functions and can be extracted from the pertaining probability functionals. We distinguish 1-point, 2-point, 3-point, $\cdots$, n-point correlation functions, where n extends up to infinity. The great prac-

tical significance of them stems from the fact that the correlation functions of low order, e.g. $n \leq 4$, carry the most relevant information about the statistical quantities of the system. Therefore it is often good enough, to consider only a few low order correlation functions instead of their infinite set or the equivalent probability density functional.

Since the primary interest in such statistical problems usually relates to averages of relevant quantities such as stress, strain, functions of these, we need the correlation functions in order to calculate those averages. This can easily be seen using the method of Green's functions. To calculate e.g. the average strain $\langle \varepsilon \rangle$, we need the modified Green's function $\underline{\underline{\Gamma}}$, or sometimes its mean $\langle \underline{\underline{\Gamma}} \rangle$. They can be gained from the correlation functions of the elastic moduli, as we have shown.

Strictly speaking we have discussed the traction boundary value problem only. It is clear, however, that the displacement and mixed boundary value problem can be treated in an analogous way.

Since the appearing series developments concern multiple integrals, the solution of our problems requires a lot of numerical effort. As far as we know, correlations of 3-rd order are sometimes tractable. There is a hope that modern computers will allow us to go beyond the 3-rd order.

This note was a very brief review of an important field within the mechanical sciences. It is clear that methods analogous to those shown here can be applied also to fields other than mechanical, e.g. to electric and heat conduction, to dielectricity, magnetic phenomena and so on. Many questions are still open, in particular where mixed correlations occur. Almost nothing has been done with the *functional* theory of random elastic media.

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UNIVERSITY OF STUTTGART, STUTTGART, GERMANY.

Received September 8, 1997.

Arch. Mech., 50, 3, pp. 459–466, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

Some properties of connections on iterated tangent bundles

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

M. KUREŠ (BRNO)

POSSIBILITIES of a generalization of the original Grifone's approach to connections are studied. Semisprays associated to connections and torsions on the iterated tangent bundle TTM are described.

1. Introduction

MANY PAPERS dealing with the theory of connections, semisprays and mutual relations are motivated by mechanics, especially by Lagrangian dynamics. GRIFONE [5], gave a new definition of the connection on a manifold M as a certain special $(1,1)$-tensor field on TM. There is a semispray with the same paths associated with each such connection. The converse is also proved; with each semispray we can associate a connection and hence we are provided with connections attached to regular Lagrangians. DE ANDRÉS, DE LEÓN and RODRIGUES [2, 3], generalized Grifone's results to tangent bundles of higher order T^rM. The applicability of their construction in higher order mechanics is known.

We study the case of iterated tangent bundle TTM, especially the possibilities of a further generalization of Grifone's results. A nice discussion of the structure of the bundle TTM is presented in the monograph of ABRAHAM and MARSDEN [1], where it is also possible to find mechanical interpretations. Furthermore, we present torsions of connections on TTM defined by the Fröhlicher–Nijenhuis bracket of the associated horizontal projection and natural affinors on this bundle. The torsion is also a subject of interest for mathematical physics. It plays an important role in the Einstein–Cartan theory of gravitation, in modern development of field theories, etc. Our approach makes use of the theory of natural operations in differential geometry. The techniques of finding the natural objects are studied in the monograph of KOLÁŘ, MICHOR and SLOVÁK [7].

2. Natural affinors and natural vector fields

In general, by an *affinor* A on a manifold M we mean a (1,1)-tensor field, i.e. a linear morphism $A : TM \to TM$ over id_M. A *natural affinor* on a natural bundle F over m-dimensional manifolds is a system of (1,1)-tensor fields $A_M : TFM \to TFM$ for every m-dimensional manifold M satisfying $TFf \circ A_M = A_N \circ TFf$

for every local diffeomorphism $f : M \to N$. Analogously, a *natural vector field* on a natural bundle F over m-dimensional manifolds is a system of vector fields $\xi_M : FM \to TFM$ for every m-dimensional manifold M satisfying $TFf \circ \xi_M = \xi_N \circ TFf$ for every local diffeomorphism $f : M \to N$. The natural vector fields on F can be interpreted as the so-called absolute natural operators $C^\infty TM \to C^\infty TFM$ transforming vector fields on M into vector fields on FM. Now, let G be another natural bundle such that $\pi : FM \to GM$ is a fibered manifold (it is possible that $GM = M$). We denote by $V^\pi FM \subset TFM$ the vertical bundle with respect to the tangent projection $T\pi$. If A is an affinor such that $\operatorname{im} A \in V^\pi FM$ and $\operatorname{rank} A = \dim V^\pi FM$, then we call it the *$\pi$-affinor*. Analogously, if ξ is a vector field such that $\operatorname{im}\xi \in V^\pi FM$ and $\operatorname{rank}\operatorname{im}\xi = \dim V^\pi FM$, then we call it the *$\pi$-vector field*.

WEIL bundles, [13], which we can see as generalizations of bundles T^r_k of k-dimensional velocities of order r, play an important role in the theory of natural operations, cf. [5]. We call reader's attention to KOLÁŘ'S papers [6, 8], in which all natural affinors and all natural vector fields, respectively, on an arbitrary Weil bundle are described. In the case of TTM, we obtain these natural objects in a geometrical way here. Because the iterated tangent bundle is the Weil bundle, our results are included in Kolář's classifications for $F = TT$ and represent their geometrical interpretations.

We denote by $\pi^1 : TM \to M$ the tangent bundle of a smooth m-dimensional manifold M. The *(second) iterated tangent bundle* $TTM = T(TM)$ obtained by the additional application of the functor T disposes of the following bundle structures: $\pi^2 : TTM \to M$, $\pi^1_1 := \pi^1_{TM} : T(TM) \to (TM)$, ${}_1\pi^1 := T\pi^1_M : T(TM) \to T(M)$ (for more details see e.g. [14]). Given some local coordinates x^i on M, let us denote by x^i, y^i the induced coordinates on TM and by x^i, y^i, X^i, Y^i the induced coordinates on TTM. Then $\pi^2 : (x^i, y^i, X^i, Y^i) \mapsto (x^i)$, $\pi^1_1 : (x^i, y^i, X^i, Y^i) \mapsto (x^i, y^i)$, ${}_1\pi^1 : (x^i, y^i, X^i, Y^i) \mapsto (x^i, X^i)$.

Firstly, we shall construct canonical affinors on TTM. We have the following exact sequence of vector bundles over TTM:

$$0 \longrightarrow V^{\pi^2}TTM \xrightarrow{i} TTTM \xrightarrow{s} TM \times_M TTM \longrightarrow 0.$$

Because there exists the canonical isomorphism

$$h : \pi^{2*}TTM = TM \times_M TTM \longrightarrow V^{\pi^2}TTM,$$

the canonical affinor is defined $A^{\pi^2} = i \circ h \circ s$. Similarly, if we take the exact sequences of vector bundles

$$0 \longrightarrow V^{\pi^1_1}TTM \longrightarrow TTTM \longrightarrow TTM \times_{TM} TTM \longrightarrow 0,$$
$$0 \longrightarrow V^{{}_1\pi^1}TTM \longrightarrow TTTM \longrightarrow TTM \times_{TM} TTM \longrightarrow 0,$$

and isomorphisms

$$\pi_1^{1*}TTM = TTM \times_{TM} TTM \longrightarrow V^{\pi_1^1}TTM,$$
$$_1\pi^{1*}TTM = TTM \times_{TM} TTM \longrightarrow V^{_1\pi^1}TTM,$$

we obtain the canonical π_1^1-affinor $A^{\pi_1^1}$ and the canonical $_1\pi^1$-affinor $A^{_1\pi^1}$, respectively. Furthermore, let A_0 denote the identical affinor. All natural affinors on TTM constitute a 4-parameter family linearly generated by A_0, $A^{\pi_1^1}$, $A^{_1\pi^1}$, A^{π^2}.

Secondly, we shall construct canonical vector fields on TTM. For the projection π^2 let $\alpha := \pi_1^1 \times_M \mathrm{id}_{TTM}$, $\beta := {}_1\pi^1 \times_M \mathrm{id}_{TTM}$, be two canonical sections of the vector bundle $TM \times_M TTM$; the canonical vector fields are defined $\xi_1^{\pi^2} = i \circ h \circ \alpha$, $\xi_2^{\pi^2} = i \circ h \circ \beta$. Similarly, for the projection π_1^1 ($_1\pi^1$, respectively) we take the canonical section $\gamma := \mathrm{id}_{TTM} \times_{TM} \mathrm{id}_{TTM}$, and by the analogous composition we obtain the π_1^1-vector field $\xi^{\pi_1^1}$ ($_1\pi^1$-vector field $\xi^{_1\pi^1}$, respectively). All natural vector fields on TTM constitute a 4–parameter family linearly generated by $\xi^{\pi_1^1}$, $\xi^{_1\pi^1}$, $\xi_1^{\pi^2}$, $\xi_2^{\pi^2}$.

REMARK 1. The Weil algebra for TT is $D_2 = D \otimes D$ (D is the algebra of dual numbers) with generators 1, δ_1, δ_2 and with relations $\delta_1^2 = \delta_2^2 = 0$.

REMARK 2. It is easy to verify identities $A^{\pi_1^1} \circ A^{_1\pi^1} = A^{_1\pi^1} \circ A^{\pi_1^1} = A^{\pi^2}$, $A^{\pi_1^1} \circ \xi^{_1\pi^1} = \xi_1^{\pi^2}$, $A^{_1\pi^1} \circ \xi^{\pi_1^1} = \xi_2^{\pi^2}$, etc.

3. Grifone's connections

Trying to follow the original Grifone's procedure, we must put necessary general questions. A *Grifone's semiconnection* on an arbitrary fibered manifold $Y \to M$ means any $(1,1)$-tensor field $\widehat{\Gamma}$ on Y satisfying

$$J_A \widehat{\Gamma} = J_A\,,$$
$$\widehat{\Gamma} J_B = -J_B\,,$$

for any chosen natural affinors J_A, J_B on Y. A Grifone's semiconnection $\widehat{\Gamma}$ is said to be the *Grifone's connection*, if the $(1,1)$-tensor field $\widehat{\gamma} = \frac{1}{2}(\mathrm{id} + \widehat{\Gamma})$ corresponds to the horizontal lifting $\gamma : Y \times_M TM \to TY$ of the general connection Γ which is defined as a section $\Gamma : Y \to J^1Y$ of the first jet prolongation of $J^1Y \to Y$ of Y, see [12]. In this case J_A and J_B are called *A-affinor* and *B-affinor*, respectively. Let us study conditions of their existence.

PROPOSITION 1. An A-affinor exists on an arbitrary Weil bundle.

P r o o f. We denote by x^i the local coordinates on M, $i = 1, \ldots, m$, and by y^p, the fiber coordinates on Y, $p = 1, \ldots, n$, and $z = 1, \ldots, m, m+1, \ldots, m+n$.

The corresponding horizontal lifting of a general connection Γ has the coordinate form

$$dy^p = \Gamma_i^p dx^i.$$

By a direct application of the definition of the A-affinor we obtain the coordinate form of J_A as

$$A_j^i \frac{\partial}{\partial x^i} \otimes dx^j + A_i^p \frac{\partial}{\partial y^p} \otimes dx^i.$$

Moreover, the rank A_i^z must be maximal, i.e. it equals m. Really, if rank $A_i^z < m$, than there exists at least one zero column $A_{i_0}^z$ or it is possible to obtain it after linear transformations. But it means $dx^{i_0} = \Gamma_j^{i_0} dx^j + \Gamma_p^{i_0} dy^p$, where we can take $\Gamma_j^{i_0}$, $\Gamma_p^{i_0}$ arbitrarily.

Further, elements of Weil algebra are sums of monomials of the form

$$a_{p_1 \dots p_k} \delta_1^{p_1} \dots \delta_k^{p_k},$$

where a are real numbers and δ are generators. There exist so-called maximal monomials, i.e. non-zero monomials, which vanish after multiplication by an arbitrary δ_i. For any such maximal monomial

$$a_{\bar{p}_1 \dots \bar{p}_k} \delta_1^{\bar{p}_1} \dots \delta_k^{\bar{p}_k},$$

we put $a_{\bar{p}_1 \dots \bar{p}_k} = 1$ and all other numbers $a = 0$. Natural affinors correspond to the multiplication by the elements of Weil algebra. Multiplication by our special element provides an affinor satisfying conditions for the coordinate form and for the rank, too. □

PROPOSITION 2. *B-affinors are just natural π-affinors (with respect to the investigated projection π).*

P r o o f. As in the proof of the previous proposition, we make sure that the coordinate form of J_B is

$$B_i^p \frac{\partial}{\partial y^p} \otimes dx^i + B_q^p \frac{\partial}{\partial y^p} \otimes dy^q,$$

and rank B_z^p must be maximal, i.e. it equals n. □

REMARK 3. A-affinors and B-affinors also exist on T^*M, TT^*M, higher order cotangent bundles $T^{r*}M$ and higher order frame bundles P^rM, cf. [8, 4, 9, 10]. The A-affinor exists on TTM, it is the affinor A^{π^2}. But we immediately see, that B-affinor does not exist on TTM.

We can state that using of the definition of the general connection Γ as a section $\Gamma : Y \to J^1Y$ of the first jet prolongation of $J^1Y \to Y$ of Y, removes the problem of the incidental non-existence of Grifone's connection.

4. Connections and associated semisprays

We denote by Γ^π a connection with respect to the projection π. So, we have connections Γ^{π^2}, $\Gamma^{\pi^1_1}$, $\Gamma^{1\pi^1}$ on TTM. But we confine ourselves to connections with respect to the projection π^2 it this chapter, because the cases $TTM \to TM$ represent, roughly speaking, the case $TM \to M$ described by Grifone. We shall call *tensions* of Γ^{π^2} the $(1,1)$-tensor fields $H_1^{\pi^2}$, $H_2^{\pi^2}$ on TTM given by $H_1^{\pi^2} = [\xi^{1\pi^1}, \Gamma^{\pi^2}]$, $H_2^{\pi^2} = [\xi^{\pi^1_1}, \Gamma^{\pi^2}]$.

Vector fields $\sigma_1^{\pi^2}$, $\sigma_2^{\pi^2}$ on TTM are said to be *semisprays* if $A^{\pi^2} \circ \xi_1^{\pi^2} = \sigma_1^{\pi^2}$, $A^{\pi^2} \circ \xi_2^{\pi^2} = \sigma_2^{\pi^2}$, respectively. We shall call *deviation* of $\sigma_1^{\pi^2}$ ($\sigma_2^{\pi^2}$) the vector field $\sigma_1^{\pi^2 *}$ ($\sigma_2^{\pi^2 *}$) defined by $\sigma_1^{\pi^2 *} = [\xi^{1\pi^1}, \sigma_1^{\pi^2}] - \sigma_1^{\pi^2}$ ($\sigma_2^{\pi^2 *} = [\xi^{\pi^1_1}, \sigma_2^{\pi^2}] - \sigma_2^{\pi^2}$, respectively).

A $(1,l)$-tensor field L on TTM, with $l \geq 1$, is said to be *semibasic*, if

(1) $L(\xi_1, \ldots, \xi_l) \in V^{\pi^2} TTM$, for every vector fields $\xi_1, \ldots, \xi_l$ on TTM, and

(2) $L(\xi_1, \ldots, \xi_l) = 0$, if ξ_1 belongs to $V^{\pi^2} TTM$.

Let L be a semibasic $(1,l)$-tensor field. We call *potentials* of L the semibasic $(1, l-1)$-tensor fields L_1^0, L_2^0 given by $L_1^0 = \mathrm{i}_{\sigma_1^{\pi^2}} L$, $L_2^0 = \mathrm{i}_{\sigma_2^{\pi^2}} L$.

Let $\sigma_1^{\pi^2}$, $\sigma_2^{\pi^2}$ be arbitrary semisprays. We denote the horizontal projector of Γ^{π^2} by the same symbol. Let us consider the semisprays $\underline{\sigma_1}$, $\underline{\sigma_2}$ given by $\underline{\sigma_1} = \Gamma^{\pi^2} \circ \sigma_1^{\pi^2}$, $\underline{\sigma_2} = \Gamma^{\pi^2} \circ \sigma_2^{\pi^2}$, respectively. These semisprays are said the *first* and the *second associated semisprays* to Γ^{π^2}.

PROPOSITION 3. For any connection Γ^{π^2} on $TTM \to M$ and their associated semisprays $\underline{\sigma_1}$, $\underline{\sigma_2}$, the identities

$$\underline{\sigma_1}^* = (H_1^{\pi^2})_1^0,$$
$$\underline{\sigma_2}^* = (H_2^{\pi^2})_2^0,$$

are satisfied.

P r o o f. If

$$dy^i = F_j^i dx^j,$$
$$dX^i = G_j^i dx^j,$$
$$dY^i = H_j^i dx^j,$$

are the local equations of Γ^{π^2}, then a direct evaluation gives the following coordinate expression of $(H_1^{\pi^2})_1^0$:

$$dy^i = y^j y^k \frac{\partial F_k^i}{\partial y^j} + Y^j y^k \frac{\partial F_k^i}{\partial Y^j} - y^k F_k^i,$$

$$dX^i = y^j y^k \frac{\partial G^i_k}{\partial y^j} + Y^j y^k \frac{\partial G^i_k}{\partial Y^j},$$
$$dY^i = y^j y^k \frac{\partial H^i_k}{\partial y^j} + Y^j y^k \frac{\partial H^i_k}{\partial Y^j} - y^k H^i_k.$$

If we evaluate the deviation of the first associated semispray

$$\sigma_1^{\pi^2} \equiv y^i \otimes \frac{\partial}{\partial x^i} + F^i_j y^j \otimes \frac{\partial}{\partial y^i} + G^i_j y^j \otimes \frac{\partial}{\partial X^i} + H^i_j y^j \otimes \frac{\partial}{\partial Y^i},$$

we come directly to the same expression. The procedure is the same for the second associated semispray. Application of local coordinates is not necessary, see the proof of an analogous assertion for T^2M in [11]. □

A parametric curve $c : I \to M$ is called a *path* of a connection Γ, if $j^1(j^1c)$ is a horizontal curve in TTM. The connection Γ is said to be *homogeneous* if its tension vanishes. Paths of a homogeneous connection are called *geodesics.*

A *path* of a semispray σ is a parametric curve $c : I \to M$ such that $j^1(j^1c)$ is an integral curve of σ. A semispray σ is called *spray*, if σ has zero deviation. If σ is a spray then their paths are called *geodesics.*

PROPOSITION 4. The paths of a connection Γ are the same as the paths of the first and the second associated semisprays.

P r o o f. The paths of a connection Γ^{π^2} satisfy the system of ordinary differential equations

$$\frac{d^2x^i}{dt^2} = F^i_j \frac{dx^j}{dt},$$
$$\frac{d^2x^i}{dt^2} = G^i_j \frac{dx^j}{dt},$$
$$\frac{d^3x^i}{dt^3} = H^i_j \frac{dx^j}{dt}.$$

If we evaluate the paths of the first (of the second) associated semispray, we come to the same equations. □

5. Torsions

We recall that the Fröhlicher – Nijenhuis bracket $[\Gamma, A]$ of Γ and an arbitrary natural affinor is called the *(general) torsion* of Γ, see [8, 10]. The geometrical interpretation of such general torsions may be complicated and their applicability may be very questionable. That is why we study only *weak torsions* as a special case here: they represent brackets of a type $[\Gamma^\pi, A^\pi]$. Thus, we have three weak torsions on TTM: $t^{\pi^1_1} = [\Gamma^{\pi^1_1}, A^{\pi^1_1}]$, $t^{\imath\pi^1} = [\Gamma^{\imath\pi^1}, A^{\imath\pi^1}]$, $t^{\pi^2} = [\Gamma^{\pi^2}, A^{\pi^2}]$.

REMARK 4. We differ from original Grifone's notations of torsions purposely, because we prefer the definition from [8].

PROPOSITION 5. The weak torsion t^{π^2} has the coordinate expression

$$\frac{\partial F^i_k}{\partial Y^j} dx^j \wedge dx^k \otimes \frac{\partial}{\partial y^i} + \frac{\partial G^i_k}{\partial Y^j} dx^j \wedge dx^k \otimes \frac{\partial}{\partial X^i} + \frac{\partial H^i_k}{\partial Y^j} dx^j \wedge dx^k \otimes \frac{\partial}{\partial Y^i} .$$

Geometrically, we can characterize t^{π^2} by a bracket expression

$$t^{\pi^2}(\eta, \theta) = [\Gamma^{\pi^2} \eta, \pi^{2*} \theta] - [\Gamma^{\pi^2} \theta, \pi^{2*} \eta] - \pi^{2*}[\eta, \theta]$$

for every vector fields η, θ on M.

P r o o f. We obtained the formula by a direct evaluation of the Fröhlicher–Nijenhuis bracket in local coordinates. The idea of geometrization is from [8]. □

Because analogous calculations for $t^{\pi^1_1}$ and $t^{1^{\pi^1}}$ are equally technical, we do not go into details here.

The *strong torsion* of Γ is the $(1,1)$-tensor field T given by $H + t^0$, where H is the tension of Γ and t^0 is the potential of the weak torsion of Γ. So we obtain $T^{\pi^2}_1 = H^{\pi^2}_1 + (t^{\pi^2})^0_1$, $T^{\pi^2}_2 = H^{\pi^2}_2 + (t^{\pi^2})^0_2$ for Γ^{π^2}. Closing this paper, we view the coordinate expression of $T^{\pi^2}_1$

$$\left(y^j \left(\frac{\partial F^i_k}{\partial y^j} + \frac{\partial F^i_k}{\partial Y^j} - \frac{\partial F^i_j}{\partial Y^k} \right) + Y^j \frac{\partial F^i_k}{\partial Y^j} - F^i_k \right) dx^k \otimes \frac{\partial}{\partial y^i}$$

$$+ \left(y^j \left(\frac{\partial G^i_k}{\partial y^j} + \frac{\partial G^i_k}{\partial Y^j} - \frac{\partial G^i_j}{\partial Y^k} \right) + Y^j \frac{\partial G^i_k}{\partial Y^j} \right) dx^k \otimes \frac{\partial}{\partial X^i}$$

$$+ \left(y^j \left(\frac{\partial H^i_k}{\partial y^j} + \frac{\partial H^i_k}{\partial Y^j} - \frac{\partial H^i_j}{\partial Y^k} \right) + Y^j \frac{\partial H^i_k}{\partial Y^j} - H^i_k \right) dx^k \otimes \frac{\partial}{\partial Y^i}$$

as a show-piece, but we recall that some bundle projections provide to associate a connection to a given semispray and a strong torsion, and it is the way how to construct a connection having the generalized Euler–Lagrange vector field as an associated semispray, [3].

This contribution was presented at the 4th Meeting on Current Ideas in Mechanics and Related Fields. The author was supported by GA CR, grant No. 201/96/0079.

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DEPARTMENT OF MATHEMATICS,
TECHNICAL UNIVERSITY OF BRNO,
Technická 2, 616 69 Brno, Czech Republic
e-mail: kures@mat.fme.vutbr.cz

Received October 7, 1997.

Arch. Mech., 50, 3, pp. 467–482, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

Dynamics of quantum vortices in superfluid ^{4}He

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

T. LIPNIACKI (WARSZAWA)

THE DISSIPATIVE motion of quantized vortex line, after reconnection, is studied within the localized induction approximation. The numerical simulations of vortex line evolution help to determine the rate of the line-length changes. In the absence of counterflow, the vortex line shortens after each reconnection and line-length reduction is calculated as a function of friction parameter α and reconnection angle φ. The obtained results sugest that the decay of quantized vortex tangle is due to line-length reduction which occurs after each reconnection of vortex lines. In the presence of the counterflow, however, the reconnection may initiate a generation of a cascade of vortex loops. These loops blow up, so the total length of vortices grows up and the quantum turbulence can be generated.

1. Introduction

THE LANDAU'S two-fluid theory [1] is the basis of our understanding of the peculiar flow properties of ^{4}He below the λ-point. Acording to this theory, He II (superfluid ^{4}He) is a sum of the Bose condensate (superfluid component) and the gas of thermal excitation (normal component). The rotationless flow of the superfluid component is violated on one-dimensional singularities called quantum vortices (Fig. 1), (FEYNMAN [3], ONSAGER [2]). The circulation of the superfluid

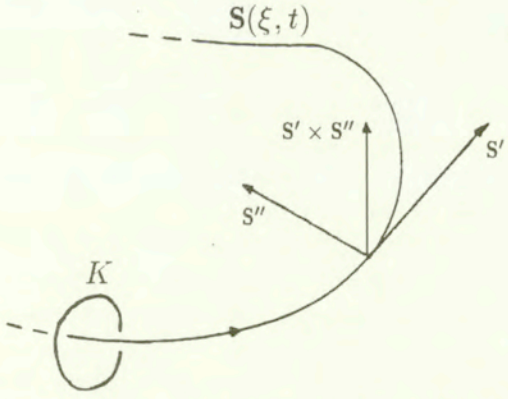

FIG. 1. Vortex line with a triad of vectors characterizing the instantaneous local configuration of the curve $s(\xi, t)$.

velocity about these lines remains constant, $\kappa = h/m_{\mathrm{He}} = 9.97 * 10^{-4}\mathrm{cm}^2/\mathrm{s}$, where h is Planck's constant, and m_{He} is the mass of helium atom. The curve traced out by a vortex filament may be specified in the parametric form $s(\xi, t)$ with t and ξ denoting time and arc length, respectively. Then the instantaneous velocity of a given point of the filament in the localized induction approximation is

$$\dot{s} = \beta s' \times s'' + V_s + \alpha s' \times (V_{ns} - \beta s' \times s'') - \alpha' s' \times [s' \times (V_{ns} - \beta s' \times s'')], \tag{1.1}$$

where prime denotes instantaneous derivative with respect to ξ, α and α' are temperature-dependent parameters which measure the frictional force exerted by the normal fluid on the vortex line. $V_{ns} = V_n - V_s$ is the difference between normal and superfluid velocities, and

$$\beta = \frac{\kappa}{4\pi} \ln\left(\frac{c}{a_0 \langle s'' \rangle}\right) \approx \kappa, \tag{1.2}$$

where κ is the quantum of circulation, c is a constant of order one, $\langle s'' \rangle$ is the average curvature of the vortices in the tangle and $a_0 \simeq 1.3 * 10^{-8}$ cm is the effective core radius of a quantized vortex. Although β has the logarithmic dependence on the tangle density since $\langle s'' \rangle$ increases as the tangle density increases, it is usually treated as a constant. The localized induction aproximation, which describes vortex motion in a much simpler way than the Biot–Savart law, is well justified when the local curvature is big enough that term $\beta s' \times s''$ is greater than the velocity induced by other vortices, or original vortex segments. Here we will base on the localized induction aproximation because of its numerical simplicity.

When the magnitude of relative velocity (counterflow) $V_{ns} = |V_n - V_s|$ becomes sufficiently large, superfluid laminar flow transforms into superfluid turbulent flow in which the quantum vortices form chaotic tangle.

The pioneerning studies of superfluid turbulence were conducted by VINEN [4], who proposed the mechanisms of vortex generation and decay. He observed that in the presence of the counterflow velocity V_{ns}, the vortex ring can blow up, and that line-line reconnections (predicted by Feynman) can give rise to new rings. Since then considerable progress has been made and the new methodology based on careful analysis of the motion of quantized vortices using extensive numerical simulation has been developed.

SCHWARZ simulated [6] the evolution of a vortex tangle basing on Eq. (1.1) describing vortex motion in the localized induction approximation, and on the assumption that vortex lines reconnect when they get close enough. Although the obtained results are in general agreement with observation, the problem is not yet sufficiently understood. The vortex tangle is characterized by its line-length density L and anisotropy coefficients. Knowing those coefficients, one can calculate the rate of vortex density growth or decay (Vinen equation). Schwarz has

found those quantities for various α (friction parameter) as the result of numerical simulations, and so has deduced the coefficients in the Vinen equation. It is still interesting to calculate the growth and decay rates in a "simpler" way – without time-consuming simulations of the whole vortex tangle.

The most important process which governs the vortex tangle evolution is the line-line reconnection (Fig. 2). Schwarz simulations confirm the observation that the density of vortex tangle depends dramatically on the assumed reconnection probability. To see why the reconnections play a crucial role in quantum turbulence, let us consider the simple evolution of a single circular vortex ring.

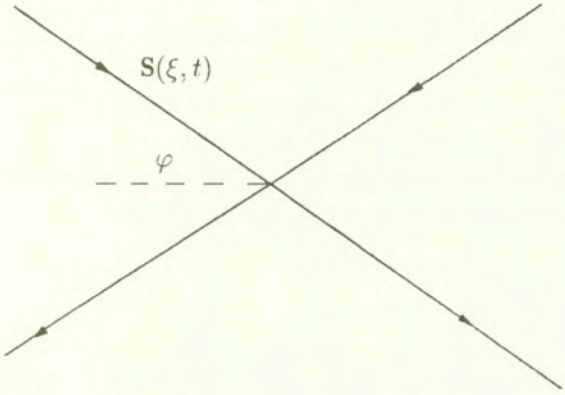

FIG. 2. Line-line reconnection configuration.

According to Eq. (1.1) we have:

$$\frac{dR}{dt} = -\frac{\alpha\beta}{R} + \alpha V_{ns}\cos\Theta\,, \tag{1.3}$$

$$\frac{d\Theta}{dt} = -\frac{\alpha V_{ns}}{R}\sin\Theta\,, \tag{1.4}$$

where R is the vortex ring radius and Θ is the angle between V_{ns} and normal to the surface containing the vortex ring. Dividing (1.3) by (1.4) and multiplying the resulting equation by $\sin\Theta$, one gets:

$$\frac{dR}{d\Theta}\sin\Theta = -R\cos\Theta + \frac{\beta}{V_{ns}}\,, \tag{1.5}$$

$$\frac{d(R\sin\Theta)}{d\Theta} = \frac{\beta}{V_{ns}}\,, \tag{1.6}$$

$$R = \frac{\beta\Theta + C}{V_{ns}\sin\Theta}\,. \tag{1.7}$$

The line $R = \beta\Theta/(V_{ns}\sin\Theta)$ in (Θ, R)-plane starting at the singular point ($R = \beta/V_{ns}$, $\Theta = 0$) separates the solutions in which R tends to infinity, from the

solutions in which R tends to zero. Namely, if

$$R > R_0(\Theta) = \frac{\beta\Theta}{V_{ns}\sin\Theta}, \tag{1.8}$$

the ring will blow up and die on the boundaries, and if $R < R_0(\Theta)$, the ring will contract to a point. The picture is not very different when instead of rings, one considers ovals. This simple example shows that to sustain turbulence, the reconnections are needed to produce new kinks which can develop into new loops (arc segments).

The aim of this paper is to consider the vortex evolution after an idealized reconnection, in the absence and in the presence of the counterflow V_{ns}. In the first case we calculate the line-length reduction resulting from a single reconnection as a function of friction coeficient α and reconnenction angle φ.

The analysis of Eq. (1.1) can be done in two steps (Schwarz). First, the factor β is absorbed into reduced time and velocity scales $\tau = \beta t$, $v = V/\beta$ to yield

$$\frac{\partial s}{\partial \tau} = s' \times s'' + v_s + \alpha s' \times (v_{ns} - s' \times s'') - \alpha' s' \times [s' \times (v_{ns} - s' \times s'')]. \tag{1.9}$$

Second, this equation is invariant under the transformation in which spatial dimensions are multiplied by a scale factor λ, time by λ^2, and velocities by λ^{-1}. If a vortex line evolution subject to the same particular velocities v_s, v_n is $s(\xi, \tau)$, then

$$s^\star(\lambda\xi, \lambda^2\tau) = \lambda s(\xi, \tau) \tag{1.10}$$

is the solution appropriate to the imposed velocities v_s/λ, v_n/λ. It means that, if all coordinates are magnified by a factor λ, and all applied velocities divided by λ, then the vortex motion will look the same, except that the time of the process increases by the factor of λ^2.

The instantaneous fractional rate of change of the line length at some particular point on a vortex is equal to $s' \cdot \dot{s}' = (s' \cdot v_s)' - \dot{s} \cdot s''$. Consequently, a given element of length $\Delta\xi$ obeys the law (SCHWARZ [6])

$$\frac{1}{\Delta\xi}\frac{\partial \Delta\xi}{\partial \tau} = \alpha[v_{ns} \cdot (s' \times s'') - |s' \times s''|^2] - \alpha' v_{ns} \cdot s'', \tag{1.11}$$

provided v_s is constant in space. As a result, line-length of vortex filament $l = \int d\xi$ satisfies the equation

$$\frac{\partial l}{\partial \tau} = \int [v_{ns} \cdot (\alpha s' \times s'' - \alpha' s'') - \alpha |s''|^2]\, d\xi. \tag{1.12}$$

2. Line evolution after reconnection

For the sake of simplicity we consider the reconnection problem of two infinite straight vortex filaments (Fig. 2). After reconnection two angles are formed. We analyse the evolution of a vortex line formed at the initial state ($\tau = 0$) angle 2φ. In fact the dynamical equation (1.1) can be used after a small time interval when the characteristic radius of curvature at the vortex vertex becomes larger than the radius of vortex core which is of the order 1–2 Å. To study the reconnection event on a macroscopic scale (1 Å) one has to use equations which model the vortex core (eg. Ginzburg–Landau) – but such a problem is far from being solved.

2.1. The case $V_{ns} = 0$

With $v_n = v_s = 0$ Eqs. (1.9), (1.12) simplyfy to

$$\frac{\partial s}{\partial \tau} = (1 - \alpha')\, s' \times s'' + \alpha s'', \tag{2.1}$$

$$\frac{\partial l}{\partial \tau} = \alpha \int |s''|^2 \, d\xi \,. \tag{2.2}$$

According to our previous considerations, Eq. (2.1) is invariant under the transformation (1.10). Since the initial conditions are also invariant under that transformation, the vortex configurations for times τ and $\lambda^2\tau$ will be similar, with similarity scale λ. In other words, the vortex line for all times will have a similar shape, whose spatial scale D is growing as $\sqrt{\tau}$. It leads to the result

$$\Delta l = A\,\tau^{1/2}, \qquad \int |s''|^2 \, d\xi = \frac{A}{2\alpha}\,\tau^{-1/2}, \tag{2.3}$$

where Δl is the line reduction and $A = A(\alpha, \alpha', \varphi)$.

The numerical simulations where performed for various angles φ, and for 5 sets of (α, α') $[(0.01, 0.005), (0.03, 0.0125), (0.1, 0.016), (0.3, 0.010), (1, -0.270)]$ corresponding to 5 different temperatures from 1.07 K° to 2.15 K°. (See also SCHWARZ [5], where line-line and line-boundary reconnections are considered.) Also the dependence of line-length reduction on parameter α' (with $\alpha = 1$) has been examined. The vortex line evolution for $\varphi = \pi/4$ and $\alpha = 0.1$ is shown in Fig. 3, the subsequent plots correspond to the vortex position at $\tau = \tau_0 i^2$ where τ_0 is arbitrary time constant and $i = 0, ..., 7$. Figure 4 shows the vortex shapes for $\varphi = \pi/6$ and two various α: 0.01 and 1. One can see that for smaller α the vortex line is more wavy.

The simulations revealed that for realistic values of $\alpha \leq 1$, $|\alpha'| < 1$, with surprising accuracy, (see Fig. 5)

Δl – does not depend of α' (to within the accuracy of 1%) (*)

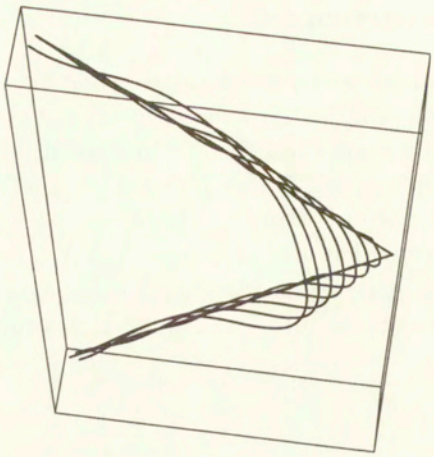

FIG. 3. Vortex line evolution after reconnection for reconnection angle $\varphi = \pi/4$, and friction coefficients $\alpha = 0.1$, $\alpha' = 0.016$. The line positions are shown at $\tau = i^2\tau_0$.

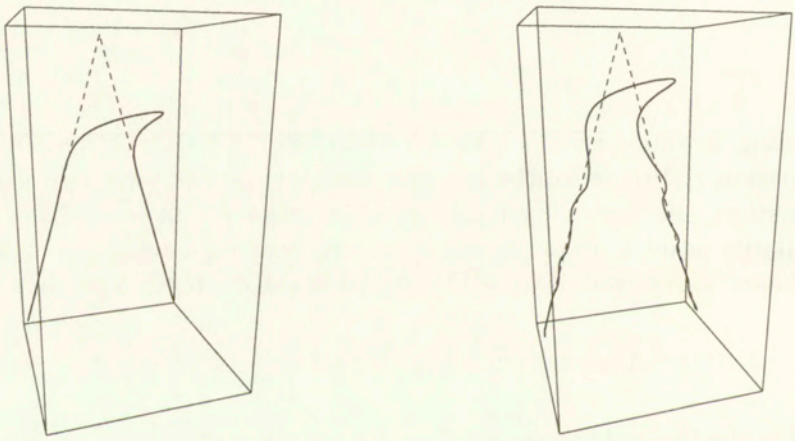

FIG. 4. The shape of vortex line for reconnection angle $\varphi = \pi/6$ and two various friction coefficients α; left – $\alpha = 1$, right – $\alpha = 0.01$. The smaller is α, the more wavy will be the vortex line.

and

$$A = B(\varphi)\,\alpha^{1/2}, \qquad \Delta l = B(\varphi)\,(\alpha\tau)^{1/2}. \tag{2.4}$$

The relations (2.4) are a simple consequence of observation (*); If line-length reduction does not depend on α' one can put $\alpha' = 1$, then the vortex evolution equation (2.1) simplifies to

$$\frac{\partial s}{\partial(\alpha\tau)} = s''. \tag{2.5}$$

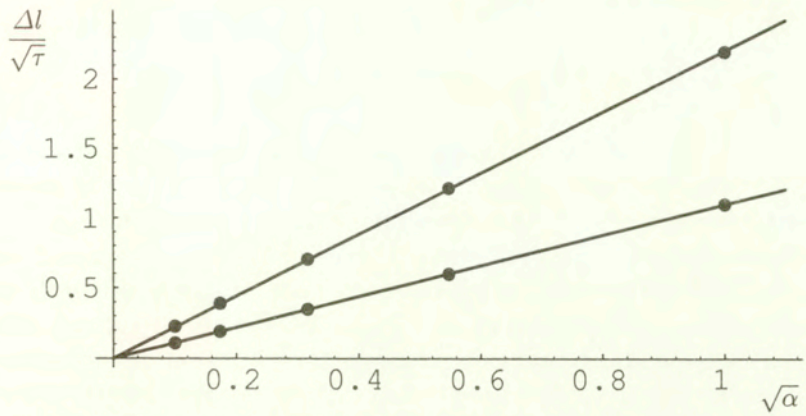

FIG. 5. $A = \Delta l/\sqrt{\tau}$ as a function of $\sqrt{\alpha}$ for two reconnection angles: $\varphi = \pi/6$ – upper line and $\varphi = \pi/4$ – lower line.

For such an evolution equation spatial dimension D and the line-length reduction Δl are proportional to $\sqrt{\alpha\tau}$.

The observation (*) and relation (2.4) can be justified as follows. Let us approximate the vortex line by the set of circular vortex segments. The line-length of the circular vortex satisfies the equation

$$\frac{\partial l}{\partial \tau} = \frac{2\pi\alpha}{R} \tag{2.6}$$

and is independent of α'. It suggests that the rate of line reduction of the whole vortex is approximately independent of α'. Moreover let us notice that for $\alpha = 0$, the vortex evolution equation (2.1) reduces to the nondissipative one,

$$\frac{\partial s}{\partial \tau} = (1 - \alpha')\, s' \times s''. \tag{2.7}$$

During the evolution governed by Eq. (2.7), the following quantities are constant in time:

$$l = \text{const}\,, \qquad \int |s''|^2 d\xi = \text{const}. \tag{2.8}$$

The first fact is the consequence of Eq. (1.8), and the second one can be proved as follows: from Eq. (2.7) one obtains

$$\dot{s}'' = s'' \times s''' + s' \times s'''' \,, \tag{2.9}$$

where the dot denotes now the instantaneous derivative with respect to $\tau^\star = (1 - \alpha')\,\tau$. Now

$$\frac{\partial}{\partial \tau^\star} \int |s''|^2 = 2 \int s'' \cdot \dot{s}'' = 2 \int s'' \cdot (s' \times s''''), \tag{2.10}$$

$$\int s'' \cdot (s' \times s'''') = \int s'' \cdot (s' \times s''')' = -\int s''' \cdot (s' \times s'''), \tag{2.11}$$

provided that

$$s'' \cdot (s' \times s''')\Big|_1^2 = 0. \tag{2.12}$$

Now, one can evaluate the vortex line step by step using the method of fractional steps. In the first half of time step we solve Eq. (2.7), in the second one we solve Eq. (2.5) using the previous result as an initial condition. The evolution governed by nondissipative Eq. (2.7) does not change the line length and does not change the squared curvature – which determine the rate of line-length changes (see Eq. (2.2)) during the evolution under Eq. (2.5). Roughly speaking, although the first term in Eq. (2.1) significantly changes the evolution of the vortex (line shape), it does not significantly influence the rate of the line-length reduction.

If we want to calculate only the length reduction, the simplified Eq. (2.5) can be used which is much simpler because the vortex line remains on a plane. Also numerically Eq. (2.5) is much more stable than Eq. (2.1), so the simulations can go faster.

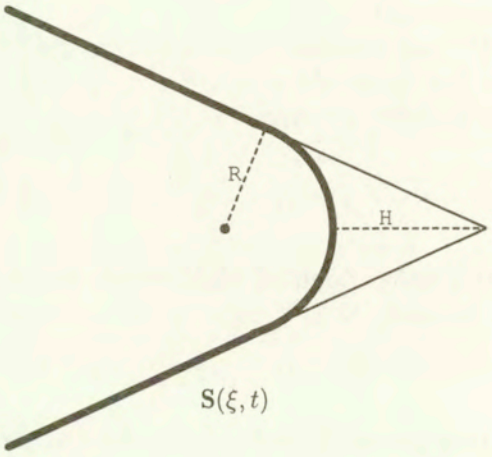

FIG. 6. The vortex line is approximated by the circle arc *plus* two semi-straight lines to calculate the rate of line reduction.

Therefore, function $B(\varphi)$, and the line-length reduction, can be estimated as follows; let us approximate the vortex line by the sum: a part of a circle tangent to the initial angle arms plus the rest of the angle (Fig. 6). As a result, we get a relation between the distance H and the radius of curvature R.

$$R = \frac{H \sin(\varphi)}{1 - \sin(\varphi)}, \tag{2.13}$$

and from Eq. (2.5)

$$\frac{\partial H}{\partial \tau} = \frac{\alpha}{R}. \tag{2.14}$$

After some algebra one gets

$$H(\tau) = \left[\frac{2\tau\alpha(1-\sin(\varphi))}{\sin(\varphi)}\right]^{1/2} \tag{2.15}$$

and

$$\Delta l = (\alpha\tau)^{1/2} B(\varphi), \tag{2.16}$$

with

$$B(\varphi) = \left[\frac{8\sin(\varphi)}{1-\sin(\varphi)}\right]^{1/2} \left(\mathrm{ctg}(\varphi) + \varphi - \frac{\pi}{2}\right). \tag{2.17}$$

Figure 7 compares the above relation with the numerical results obtained for Eq. (2.1).

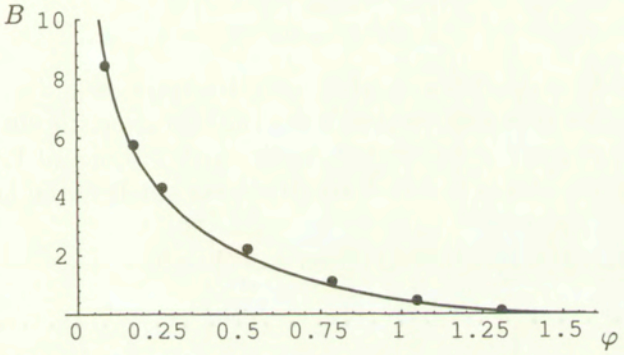

FIG. 7. Value of $B(\varphi)$ approximated by relation (2.17) (line) and calculated in numerical simulations (dots) (line reduction $\Delta l = B(\varphi)\sqrt{\alpha\tau}$).

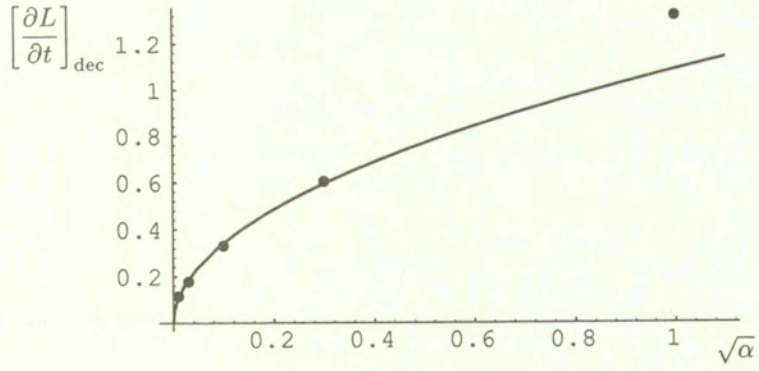

FIG. 8. α-dependence of the decaying term $[\partial L/\partial t]_{\mathrm{dec}}$ in Vinen equation (Schwarz simulation) – dots, and square root α dependence of line reduction after reconnection. The line is fitted to first four points, i.e. for $\alpha < 1$.

2.2. The case $V_{ns} = \text{const} \neq 0$

The absolute value of coefficient α' is smaller than α and unity, and the preliminary simulations show that the last term of Eq. (1.9) does not play any significant role in the vortex line evolution. In further analysis, for the sake of simplicity, we put $\alpha' = 0$.

In the superfluid reference frame with $v_{ns} = \text{const} \neq 0$, $\alpha' = 0$, Eq. (1.9) reads

$$\dot{s} = s' \times s'' + \alpha s'' + \alpha s' \times v_{ns} \,. \tag{2.18}$$

According to the scaling properties of the above equation for each configuration, the characteristic dimension D and also the line-length change Δl are given by some functions f, g.

$$D = \frac{\mathrm{f}(\tau * v_{ns}^2, \alpha, \varphi)}{v_{ns}} \,, \tag{2.19}$$

$$\Delta l = \frac{\mathrm{g}(\tau * v_{ns}^2, \alpha, \varphi)}{v_{ns}} \,. \tag{2.20}$$

The quantity $\tau * v_{ns}^2$ plays the role of an effective time.

Immediately after the reconnection, when the characteristic curvature is large, the vortex line evolution is dominated by the first 2 terms of Eq. (2.18). After some time, when the characteristic curvature gets smaller, the last term dominates the motion of a vortex.

We consider 6 characteristic configurations (Fig. 9).

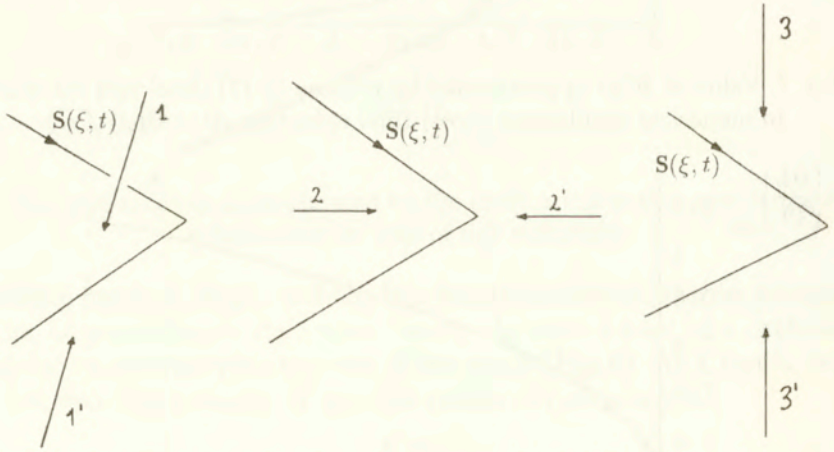

FIG. 9. Six characteristic configurations. Arrows show the direction of counterflow velocity for each configuration.

In the configuration 1 and 1′ the counterflow velocity is perpendicular to the initial vortex plane. In the first case, component $\alpha s' \times v_{ns}$ of the vortex velocity

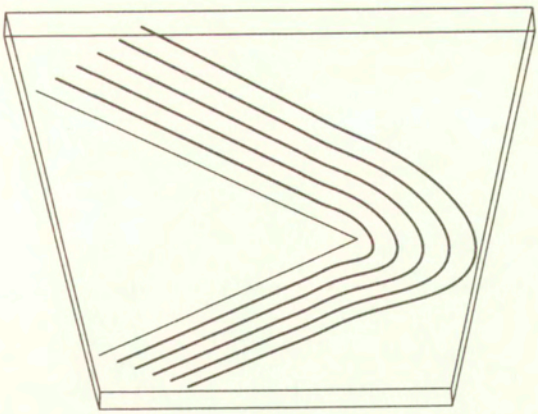

FIG. 10. The vortex evolution in configuration 1 (counterflow velocity perpendicular to the initial vortex plane).

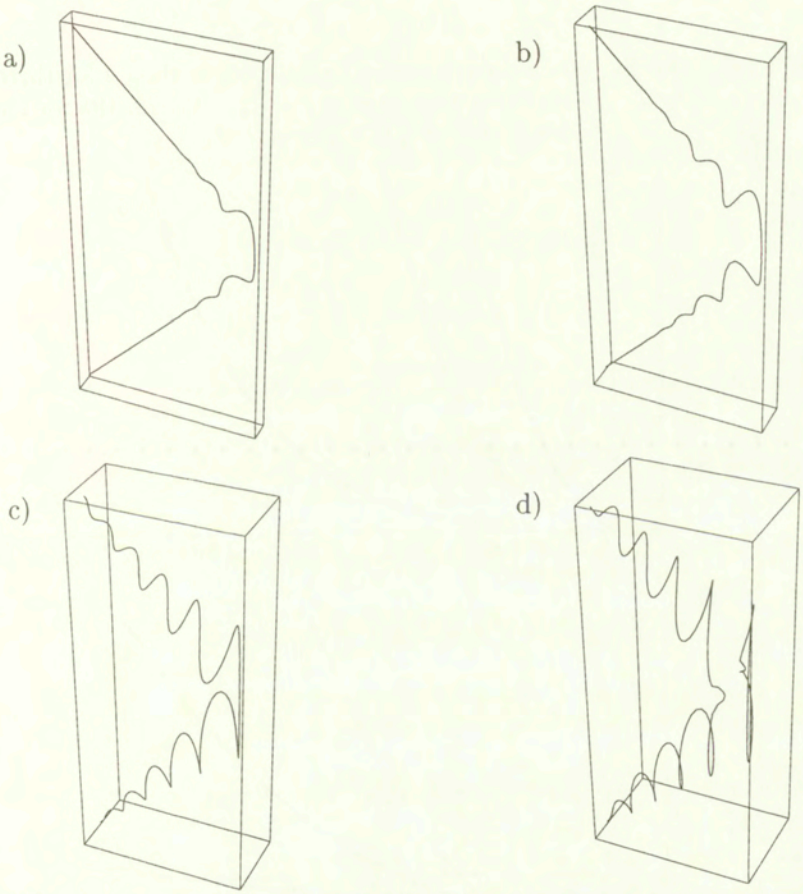

FIG. 11. The vortex evolution in configuration 2 for $\alpha = 0.3$, a) $\tau * v_{ns}^2 = 32$, b) $\tau * v_{ns}^2 = 64$, c) $\tau * v_{ns}^2 = 96$, d) $\tau * v_{ns}^2 = 128$. The separated vortex ring is seen at the bottom.

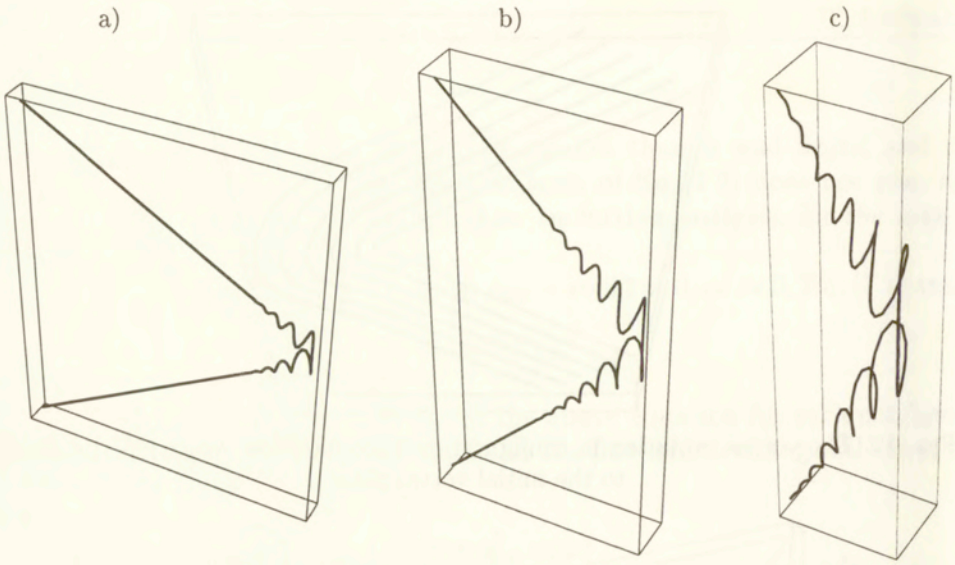

FIG. 12. The vortex line just before reconnection in configuration 2 for three different reconnection angles. The vortex ring separates at $\tau * v_{ns}^2 = 57, 79, 198$ for reconnection angles 30°, 45°, 60°, respectively.

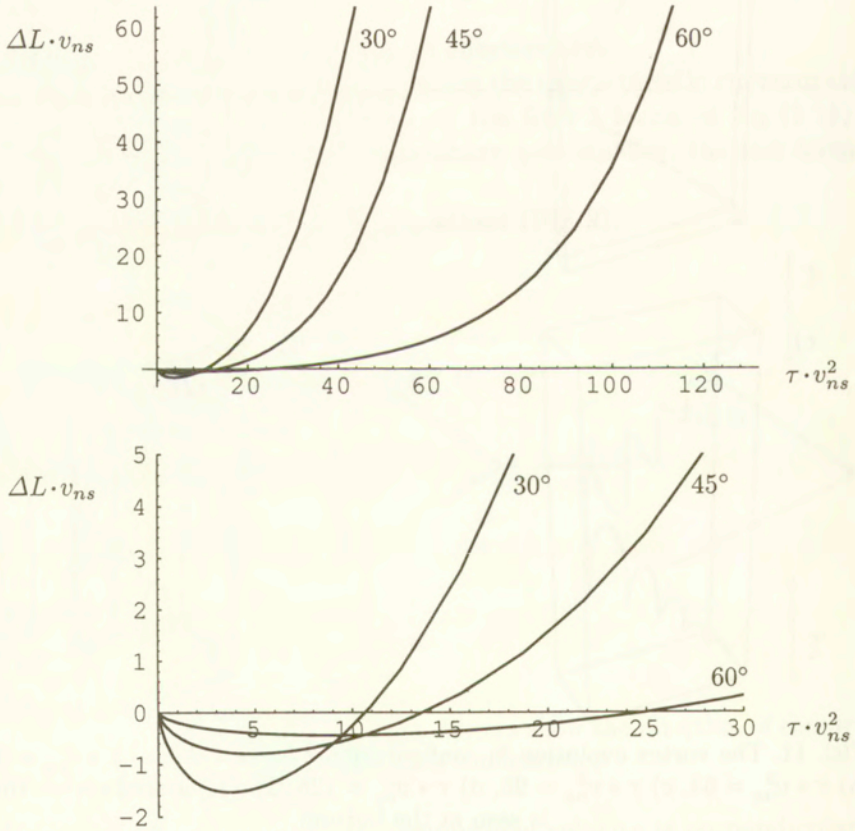

FIG. 13. Line-length changes in configuration 2 for 3 various reconnection angles 30°, 45°, 60°. Lower figure – the same functions for small $\tau * v_{ns}^2$.

is directed outwards and the vortex lengthens (Fig. 10), while in configuration $1'$ the vortex line shortens.

The vortex evolution in configurations $2, 2', 3, 3'$ is much more interesting. The magnitude of component $\alpha s' \times v_{ns}$ of the vortex velocity depends on the relative angle between the direction of the counterflow, and the local tangent to the vortex, and so it varies along the vortex line. As a result, some parts of the vortex line move faster than the others – this starts the vortex loop formation.

In the configurations 2 and $2'$ the counterflow velocity lies in the initial vortex plane and is parallel to the axis of symmetry. The self-induced velocity directs the vertex above the initial vortex plane. If the velocity component $\alpha s' \times v_{ns}$ is also (initially) directed above that plane (configuration 2), the loops form easily. After the loops are formed, the vortex reconnects with itself and vortex ring separates (Fig. 11). The time of ring separation increases with growing reconnnection angle φ (Fig. 12). Figure 13 illustrates the time dependence of total line length (with separated ring) of the vortex. Immediately after the reconnection, as we can

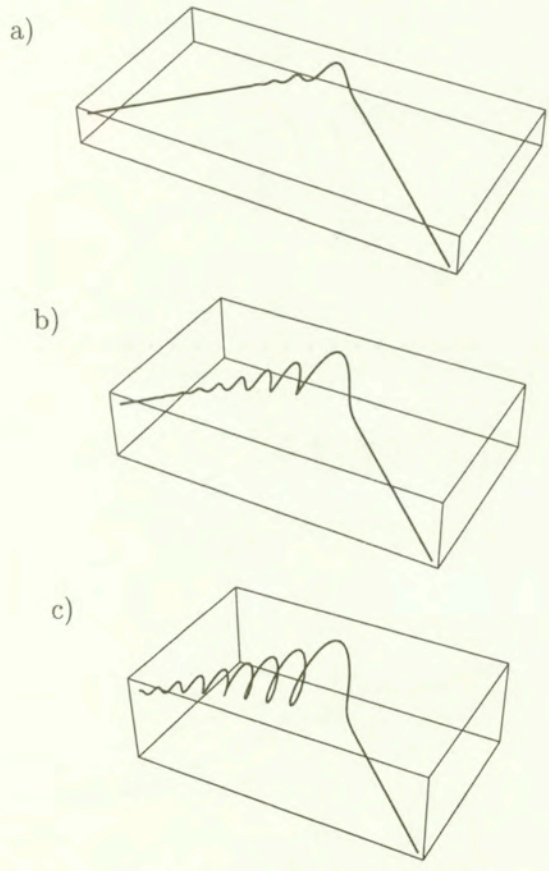

FIG. 14. The vortex evolution in configuration 3. $\alpha = 0.3$, a) $\tau * v_{ns}^2 = 50$, b) $\tau * v_{ns}^2 = 104$, c) $\tau * v_{ns}^2 = 144$.

expect from the previous section, the vortex line shortens (Fig. 13b), but for longer times the line-length increases. The smaller is the reconnection angle, the faster increases the line length (Fig. 13a).

The configurations 3 and $3'$ are symmetrical each to other. The instability propagates from the vertex of the filament onto one of angle arms on which loops are formed (Fig. 14). Even for reconnection angles φ close to $\pi/2$, the instability produces the cascade of loops (Fig. 15). For reconnection angles close to $\pi/2$, the loops lie (roughly speaking) on a cone with axis parallel to v_{ns}. The $\alpha s' \times v_{ns}$ velocity component directed outwards the cone increases the loops. Because of this mechanism, the lines parallel to counterflow velocity are very unstable, even a small kink on a line can initiate the cascade of loops. The line-length changes are growing with the growing reconnection angle up to the angle of roughly 60°, and then get smaller for larger angles (Fig. 16). The last result is due to the fact that for reconnection angles closer to $\pi/2$, longer time is needed to initiate the cascade of loops.

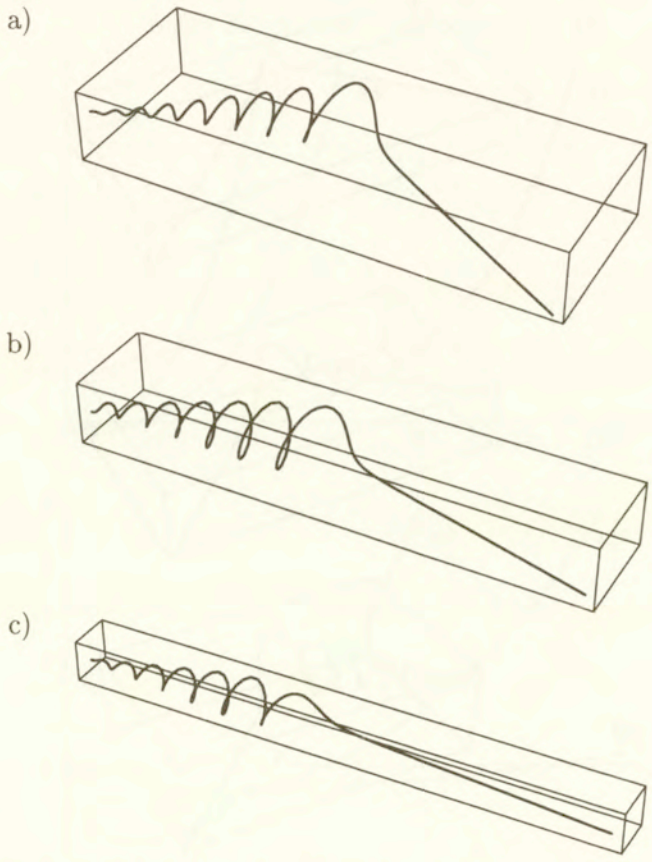

FIG. 15. Loops generation after reconnnection in configuration 3 for 3 different reconnection angles: a) $\varphi = 60°$, b) $\varphi = 75°$, c) $\varphi = 85°$ for $\alpha = 0.3$, $\tau * v_{ns}^2 = 81$.

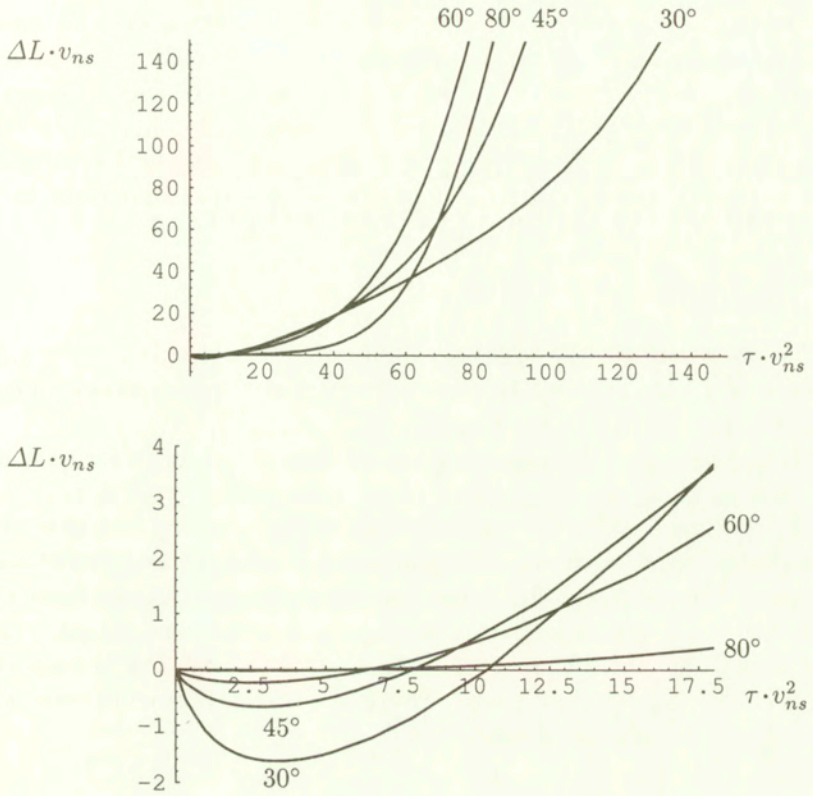

FIG. 16. Line-length changes in configuration 3 for 4 different reconnection angles: 30°, 45°, 60°, 80°. Lower figure – the same functions for small $\tau * v_{ns}^2$.

3. Conclusion

Equation (2.16), confirmed by numerical simulations, describing the line reduction $\Delta l(\alpha, \varphi, \tau)$ is the main result of the first part of the paper. Besides, we found that

$$\int |s''|^2 d\xi = \frac{B}{2\sqrt{\alpha\tau}}, \tag{3.1}$$

with B given by Eq. (2.17) with a resonable accuracy.

To interpret the main result of the first part, let us recall the Vinen equation with Schwarz coefficients

$$\frac{\partial L}{\partial \tau} = \alpha I_l V_{ns} L^{3/2} - \alpha c_2^2 L^2, \tag{3.2}$$

where is $I_l(\alpha)$ an anisotropy coefficient, and

$$c_2^2(\alpha) = \frac{\langle |s''|^2 \rangle}{L} \tag{3.3}$$

measures the average curvature of the vortex tangle. SCHWARZ [6] measured I_l and c_2^2 in numerical simulations performed for 5 various values of α. Now assume that the reconnection rate does not depend on α which seems to be resonable, at least for $\alpha \ll 1$, when vortex dynamics is dominated by the first term in Eq. (2.1). If so, the dependence of the line-length reduction on $\sqrt{\alpha}$ after reconnection should correspond to α dependence of the second term in Vinen equation describing decay of the vortex tangle. Namely

$$c_2^2 \alpha = C\sqrt{\alpha}. \tag{3.4}$$

The best fit (shown in Fig. 7) to four points (with $\alpha < 1$) gives $C = 1.1$. The good fit (for $\alpha < 1$) assures that the line reduction after reconnections plays the key role in decaying of the vortex tangle.

In the second part we have presented the mechanism of loops formation initiated by a reconnection, which probably plays an important role in rise of quantum turbulence when spacing beetwen vortices is relatively big. In a dense tangle, the reconnections occur so frequently that time of undisturbed evolution after each reconnection is too short for loops formation. As one can see from Figures 13 and 16, there is a characteristic time (t_0 for a given configuration and reconnection angle) for which the net growth is equal to zero. For the equlibrium density, the characteristic time spacing between vortex segments reconnection should correspond to average value of t_0.

Acknowledgments

This work was supported by the KBN grant 7T07A03412.

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POLISH ACADEMY OF SCIENCES
INSTITUTE OF FUNDAMENTAL TECHNOLOGICAL RESEARCH
e-mail: tlipnia@ippt.gov.pl

Received November 7, 1997.

Arch. Mech., 50, 3, pp. 483–495, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

On the general form of jump conditions for thin irregular shells

Dedicated to Prof. Henryk Zorski on the occasion of his 70-th birthday

J. MAKOWSKI (BOCHUM), W. PIETRASZKIEWICZ (GDAŃSK) and H. STUMPF (BOCHUM)

THE PAPER deals with the nonlinear theory of thin shell structures in the presence of irregularities in geometry, deformation, material properties and loading. The irregular shell is modelled by a reference network being a union of piecewise smooth surfaces and space curves, with various fields satisfying relaxed smoothness, differentiability, and regularity requirements. Transforming the virtual work principle postulated for the entire reference network, the corresponding local field equations and side conditions (boundary and jump conditions) are derived. It is shown that no more than four static and work-conjugate kinematic jump conditions can correctly be formulated whenever the shell deformation is assumed to be entirely determined by deformation of the reference network capable of resisting to stretching and bending. This assumption includes various special formulations of the Kirchhoff–Love type theory of elastic shells, as well as their substantial generalizations accounting for finite strains and inelastic deformations.

1. Introduction

THE NONLINEAR theory of thin shells is well developed for an idealized shell structure defined through a reference surface consisting of a single, smooth and regular surface element (see [1] and references given there).

Real shell structures usually contain folds, stiffeners, branches, self-intersections and additional design elements which make some fields non-smooth or discontinuous along specified curves on the reference surface. The shell deformation itself may not be smooth along some curves, and stiffeners, branching regions or technological connections may possess their own mechanical properties. All such problems of thin shells are referred to in this paper as irregular ones. In order to model and analyze such irregular shell problems it is not enough to formulate the local equilibrium equations, kinematic relations and boundary conditions supplemented by appropriate constitutive equations. In addition, we have to provide some jump conditions along the singular curves.

In an engineering approach to the problem [2–5] the irregular shell structure is first divided into regular parts, and each part is modelled separately by various known analytical or numerical methods. Then the regular parts are assembled

back into the whole shell structure by adjusting boundary conditions of the adjacent regular shell parts along the junction, with account of possibly different mechanical properties of the junction itself, if necessary. Such an approach replaces the problem of modelling and analysis of the whole irregular shell structure by another problem of an assemblage of its regular parts analyzed separately. In this alternative approach any particular assembling technique (which may depend upon the solution method applied) should be regarded as an additional mechanical postulate and can lead to different forms of the jump conditions. It is not apparent under which assumptions, or whether at all, both the problems are mechanically equivalent. Take the very popular finite element method as an example. Various shell finite elements can be used to model regular parts of the shell structure, and several techniques can be applied to assemble the regular parts modelled by the finite elements into the whole irregular shell structure. A critical review of various assembling techniques [6, 7] suggests that each of them is element-dependent and applicable to a limited class of shell problems.

The aim of this paper is to reveal the general structure of the jump conditions appropriate for the nonlinear theory of thin irregular shells. The irregular shell structure is modelled here by a material surface-like continuum, called a shell reference network, capable of resisting the stretching and bending. Such a model includes the classical Kirchhoff-Love type linear and geometrically nonlinear theories of thin elastic shells [1], finite strain theories of rubber-like shells [8, 9] and the theory of elastic-plastic shells undergoing finite strains [10]. The network is composed of piecewise smooth surfaces and space curves. Each space curve in the network may represent a singular surface curve, but also a one-dimensional continuum endowed with its own mechanical properties. Then the principle of virtual work is postulated in the entire reference network, with various fields in principle satisfying the relaxed smoothness, differentiability and regularity assumptions. The non-standard transformation of the principle leads to the local Lagrangian equilibrium equations and boundary conditions known from the theory of thin regular shells, [1]. Additionally, along the singular curves we obtain the general form of four jump conditions appropriate for the theory of thin irregular shells. The jump conditions do not depend on the solution methods or assembling techniques applied, and are valid for unrestricted displacements, rotations, strains and/or bendings of the reference network.

2. Basic postulates

A consistent formulation of field equations and side conditions (boundary and jump conditions) for thin irregular shell structures can be based on the following two postulates:

I. *The deformation of the entire thin irregular shell structure is determined, within a sufficient accuracy, by the deformation of a distinguished material surface-like continuum, called the shell reference network.*

II. *The equlibrium conditions of the entire thin irregular shell structure are determined, to within a sufficient accuracy, by the principle of virtual work for the network capable of resisting the stretching and bending.*

The first of these postulates is kinematic in nature and can be regarded as definition of the thin irregular shell structure. The second one should be regarded as the basic dynamic postulate of the theory. Both postulates are independent of specific constitutive equations needed to model particular classes of materials.

Let us denote by M an undeformed configuration of the reference network referred to in the Postulate I. Then, formally, the principle of virtual work for the irregular shell structure modelled by M can be written in the form

$$\mathcal{G} \equiv \mathcal{G}_{\text{int}} - \mathcal{G}_{\text{ext}} - \mathcal{G}_{\Gamma} = 0, \tag{2.1}$$

where $\mathcal{G}_{\text{int}}$ stands for the internal virtual work, $\mathcal{G}_{\text{ext}}$ denotes the external virtual work, while the term $\mathcal{G}_{\Gamma}$ has been included in (2.1) to account for an additional virtual work due to generalized forces and moments at the shell junctions, multiple-shell intersections and other singular curves denoted jointly by Γ.

Within the classical theory of smooth shells, the undeformed configuration $M \subset \mathcal{E}$ ($\mathcal{E}$ denotes the three-dimensional Euclidean point space, i.e. the physical space, and E denotes its translation space) of the shell reference surface is assumed to be a connected and oriented regular surface of class C^2 or higher, with a piecewise smooth boundary ∂M. A typical point of M is then identified by the position vector relative to the origin of a fixed Cartesian coordinate system in the space. For simplicity, we shall use the same symbol $\mathbf{Y}$ for points on M and their position vectors. A deformation of M is described by a map $\boldsymbol{\chi} : M \to \mathcal{E}$, which carries each surface point $\mathbf{Y} \in M$ into its spatial place

$$\mathbf{y} = \boldsymbol{\chi}(\mathbf{Y}) = \mathbf{Y} + \mathbf{u}(\mathbf{Y}) \tag{2.2}$$

in the deformed configuration $m = \boldsymbol{\chi}(M)$ of M, where the spatial vector field $\mathbf{u} : M \to E$ denotes the associated displacement field. In the classical theory of thin smooth shells one also assumes that the deformation map $\boldsymbol{\chi}$ is globally invertible (on the codomain $m = \boldsymbol{\chi}(M)$), is of class C^2 or higher and admits the extension of the same class to the boundary ∂M. Thus, the surface deformation gradient $\mathbf{F} = \mathbf{P}\,\text{Grad}_s\boldsymbol{\chi}$, where $\mathbf{P}$ is a perpendicular projection [11] on the tangent plane $T_{\mathbf{y}}m$, is well defined at each point of M including the boundary, is continuous at all interior points of M and has continuous extensions to the boundary.

In this paper all concepts, including surface differential operators relevant to the smooth surfaces, are understood in the sense defined in [11, 12]. Additionally, we assume that M can be described locally in the parametric form $\mathbf{Y} = \mathbf{Y}(\xi^{\beta})$, where $(\xi^{\beta}, \beta = 1, 2)$ are surface coordinates chosen in any convenient way. Then the natural base vectors $\mathbf{A}_{\alpha}$ and the unit normal vector $\mathbf{A}_n$ at each interior point $\mathbf{Y} \in \text{int}\,M$, the metric tensor $\mathbf{A}$ and the curvature tensor $\mathbf{B}$ are defined in the usual manner [1].

The regularity assumptions stated above for the smooth surface M are too restrictive if various geometric, material and kinematic irregularities are to be admitted. These regularity assumptions may be relaxed in many ways. For a wide class of shell structures it can be assumed that the undeformed reference surface M is only piecewise smooth of a suitable class (the relevant mathematical definition can be found in [13]). Parallelly, we may also admit the deformation $\chi : M \to \mathcal{E}$ of the reference surface to be only piecewise smooth of a corresponding class. Therefore, the theory of irregular shells developed here relies on concepts of piecewise smooth surfaces (and some generalizations thereof) and of piecewise smooth surface fields largely based on our paper [12].

3. Geometry and deformation

Various irregularities encountered in the analysis of irregular shell problems can be grouped into three broad classes, [12]: 1. The undeformed configuration of the shell reference surface is not smooth (thus it may contain folds) or it is not a surface in the classical sense (for example, two smooth intersecting surfaces do not form a surface as the whole). Such irregularities may be called geometric. 2. Deformation of the shell reference surface (smooth or not in the undeformed configuration) fails to be smooth. We may refer to this kind of irregularities as kinematic, since they are associated with the deformation. 3. The shell structure cannot be considered as a single shell (smooth or non-smooth and undergoing smooth or non-smooth deformation) but rather as a union of some number of single shells interconnected along junctions. This type of irregularities may be called mechanical, because the junctions may have their own mechanical properties possibly quite different from the properties of the adjacent shells. The basic assumption made in the three cases is that all irregularities are restricted to distinct curves and points (i.e. to sets of zero area measure) on the shell reference surface-like continuum. Under this assumption, all the three classes of irregularities can be considered at once as follows.

In the most general case, the undeformed configuration of the reference surface-like continuum can be defined to be a network $M \subset \mathcal{E}$ consisting of a finite number of surface elements $M^{(k)}$, $k = 1, 2, ..., K$, with the following properties:

1. Each $M^{(k)}$ is a bounded, oriented, connected and smooth surface of class C^n, $n \geq 2$, whose boundary $\partial M^{(k)}$ consists of a finite number of closed Jordan curves oriented consistently with $M^{(k)}$ that do not meet in cusps.

2. No two distinct surface elements $M^{(k)}$ have common interior points.

3. Two or more distinct surface elements $M^{(k)}$ may have a spatial curve $\Gamma^{(a)}$ as a common part of the boundaries. Such a curve is defined by

$$\Gamma^{(a)} = \partial M^{(k_1)} \cap \partial M^{(k_2)} \cap \ldots \cap \partial M^{(k_m)} \quad \text{if} \quad k_1 \neq k_2 \neq \ldots k_m . \tag{3.1}$$

4. Two or more distinct curves $\Gamma^{(a)}$ may have in common only single isolated points.

We then define the network M as the union of all closed surface elements $\overline{M}^{(k)} = M^{(k)} \cup \partial M^{(k)}$, and by Γ we denote the union of all curves $\Gamma^{(a)}$. It is clear that $\Gamma \subset M$. Moreover, the boundary ∂M of M, defined now by

$$\partial M = \left(\bigcup_{k=1}^{K} \partial M^{(k)} \right) \setminus \Gamma, \tag{3.2}$$

consists of a finite number of Jordan curves (not necessarily closed).

Each $M^{(k)}$ can be regarded as the reference surface of a regular shell part. Each $\Gamma^{(a)}$ can be regarded as representing a geometric surface curve (e.g. a fold or a curve in M across which some fields fail to be smooth), but also a reference axis of one-dimensional continuum (e.g. an axis of a rod-like element) representing a multiple shell intersection, a technological junction, etc., whenever they are assumed to have mechanical properties of their own. In the former case we call $\Gamma^{(a)}$ a geometric singular curve, and in the latter case – a physical singular curve. Because geometric curves are just a special case of physical curves, no distinction will be made in the general considerations and the two cases will be considered at the same time. The geometry of each smooth surface element $M^{(k)}$ and its boundary $\partial M^{(k)}$, hence the geometry of the curves $\Gamma^{(a)}$, can now be described by the methods of classical differential geometry.

In general, any deformation of the reference network M is described by two maps $\chi : M \setminus \Gamma \to \mathcal{E}$ and $\chi_\Gamma : \Gamma \to \mathcal{E}$, since the singular curve Γ may be admitted to follow its own deformation. We shall assume that the deformation χ is a continuous function over each smooth surface element $M^{(k)}$ and differentiable of class C^2 in the interior of $M^{(k)}$ (in the relative topology). Under these assumptions the surface gradient $\mathbf{F}$ exists at every point $\mathbf{Y} \in \operatorname{int} M^{(k)}$. However, we shall not assume *a priori* that the deformation χ is continuous across the singular curve Γ or some parts thereof. Accordingly, we regard χ as being defined for all points of M except possibly for points belonging to Γ. We shall then assume that the deformation map χ has a finite limit at every point $\mathbf{Y} \in \Gamma$,

$$\mathbf{y}^{(k)} = \chi^{(k)}(\mathbf{Y}) = \lim_{\mathbf{Z} \to \mathbf{Y}} \chi(\mathbf{Z}) = \mathbf{Y} + \lim_{\mathbf{Z} \to \mathbf{Y}} \mathbf{u}(\mathbf{Z}), \qquad \mathbf{Z} \in M^{(k)}, \tag{3.3}$$

whenever Γ is a part of the boundary $\partial M^{(k)}$. However, in many cases the function χ may be defined on an entire M and the deformation χ_Γ is then the restriction of χ to Γ, i.e. $\chi_\Gamma = \chi_{|\Gamma}$.

4. Virtual work expressions

Within a formal (axiomatic) approach, the internal virtual work $\mathcal{G}_{\text{int}}$ is assumed to be a real-valued, additive set function over measurable subsets of the reference network and an absolutely continuous function with respect to the area

measure (line and area measures are understood in the sense of Hausdorff measure). Under these assumptions the internal virtual work $\mathcal{G}_{\text{int}}$ can be written as the sum of virtual work expressions over all mutually disjoint smooth surface elements $M^{(k)}$:

$$\mathcal{G}_{\text{int}} = \sum_k \mathcal{G}_{\text{int}}^{(k)} = \sum_k \iint_{M^{(k)}} W_i \, dA \,, \tag{4.1}$$

where W_i denotes the internal virtual work density per unit area of the undeformed reference network M.

Similarly, the external virtual work $\mathcal{G}_{\text{ext}}$ can naturally be written as the sum of two parts, which account for the virtual work of the external surface forces and moments and the virtual work of the external boundary forces and moments, respectively:

$$\mathcal{G}_{\text{ext}} = \sum_k \iint_{M^{(k)}} W_e \, dA \,, + \int_{\partial M_f} w_e \, dS. \tag{4.2}$$

Here W_e denotes the virtual work density of external surface forces and moments measured per unit area of the undeformed reference network M, while w_e denotes the virtual work density of external forces and moments applied to a part ∂M_f of the boundary ∂M.

Consistently with the postulate (I), each regular part of the undeformed irregular shell structure is modelled by a smooth surface element $M^{(k)}$, the deformed configuration of which $m^{(k)} = \boldsymbol{\chi}(M^{(k)})$ is determined by the position vector $\mathbf{y} = \boldsymbol{\chi}(\mathbf{Y})$ and the field $\mathbf{n}(\boldsymbol{\chi}(\mathbf{Y}))$ of unit normal vectors specifying its orientation. Moreover, by virtue of the classical theorem of differential geometry, two symmetric surface tensors [1, 8–10]

$$\begin{aligned} \boldsymbol{\Gamma} &= \frac{1}{2}\left(\mathbf{F}^T\mathbf{a}\,\mathbf{F} - \mathbf{A}\right) = \Gamma_{\alpha\beta}\mathbf{A}^\alpha \otimes \mathbf{A}^\beta, \qquad \Gamma_{\alpha\beta} = \frac{1}{2}(a_{\alpha\beta} - A_{\alpha\beta}), \\ \mathbf{K} &= -\left(\mathbf{F}^T\mathbf{b}\,\mathbf{F} - \mathbf{B}\right) = K_{\alpha\beta}\mathbf{A}^\alpha \otimes \mathbf{A}^\beta, \qquad K_{\alpha\beta} = -(b_{\alpha\beta} - B_{\alpha\beta}) \end{aligned} \tag{4.3}$$

provide the Green-type measures of the local strains (stretching and bending) of the reference surface element $M^{(k)}$. Here $\mathbf{a}$ and $\mathbf{b}$ denote the metric and curvature tensors of the deformed surface element $m^{(k)}$, respectively.

When dealing with virtual deformations of the shell reference network, we may consider a one-parameter family of deformations $\mathbf{y} = \boldsymbol{\chi}(\mathbf{Y}, t)$, where t is a scalar (time-like) parameter. We then denote by $\mathbf{v} \equiv \dot{\mathbf{y}} = \dot{\mathbf{u}}$ and $\mathbf{w} \equiv \dot{\mathbf{n}}$ the virtual displacement of the reference surface and the virtual change of the unit normal, respectively. The virtual changes of the local strain measures (4.3) are $\dot{\boldsymbol{\Gamma}} = \dot{\Gamma}_{\alpha\beta}\mathbf{A}^\alpha \otimes \mathbf{A}^\beta$ and $\dot{\mathbf{K}} = \dot{K}_{\alpha\beta}\mathbf{A}^\alpha \otimes \mathbf{A}^\beta$. It is now obvious that the simplest expression for the internal virtual work density W_i must be of the form

$$W_i = \mathbf{N}\cdot\dot{\boldsymbol{\Gamma}} + \mathbf{M}\cdot\dot{\mathbf{K}} = N^{\alpha\beta}\dot{\Gamma}_{\alpha\beta} + M^{\alpha\beta}\dot{K}_{\alpha\beta}\,, \tag{4.4}$$

where $\mathbf{N} = N^{\alpha\beta}\mathbf{A}_\alpha \otimes \mathbf{A}_\beta$ and $\mathbf{M} = M^{\alpha\beta}\mathbf{A} \otimes \mathbf{A}_\beta$ are the symmetric stress resultant and couple surface tensors of the 2-nd Piola–Kirchhoff type.

The virtual work density of the external surface and boundary loads can be represented by invariant expressions as in the classical theories of thin smooth Kirchhoff–Love type shells [1]:

$$W_e = \mathbf{p}\cdot\mathbf{v} + \mathbf{h}\cdot\mathbf{w}\,, \qquad w_e = \mathbf{T}^*\cdot\mathbf{v} + \mathbf{H}^*\cdot\mathbf{w}\,. \tag{4.5}$$

Here $\mathbf{p}$ and $\mathbf{h}$ are the external surface force and moment resultant vectors referred to the undeformed surface element $M^{(k)}$, while $\mathbf{T}^*$ and $\mathbf{H}^*$ are the external boundary force and moment resultants referred to the undeformed boundary ∂M_f.

5. Equilibrium equations and boundary conditions

Derivation of the local equilibrium equations and boundary conditions for thin regular shells may be found in many papers (see e.g. [1, 8–10]). The same procedure, under suitable regularity assumptions, can essentially be applied to each smooth surface element $M^{(k)}$. Accordingly, we present below only the main steps of this derivation.

The virtual strains can be obtained by varying the components of the strain tensors (4.3). At each internal point of $M^{(k)}$, the field of unit normal vectors $\mathbf{n}$ can be expressed in terms of first derivatives of the displacement field, $\mathbf{n} = \mathbf{n}(\mathbf{u}_{,\beta})$, since it must satisfy the three geometric constraints, $\mathbf{a}_\beta\cdot\mathbf{n} = 0$ and $\mathbf{n}\cdot\mathbf{n} = 1$, where $\mathbf{a}_\beta$ are the natural base vectors of $m^{(k)} = \boldsymbol{\chi}(M^{(k)})$. Variations of these constraints lead to $\mathbf{w} = -(\mathbf{n}\cdot\mathbf{v}_{,\beta})\mathbf{a}^\beta$. Then, it is not difficult to show that the internal virtual work density (4.4) can be written in the form [1]

$$W_i = \mathbf{T}^\beta\cdot\mathbf{v}_{,\beta} + (\mathbf{H}^\beta\cdot\mathbf{w})_{|\beta}\,, \tag{5.1}$$

where the generalized stress resultants $\mathbf{T}^\beta$ and couple resultants $\mathbf{H}^\beta$ are defined by

$$\mathbf{T}^\beta = N^{\alpha\beta}\mathbf{a}_\alpha + M^{\alpha\beta}\mathbf{n}_{,\alpha} + \left[(M^{\lambda\alpha}\mathbf{a}_\lambda)_{|\alpha}\cdot\mathbf{a}^\beta\right]\mathbf{n}, \qquad \mathbf{H}^\beta = M^{\alpha\beta}\mathbf{a}_\alpha\,. \tag{5.2}$$

Here $(\cdot)_{|\alpha}$ denotes covariant differentiation in the undeformed metric $A_{\alpha\beta}$.

The tensors $\mathbf{T} = \mathbf{T}^\beta \otimes \mathbf{A}_\beta$ and $\mathbf{H} = \mathbf{H}^\beta \otimes \mathbf{A}_\beta$ are assumed to be of class C^1 in the interior of each smooth surface element $M^{(k)}$ and to have extensions of the same class to the boundary $\partial M^{(k)}$, with finite limits $\mathbf{T}^{(k)}(\mathbf{Y})$ and $\mathbf{H}^{(k)}(\mathbf{Y})$ at each point $\mathbf{Y} \in \partial M^{(k)}$. Then the surface divergence theorem can be applied on each smooth surface element $M^{(k)}$ to give

$$\iint\limits_{M^{(k)}} W_i\, dA = -\iint\limits_{M^{(k)}} (\mathrm{Div}_s\mathbf{T})\cdot\mathbf{v}\, dA + \int\limits_{\partial M^{(k)}} \left(\mathbf{T}_\nu^{(k)}\cdot\mathbf{v}^{(k)} + \mathbf{H}_\nu^{(k)}\cdot\mathbf{w}^{(k)}\right) dS, \tag{5.3}$$

where $\mathrm{Div}_s \mathbf{T} = \mathbf{T}^{\beta}{}_{|\beta}$ at every interior point of $M^{(k)}$, $\mathbf{T}_{\nu}^{(k)} \equiv \mathbf{T}^{(k)}\boldsymbol{\nu}^{(k)}$ and $\mathbf{H}_{\nu}^{(k)} \equiv \mathbf{H}^{(k)}\boldsymbol{\nu}^{(k)}$ at the boundary point $\mathbf{Y} \in \partial M^{(k)}$, with $\boldsymbol{\nu}^{(k)}$ denoting the unit outward normal vector along $\partial M^{(k)}$.

In the same manner, the external surface virtual work density $(4.5)_1$ can be rewritten in the form

$$W_e = \mathbf{l}\cdot\mathbf{v} - [(\mathbf{h}\cdot\mathbf{a}^{\beta})\mathbf{n}\cdot\mathbf{v}]_{|\beta}, \qquad \mathbf{l} \equiv \mathbf{p} + [(\mathbf{h}\cdot\mathbf{a}^{\beta})\mathbf{n}]_{|\beta} \tag{5.4}$$

and

$$\iint_{M^{(k)}} (\mathbf{p}\cdot\mathbf{v} + \mathbf{h}\cdot\mathbf{w})\,dA = \iint_{M^{(k)}} \mathbf{l}\cdot\mathbf{v}\,dA - \int_{\partial M^{(k)}} \left((\mathbf{h}^{(k)}\cdot\boldsymbol{\mu}^{(k)})\mathbf{n}^{(k)}\cdot\mathbf{v}^{(k)}\right) dS, \tag{5.5}$$

where $\boldsymbol{\mu} = \mathbf{a}^{\beta}\nu_{\beta}$.

Along the boundary $\partial M^{(k)}$ of each smooth surface element $M^{(k)}$, the surface gradient $\mathrm{Grad}_s \mathbf{u}$ of the displacement field can be decomposed into tangential and normal derivatives (under the assumption that $\mathrm{Grad}_s \mathbf{u}$ admits a continuous extension to the boundary $\partial M^{(k)}$):

$$\begin{gathered} \mathrm{Grad}_s \mathbf{u} = \mathbf{u}_{,\nu} \otimes \boldsymbol{\nu} + \mathbf{u}' \otimes \boldsymbol{\tau}, \\ \mathbf{u}_{,\nu} \equiv (\mathrm{Grad}_s \mathbf{u})\boldsymbol{\nu} = \mathbf{u}_{,\beta}\nu^{\beta}, \qquad \mathbf{u}' \equiv (\mathrm{Grad}_s \mathbf{u})\boldsymbol{\tau} = \mathbf{u}_{,\beta}\tau^{\beta}, \end{gathered} \tag{5.6}$$

where $\boldsymbol{\tau}$ is the unit tangent vector of $\partial M^{(k)}$. From (5.6) it follows that the field of unit normal vectors $\mathbf{n}$ along $\partial m^{(k)} = \boldsymbol{\chi}(\partial M^{(k)})$ can be regarded as a function of $\mathbf{u}_{,\nu}$ and $\mathbf{u}'$, i.e. $\mathbf{n} = \mathbf{n}(\mathbf{u}_{,\nu}, \mathbf{u}')$, subjected to only two independent constraints

$$\mathbf{y}'\cdot\mathbf{n} = (\boldsymbol{\tau} + \mathbf{u}')\cdot\mathbf{n} = 0, \qquad \mathbf{n}\cdot\mathbf{n} = 1. \tag{5.7}$$

As a result, $\mathbf{n} = \mathbf{n}(\mathbf{u}_{,\nu}, \mathbf{u}')$ along $\partial M^{(k)}$ is expressible through $\mathbf{u}'$ and a scalar function $\phi = \phi(\mathbf{u}_{,\nu}, \mathbf{u}')$ describing the rotational deformation of the shell lateral boundary surface. The structure of the function $\phi(\mathbf{u}_{,\nu}, \mathbf{u}')$ was discussed in [14, 15], where the general expression for $\mathbf{w} \equiv \dot{\mathbf{n}}$ in terms of $\varphi \equiv \dot{\phi}$ and $\mathbf{v}'$ was derived in the form

$$\mathbf{w} = \mathbf{q}\varphi + \mathbf{L}\,\mathbf{v}', \qquad \mathbf{q}(\phi, \mathbf{u}') \equiv \partial_{\phi}\mathbf{n}, \qquad \mathbf{L}(\phi, \mathbf{u}') \equiv \partial_{\mathbf{u}'}\mathbf{n}. \tag{5.8}$$

Explicit expressions for the vector-valued function $\mathbf{q} = \mathbf{q}(\mathbf{u}_{,\nu}, \mathbf{u}')$ and the tensor-valued function $\mathbf{L} = \mathbf{L}(\mathbf{u}_{,\nu}, \mathbf{u}')$ depend on the particular definition of the scalar-valued function $\phi = \phi(\mathbf{u}_{,\nu}, \mathbf{u}')$ employed.

With the help of (5.8), the second term in the line integral of (5.3) can be transformed further to

$$\int_{\partial M^{(k)}} \mathbf{H}_{\nu}^{(k)}\cdot\mathbf{w}^{(k)}\,dS = \int_{\partial M^{(k)}} \left(-\mathbf{f}^{(k)}\cdot(\mathbf{v}^{(k)})' + H^{(k)}\varphi^{(k)}\right) dS, \tag{5.9}$$

where

$$\mathbf{f}^{(k)} = -\mathbf{L}^T \mathbf{H}_\nu^{(k)}, \qquad H^{(k)} = \mathbf{q} \cdot \mathbf{H}_\nu^{(k)}. \tag{5.10}$$

Along each $\partial M^{(k)}$ there may be singular points (e.g. corner points) P_a, $a = 1, ..., A$, described by $S = S_a$, at which the field $\mathbf{f}^{(k)} \cdot \mathbf{v}^{(k)}$ is not differentiable. At such points we assume the existence of finite limits of $\mathbf{f}^{(k)}$ and $\mathbf{v}^{(k)}$ defined by

$$\mathbf{f}_a^{(k)\pm} = \lim_{h \to 0} \mathbf{f}^{(k)}(S_a \pm h), \qquad \mathbf{v}_a^{(k)\pm} = \lim_{h \to 0} \mathbf{v}^{(k)}(S_a \pm h). \tag{5.11}$$

Then the line integral (5.9) can be transformed by applying the integration by parts leading to

$$\iint_{M^{(k)}} W_i \, dA = -\iint_{M^{(k)}} (\mathrm{Div}_s \mathbf{T}) \cdot \mathbf{v} \, dA + \int_{\partial M^{(k)}} (\mathbf{P}_\nu^{(k)} \cdot \mathbf{v}^{(k)} + H^{(k)} \varphi^{(k)}) \, dS + \sum_{P_a \in \partial M^{(k)}} \left(\mathbf{f}_a^{(k)+} \cdot \mathbf{v}_a^{(k)+} - \mathbf{f}_a^{(k)-} \cdot \mathbf{v}_a^{(k)-} \right), \tag{5.12}$$

where

$$\mathbf{P}_\nu^{(k)} = \mathbf{T}_\nu^{(k)} + (\mathbf{f}^{(k)})'. \tag{5.13}$$

By virtue of (5.12) and (4.1), the internal virtual work for the entire reference network M can be written in the form

$$\mathcal{G}_{\mathrm{int}} = -\iint_M (\mathrm{Div}_s \mathbf{T}) \cdot \mathbf{v} \, dA + \int_{\partial M} (\mathbf{P}_\nu \cdot \mathbf{v} + H\varphi) \, dS + \int_\Gamma (\llbracket \mathbf{P}_\nu \cdot \mathbf{v} \rrbracket + \llbracket H\varphi \rrbracket) \, dS + \sum_{P_i \in \Gamma} [\mathbf{f} \cdot \mathbf{v}]_i + \sum_{P_b \in \partial M_f} [\mathbf{f} \cdot \mathbf{v}]_b . \tag{5.14}$$

Here the jump $\llbracket \mathbf{P}_\nu \cdot \mathbf{v} \rrbracket$ at each regular point $\mathbf{Y} \in \Gamma^{(a)} \equiv \Gamma^{(1,2,...,n)}$ of the common curve for $n \geq 2$ adjacent surface elements $M^{(k)}$ is defined by

$$\llbracket \mathbf{P} \cdot \mathbf{v} \rrbracket = \pm \mathbf{P}_\nu^{(1)} \cdot \mathbf{v}^{(1)} \pm \mathbf{P}_\nu^{(2)} \cdot \mathbf{v}^{(2)} \pm \ldots \pm \mathbf{P}_\nu^{(n)} \cdot \mathbf{v}^{(n)}, \tag{5.15}$$

with the jump $\llbracket H\varphi \rrbracket$ being defined in the same way. The signs in the definition (5.15) must be chosen consistently with a fixed orientation of the curve $\Gamma^{(a)}$. If the orientation of $\Gamma^{(a)}$ coincides with the orientation of the boundary curve $\partial M^{(k)}$, then the sign "$-$" must be chosen for the corresponding term and the "$+$" sign otherwise. If we denote by $\boldsymbol{\tau}_\Gamma$ the unit tangent vector specifying the orientation of the curve $\Gamma^{(a)}$, then $\boldsymbol{\nu}^{(k)} = \pm \boldsymbol{\tau}_\Gamma \times \mathbf{A}_n^{(k)}$, and the sign must be chosen in such a way that the boundary $\partial M^{(k)}$ be consistently oriented with $M^{(k)}$.

The jumps at all singular points of M have been divided in (5.14) into the jumps $[\mathbf{f} \cdot \mathbf{v}]_i$ at the internal points $P_i \in \Gamma$, $i = 1, ..., I$, and the jumps $[\mathbf{f} \cdot \mathbf{v}]_b$ at the

boundary points $P_b \in \partial M$. At each internal point P_i being the common point of $m \geq 2$ adjacent branches $\Gamma^{(a)}$ of Γ, and at each boundary point P_b being the common point of $t \geq 2$ adjacent parts $\partial M^{(t)}$ of ∂M and adjacent branches $\Gamma^{(q)}$ of Γ approaching P_b from inside of M, these jumps are defined by

$$
\begin{aligned}
[\mathbf{f}\cdot\mathbf{v}]_i &= \pm\mathbf{f}_i^{(1)\pm}\cdot\mathbf{v}_i^{(1)\pm} \pm \mathbf{f}_i^{(2)\pm}\cdot\mathbf{v}_i^{(2)\pm} \pm \ldots \pm \mathbf{f}_i^{(m)\pm}\cdot\mathbf{v}_i^{(m)\pm}, \\
[\mathbf{f}\cdot\mathbf{v}]_b &= \pm\mathbf{f}_b^{(1)\pm}\cdot\mathbf{v}_b^{(1)\pm} \pm \mathbf{f}_b^{(2)\pm}\cdot\mathbf{v}_b^{(2)\pm} \pm \ldots \pm \mathbf{f}_b^{(t)\pm}\cdot\mathbf{v}_b^{(t)\pm} \\
&\quad \pm\mathbf{f}_i^{(1)\pm}\cdot\mathbf{v}_b^{(1)\pm} \pm \mathbf{f}_i^{(2)\pm}\cdot\mathbf{v}_b^{(2)\pm} \pm \ldots \pm \mathbf{f}_i^{(q)\pm}\cdot\mathbf{v}_b^{(q)\pm}.
\end{aligned} \tag{5.16}
$$

Similar transformations can be applied to the external virtual work, which gives

$$
\begin{aligned}
\mathcal{G}_{\text{ext}} = \iint_{M\setminus\Gamma} \mathbf{l}\cdot\mathbf{v}\,dA - \int_{\Gamma} [\![(\mathbf{h}\cdot\boldsymbol{\mu})\mathbf{n}\cdot\mathbf{v}]\!]\,dS + \int_{\partial M_f} (\{\mathbf{P}^* - (\mathbf{h}\cdot\boldsymbol{\mu})\mathbf{n}\}\cdot\mathbf{v} + H^*\varphi)\,dS \\
- \int_{\partial M_d} (\mathbf{h}\cdot\boldsymbol{\mu})\mathbf{n}\cdot\mathbf{v}\,dS + \sum_{P_b\in\partial M_f} [\mathbf{f}^*\cdot\mathbf{v}]_b,
\end{aligned} \tag{5.17}
$$

where $\partial M_d = \partial M\setminus\partial M_f$ is the complementary part of ∂M, and

$$
\mathbf{f}^* = -\mathbf{L}^T\mathbf{H}^*, \qquad H^* = \mathbf{q}\cdot\mathbf{H}^*, \qquad \mathbf{P}^* = \mathbf{T}^* + (\mathbf{f}^*)'. \tag{5.18}
$$

The jumps $[\![(\mathbf{h}\cdot\boldsymbol{\mu})\mathbf{n}\cdot\mathbf{v}]\!]$ along the common curve $\Gamma^{(a)}$ for $n \geq 2$ adjacent surface elements are defined analogously to (5.15). However, the jumps $[\mathbf{f}^*\cdot\mathbf{v}]_b$ in (5.17) take into account only those limiting values which are obtained by approaching P_b along branches of the boundary ∂M_f. If the boundary point P_b is a common point of $t \geq 2$ adjacent parts $\partial M^{(t)}$ of ∂M and q adjacent branches of $\Gamma^{(q)}$ of Γ, then

$$
[\mathbf{f}^*\cdot\mathbf{v}]_b = \pm\mathbf{f}_b^{*(1)\pm}\cdot\mathbf{v}_b^{(1)\pm} \pm \mathbf{f}_b^{*(2)\pm}\cdot\mathbf{v}_b^{(2)\pm} \pm \ldots \pm \mathbf{f}_b^{*(t)\pm}\cdot\mathbf{v}_b^{(t)\pm}. \tag{5.19}
$$

Introducing (5.14) and (5.17) into the principle of virtual work (2.1) we obtain

$$
\begin{aligned}
&-\iint_{M\setminus\Gamma} (\mathrm{Div}_s\mathbf{T} + \mathbf{l})\cdot\mathbf{v}\,dA \\
&+ \int_{\partial M_f} (\{\mathbf{P}_\nu - \mathbf{P}^* + (\mathbf{h}\cdot\boldsymbol{\mu})\mathbf{n}\}\cdot\mathbf{v} + (H - H^*)\varphi)\,dS + \sum_{P_b\in\partial M_f} [(\mathbf{f} - \mathbf{f}^*)\cdot\mathbf{v}]_b \\
&+ \int_{\partial M_d} (\{\mathbf{P}_\nu + (\mathbf{h}\cdot\boldsymbol{\mu})\mathbf{n}\}\cdot\mathbf{v} + H\varphi)\,dS + \sum_{P_b\in\partial M_d} [\mathbf{f}\cdot\mathbf{v}]_b \\
&+ \int_{\Gamma} ([\![\{\mathbf{P}_\nu + (\mathbf{h}\cdot\boldsymbol{\mu})\mathbf{n}\}\cdot\mathbf{v}]\!] + [\![H\varphi]\!])\,dS + \sum_{P_i\in\Gamma} [\mathbf{f}\cdot\mathbf{v}]_i - \mathcal{G}_\Gamma = 0.
\end{aligned} \tag{5.20}
$$

For arbitrary but kinematically admissible virtual deformations, the fields $\mathbf{v}$ and φ vanish identically along ∂M_d. Then, from (5.20) we obtain the Lagrangian local equilibrium equations

$$\text{Div}_s \mathbf{T} + \mathbf{l} = \mathbf{0} \qquad \text{at each regular } \mathbf{Y} \in M, \tag{5.21}$$

and the static boundary and corner conditions

$$\begin{aligned} &\mathbf{P}_\nu - \mathbf{P}^* + (\mathbf{h}\cdot\boldsymbol{\mu})\mathbf{n} = \mathbf{0}, \qquad H - H^* = 0 \quad \text{along regular parts of } \partial M_f, \\ &\mathbf{f}_b - \mathbf{f}_b^* = \mathbf{0} \qquad \text{at each singular point } P_b \in \partial M_f. \end{aligned} \tag{5.22}$$

Correspondingly, the work-conjugate geometric boundary conditions take the form

$$\mathbf{u} = \mathbf{u}^*, \qquad \phi = \phi^* \quad \text{along } \partial M_d. \tag{5.23}$$

As it has been expected, the local equilibrium conditions for thin irregular shells are the same as in the classical nonlinear theory of thin smooth shells [1].

6. General form of jump conditions

The new aspects of the theory of thin irregular shells, as compared with regular ones, lie exclusively in the concept of jump conditions needed, besides the constitutive relations, to obtain the complete formulation of the boundary value problem. The considerations of the previous section have shown that if the equilibrium equations and boundary conditions hold, then the principle of virtual work (5.20) asserts that

$$\int_\Gamma \left([\![\{\mathbf{P}_\nu + (\mathbf{h}\cdot\boldsymbol{\mu})\mathbf{n}\}\cdot\mathbf{v}]\!] + [\![H\varphi]\!] \right) dS + \sum_{P_i \in \Gamma} [\mathbf{f}\cdot\mathbf{v}]_i - \mathcal{G}_\Gamma = 0. \tag{6.1}$$

Equation (6.1) expresses the most general form of jump conditions in the weak form, and all considerations leading to (6.1) provide an unambiguous interpretation of the final results. No other results or consequences can be obtained when one applies the two hypotheses from Sec. 2, on which the whole theory of thin irregular shells is based. The weak form (6.1) of the jump conditions must hold for all cases, whether the irregularities are of geometric, kinematic or static nature, and (6.1) is entirely independent of the mechanical properties assigned to the curve Γ and the points P_i, P_b. Of course, so far we have not said anything about the possible physical meaning of the curve Γ and the points P_i, P_b, because our aim has been to include as many special cases as possible within this general framework. Moreover, at the beginning of the analysis, no *a priori* information about the form of $\mathcal{G}_\Gamma$ has been at our disposal.

In general, the $\Gamma^{(a)}$ are either geometric or physical curves embedded in the shell reference network M. In the first case, each $\Gamma^{(a)}$ represents simply a geometric curve on M, across which some surface fields fail to be continuous or smooth of the required class. In the second case, each $\Gamma^{(a)}$ is said to be a physical curve in the sense that it can be equipped with specific physical properties possibly quite distinct from the mechanical properties of the regular shell parts. Such a $\Gamma^{(a)}$ can model various physical situations encountered in real shell structures. The same applies to points P_i and P_b. In either case, it becomes obvious that the most general form of the virtual work expression $\mathcal{G}_\Gamma$ allowed within the theory of thin irregular shells is

$$\mathcal{G}_\Gamma = \int_\Gamma \sigma_\Gamma(\mathbf{Y})\, dS + \sum_{P_i \in \Gamma} \sigma_i\,, \tag{6.2}$$

where σ_Γ is the virtual work density along regular parts of the curve Γ, and σ_i is the virtual work at any singular point of Γ. The functions σ_Γ and σ_i must be specified in each particular case of the irregularity.

In view of (6.2), and taking further into account that the equation (6.1) must hold for each curve $\Gamma^{(a)}$ as well as for every part of it, we obtain the corresponding local form of the jump conditions:

$$[\![\{\mathbf{P}_\nu + (\mathbf{h}\cdot\boldsymbol{\mu})\mathbf{n}\}\cdot\mathbf{v}]\!] + [\![H\varphi]\!] - \sigma_\Gamma = 0, \quad \text{at regular points of } \Gamma, \tag{6.3}$$

$$[\mathbf{f}\cdot\mathbf{v}]_i - \sigma_i = 0, \quad \text{at each internal singular point } P_i \in \Gamma. \tag{6.4}$$

The jump conditions (6.3) and (6.4) constitute the additional set of local relations for thin irregular shell structures to be satisfied along the singular curves Γ.

The jump conditions (6.3) and (6.4) are valid for unrestricted displacements, rotations, strains and/or bending of the reference network M. Their general form depends neither on the assembling techniques nor on the solution methods applied. For special types of irregularities, the jump conditions can be considerably simplified and presented in a more explicit uncoupled form. Such particular forms of the jump conditions appropriate for only geometric irregularities (folds, intersections, rigid junctions) and for some simple kinematic irregularities (elastic and visco-elastic junctions) will be discussed in [16].

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LEHRSTUHL FÜR ALLGEMEINE MECHANIK,
RUHR - UNIVERSITÄT BOCHUM, GERMANY
and
POLISH ACADEMY OF SCIENCES,
INSTITUTE OF FLUID-FLOW MACHINERY, GDAŃSK, POLAND.

Received October 7, 1997.

Arch. Mech., 50, 3, pp. 497–508, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

Superconducting fullerenes in a nonconventional thermodynamical model

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

B. MARUSZEWSKI (POZNAŃ)

A CRYSTALLINE SOLID of C_{60} (a fullerene) is expected to be an insulator or a semiconductor. However, one of the most striking properties of C_{60} – related materials is the observation of relatively high temperature superconductivity in alkali metal doped M_3C_{60} and in various alkaline earth doped compounds. So, the interstitial diffusion of impurities considerably influences the superconductivity phase. The value of the critical temperature below which the superconducting phase exists, strongly depends on many other external influences (electromagnetic, thermal, mechanical, etc.). The paper deals with construction of a phenomenological macroscopic model of interactions between physical fields in fullerenes, basing on the extended thermodynamics with internal variables and with the use of Liu's theorem in order to apply the entropy inequality.

1. Introduction

MATERIALS of specific properties, particularly smart materials very sensitive to external influences which vary due to mutual interactions between physical fields and such materials, are of great interest for researchers and engineers. One of the most spectacular examples of such materials are fullerenes, the allotropic variety of carbon. Fullerenes have large closed cage polyhedral molecules of carbon atoms, the most common fullerene being C_{60}. As the molecular crystal they form a *fcc* or *bcc* lattice. Since each carbon atom has its valence requirements fully satisfied (each carbon atom has four valence electrons), a crystalline solid of C_{60} is expected to be an insulator or a semiconductor. However, one of the most striking properties of C_{60}-related materials is the observation of relatively high temperature superconductivity in alkali metal doped M_3C_{60} and in various alkaline earth doped compounds. In the synthesis of C_{60}, larger fullerenes are also formed, e.g. C_{70}, C_{76}, C_{78}, C_{80}, C_{84}, C_{240}, C_{330}. In principle, the smallest possible fullerene is C_{20} though no C_{20} fullerenes have been reported experimentally. Thus, C_{60} is the only fullerene host for which superconductivity has been identified. For the physical properties of fullerenes see [1]. There are three ways to introduce foreign atoms into a C_{60}-based solid. One of them involves the addition of a rare earth, an alkaline earth or an alkali metal ion into the interior

of the fullerene molecule. However, no superconductivity has been observed in such doped fullerene and it may remain the insulator or the semiconductor.

The second method is the substitutional doping of an impurity atom in a different valence state for a carbon atom on the surface of a fullerene molecule. However, because of atom diameters and distances on the C_{60} surface, only boron and nitrogen might be dopants in that case. And again, no superconductivity has been observed in the above structure.

In the third method of doping fullerene solids, the dopant is introduced into the interstitial positions between adjacent molecules. In this doping, a charge transfer can take place between the impurities and the molecules. That transfer forms a situation when superelectrons (the Cooper pairs) self-consistently coexist with each other creating (being) the carriers of the supercurrent. It is known that within the region of one Cooper pair, there are many centers of the other pairs. Thus the Cooper pairs (superelectrons) cannot be treated independently since they form a very complicated interlaced structure, the stability of which is extremely important for the existence of the superconducting state. There are numerous examples of superconductivity in such doped C_{60}.

The last method is most important for us since the interstitial mass diffusion processes (the intermolecular diffusion in the fullerene molecular crystal) might considerably influence conductivity properties of fullerenes; those properties can vary during such a process. However, not only diffusion of impurities and their concentration influence the value of critical temperature below which the superconducting phase exists. That value and even the existence of superconducting phase strongly depend also on many other external influences, like the magnitude of applied magnetic or electric fields, the density of electric current existing in the fullerene, the thermal conditions and properties (heat flux, temperature, heat capacity or heat conductivity vs. temperature) which accompany the processes running in the C_{60} as superconductors [2].

In nonequilibrium (and even in equilibrium) states of superconductors, in temperatures different from zero, a part of the pairs is thermally dissociated and the density of superelectrons depends on the number of nondissociated pairs. Since the process of the Cooper pairs creation is selfconsistent, any change of their number produced by external fields, like temperature, electromagnetic field and diffusion of impurities, strongly influences characteristic properties of superelectrons. If the quantities characteristic for the above fields reach their critical values, the continuous transition from superconducting to normal state of the fullerene occurs.

The dependence of the constitutive superconductor parameters on pressure or mechanical stresses are also interesting. Great number of various properties of the fullerenes shown above, strong dependence of material coefficients in superconducting phase on many physical fields, phase transitions occurring during processes, and the like, indicate that any description of thermodynamical states and processes is rather very complicated. There exist several attempts to de-

scribe physical interactions in deformable superconductors in the framework of nonequilibrium thermodynamical phenomenological models. For the most characteristic ones see [3–9, 15–17].

The paper deals with construction of a model of interactions between physical fields in fullerenes within their superconducting phase. A specific definition of the state vector has been proposed. It consists of field controllable variables and additionally, of internal variables responsible for the electrical conductivity properties of the M_xC_{60} material. An extended-like thermodynamical model [10] with the use of that state vector and consequences of its introduction are presented. The superscripts N and S concern the "normal" and "superconducting" states of the fullerene, respectively.

2. Conductivity phases of fullerenes

As we have mentioned before, a pure molecular crystal C_{60} is expected to be an insulator and/or semiconductor when doped. Dopants change its conductivity properties according to their positions in the lattice. Those positions depend on the impurity concentration. Doping, for instance, with an alkaline earth impurity, e.g. Ca, when two Ca atoms are placed at the tetrahedral sites of the *fcc* C_{60} lattice and the third Ca atom is placed either at an on-center or at an off-center position of the octahedral interstitial site, causes that Ca_3C_{60} becomes a semiconductor. In the case of the superconducting phase, three Ca atoms are at off-centered positions of the octahedral interstitial site [1]. So, two different properties of the fullerene depend on the concentration of impurities:

i) the conductivity property – whether it is a semiconductor or a superconductor,

ii) the conductivity property – the existence of the superconducting phase in the normal semiconducting phase where the former one results from the density of the Cooper pairs.

Thus, any description of state of the fullerene when the superconducting phase also exists, seems to be very complicated. For the thermoelastic and doped fullerene C_{60} in which relaxation of thermal field, diffusion and electric current is observed, the vector of state (the set of independent variables) concerning any conductivity phase can be generally presented in the form (extended irreversible thermodynamical (EIT) model)

$$\mathcal{A} = \{\varepsilon, \boldsymbol{\mathcal{R}}, T, \nabla T, c, \nabla c, \mathbf{q}, \mathbf{j}^c, \aleph, \mathbf{j}\}, \tag{2.1}$$

where ε is the linear small strain tensor, because it is difficult to expect that within the superconducting phase existing in the relatively low temperature, large elastic deformations are possible, $\boldsymbol{\mathcal{R}}$ is a vector of electromagnetic field variables (see comments below), T is the temperature and $\mathbf{q}$ is the heat flux, c is the concentration of impurities and $\mathbf{j}^c$ is the flux of impurity mass (cf. [12]),

$\aleph$ is an internal variable responsible for the generally understood electric charge carrier density, and $\mathbf{j}$ is the flux of the carrier field, i.e. the electric current. The vector $\boldsymbol{\mathcal{R}}$ is defined as

$$\boldsymbol{\mathcal{R}} = \begin{cases} \{\mathcal{E}, \mathbf{B}\} \\ \text{or} \\ \{\varphi, \mathbf{A}, \nabla\varphi, \nabla\mathbf{A}\}, \end{cases} \tag{2.2}$$

where $\mathcal{E}$ – the electromotive intensity in the moving frame and $\mathbf{B}$ – the magnetic induction, φ – the scalar and $\mathbf{A}$ – the vector electromagnetic potentials, respectively. They can be equivalently chosen as independent electromagnetic variables [3–9, 15–17]. Situation with the internal variable $\aleph$ and its flux $\mathbf{j}$ is much more complicated. They can be defined as

$$\aleph = \begin{cases} \{n, p, \nabla n, \nabla p\} \quad \text{for the normal semiconducting phase [11]} \\ \text{and/or} \\ \{\psi, \psi^*, \nabla\psi, \nabla\psi^*\} \quad \text{for the superconducting phase [4–9]}, \end{cases} \tag{2.3}$$

$$\mathbf{j} = \begin{cases} \{\mathbf{j}^n, \mathbf{j}^p\} \quad \text{for the normal semiconducting phase [11]} \\ \text{and/or} \\ \left\{\mathbf{j}^S\right\} \quad \text{for the normal superconducting phase [3]}, \end{cases} \tag{2.4}$$

where n and p are the mass densities of electrons and holes in a semiconductor, respectively, ψ denotes the complex wave function describing the entire ensemble of superelectrons such that [2]

$$n^S = \psi\psi^* = |\psi|^2 \tag{2.5}$$

is the probability density or local density of superelectrons (ψ^* is the complex conjugate to ψ) [2], then $\mathbf{j}^n$ and $\mathbf{j}^p$ are the fluxes of electrons and holes in the semiconducting phase and $\mathbf{j}^S$ is the flux of superelectrons (the Cooper pairs) or simply supercurrent. Remark that in $\boldsymbol{\mathcal{R}}$ (2.2), either electromagnetic variables or electromagnetic potentials are responsible for electromagnetic field, contrary to $\aleph$ (2.3) and $\mathbf{j}$ (2.4). $\aleph$ and $\mathbf{j}$ can be taken in their full not alternative forms creating the set of independent variables (the vector of state) for the semiconducting normal phase and the superconducting one.

Another comment is necessary to be mentioned here. It deals with the time evolution of $\aleph$ and $\mathbf{j}$. In a case of the semiconducting phase we have the laws of conservation of electron and hole as the evolution equations for $\mathbf{j}^n$ and $\mathbf{j}^p$ as related to relaxation semiconductors [11]. For the superconducting phase, the evolution equation of the wave function ψ is the generalized Schrödinger equation, then the generalized first London equation describes the evolution of the supercurrent $\mathbf{j}^S$ [2].

3. Extended-like thermodynamical model

From now on we confine our considerations only to the semiconducting phase of a fullerene. The semiconducting normal phase of that material can be described within one of the existing thermodynamical models of deformable semiconductors (see [11], for instance). To obtain a description of both the semiconducting and superconducting coexisting phases of the fullerene, one has to superpose the model presented below with that proposed, among others, in [11]. We aim at investigating a thermoelastic (for the reason mentioned before) superconducting fullerene in which the impurity (mass) diffusion occurs and the relaxation features of supercurrent, thermal and diffusion fields are taken into account. The latter one is included in the model only for formal reasons. Finally, it will be dropped out by the use of a proper gauging (the relaxation time of the mass diffusion field is too long as compared to the remaining two relaxation times concerning the supercurrent and the thermal fields). Electromagnetic properties resulting from possible electrical polarization or magnetization are excluded from our considerations. For such a fullerene body, its superconducting state is described by the following set of independent variables (the vector of state) selected from (2.1) – (2.4):

$$\mathcal{C} = \left\{\varepsilon_{ij}, \varphi, A_i, T, T_{,i}, c, c_{,i}, \psi, \psi^*, \psi_{,i}, \psi^*_{,i}, q_i, j^c_i, j^S_i\right\} \tag{3.1}$$

and all of them are evaluated at the same point and time. Also all the fields in (3.1) as well as the fullerene are assumed to be continuous. The physical processes occurring in the above-defined situation are governed by three groups of fundamental laws. The first group concerns the balances of mass, momentum, moment of momentum and internal energy.

The balance of diffusing (impurity) mass resulting from the continuity equations for the constituents (impurities and a fullerene) reads [12]

$$\varrho\dot{c} + j^c_{k,k} = 0. \tag{3.2}$$

The superimposed dot denotes the material time derivative.

The momentum balance for nonpolarized and nonmagnetized body with other electromagnetic interactions takes the form (cf.[13, 15–17])

$$\varrho\dot{v}_k - \sigma_{jk,j} - \epsilon_{kij} j_i B_j - f_k = 0, \tag{3.3}$$

where v_k is the velocity of the body point, σ_{ik} denotes the stress tensor and f_k is a body force density.

The moment of momentum balance is assumed in its classical form that indicates the symmetry of the stress tensor for any spin, and skew-symmetric features can be omitted in the fullerene crystal entity [1, 13, 14]:

$$\epsilon_{ijk}\sigma_{jk} = 0. \tag{3.4}$$

However, we must remember about the domain structure of superconductors, because the conductivity and superconductivity phases coexist. Hence skew-symmetric features of the fullerene may occur during deformation processes. Moreover, the vortex properties of the magnetic flux in the superconductors also give a contribution to the moment of momentum [2]. So, the balance (3.4) is understood as the first approximation in the description of interactions between the mechanical and other physical fields in fullerenes.

The internal energy balance is taken in the following form [3–9, 12, 15–17]:

$$\varrho\dot{U} - \sigma_{ji}v_{i,j} + q_{k,k} - j_i\mathcal{E}_i - \varrho r = 0, \tag{3.5}$$

where U denotes the internal energy density per unit mass and r is the heat source distribution density.

The second group of laws deals with the electromagnetic field. *The Maxwell equations* are taken in their classical form disregarding the displacement current and the free charge density [2]:

$$\epsilon_{ijk}E_{k,j} + \frac{\partial B_i}{\partial t} = 0, \tag{3.6}$$

$$\epsilon_{ijk}H_{k,j} - j_i = 0, \tag{3.7}$$

$$B_{k,k} = 0, \tag{3.8}$$

$$D_{k,k} = 0. \tag{3.9}$$

The above laws must be complemented by the relations

$$\mathcal{E}_i = E_i + \epsilon_{ijk}v_jB_k\,, \tag{3.10}$$

$$j_i = j_i^n + j_i^p + j_i^S = j_i^N + j_i^S\,, \tag{3.11}$$

$$E_k = -\varphi_{,k} - \frac{\partial A_k}{\partial t}\,, \tag{3.12}$$

$$B_k = \epsilon_{kij}A_{j,i}\,, \tag{3.13}$$

$$D_k = \epsilon E_k\,, \tag{3.14}$$

$$B_k = \mu_0 H_k\,. \tag{3.15}$$

j_i^N denotes the *normal* current which satisfies Ohm's law in conductors and additionally in semiconductors, the diffusion law of the charge carriers, ϵ is the permittivity of the fullerene and μ_0 is the permeability of vacuum.

The third group of fundamental laws concerns the time evolution of internal variables and fluxes. So, we postulate the following equations:

- *the evolution equation for the heat flux*

$$\overset{*}{q}_k - Q_k(\mathcal{C}) = 0, \tag{3.16}$$

- *the evolution equation for the wave function*

$$\dot{\psi} - \Psi(\mathcal{C}) = 0, \tag{3.17}$$

and *its complex conjugate*

$$\dot{\psi}^* - \Psi^*(\mathcal{C}) = 0, \tag{3.18}$$

- *the evolution equation for the mass flux*

$$\overset{*}{j_k^c} - J_k^c(\mathcal{C}) = 0, \tag{3.19}$$

and *the evolution equation for the supercurrent*

$$\overset{*}{j_k^S} - J_k^S(\mathcal{C}) = 0. \tag{3.20}$$

The superimposed asterisk denotes the Zaremba–Jaumann time derivative. We must comment on the relation of Eqs. (3.17) and (3.18) with the supercurrent density j_k^S, the density of the superelectrons n^S and eventually Eq. (3.20). On using the relation (2.5) and the evolution equations (3.17) and (3.18), we obtain [2]

$$\frac{\partial n^S}{\partial t} + j_{k,k}^S = N^S(\mathcal{C}) \tag{3.21}$$

which may be treated as the balance of superelectrons, where

$$j_{k,k}^S - N^S(\mathcal{C}) = \left(\psi^* \psi_{,k} + \psi \psi_{,k}^*\right) - \left[\psi^* \Psi(\mathcal{C}) + \psi \Psi^*(\mathcal{C})\right]. \tag{3.22}$$

Equation (3.21) is a generalization of the conservation law for the Cooper pairs [2] to external influences of various physical fields. The source-like term in (3.21) $N^S(\mathcal{C})$ is assumed to vanish if there are no influences of the elastic, thermal and mass diffusion fields on the state of the fullerene. It means that in such situation the superelectron charge is conserved. If we want to describe the processes considered above in a proper way, we must demand that they should be admissible from the thermodynamical point of view, i.e. they should not contradict the second law of thermodynamics. The latter written in local form, takes the form of the entropy inequality

$$\varrho \dot{S} + \Phi_{k,k} - \frac{\varrho r}{T} \geq 0, \tag{3.23}$$

where S denotes the entropy density and Φ_k is the entropy flux associated with the fields of the set $\mathcal{C}$. As a matter of fact, if we define the set

$$\mathcal{Z}\left\{\sigma_{ij}, \mu^c, U, Q_k, \Psi, \Psi^* J_k^c, J_k^S, S, \Phi_k\right\}, \tag{3.24}$$

then we must look for general constitutive equations in the form

$$\mathcal{Z} = \mathcal{Z}(\mathcal{C}), \tag{3.25}$$

where both $\mathcal{C}$ and $\mathcal{Z}$ are evaluated at the same point and time (we ignore hereditary and nonlocal effects).

To determine the explicit forms of (3.25), Liu's theorem [18] seems to be the most convenient tool to use for the analysis of the inequality (3.23). For the sake of simplicity the body forces and heat sources will be omitted in our discussion. μ^c will be defined in the sequel.

According to Liu's theorem, where all the balance and evolution equations are considered as mathematical constraints for the general validity of (3.23), we must introduce the so-called Lagrange – Liu's multipliers to account for equations (3.2), (3.3), (3.5)–(3.9), (3.16)–(3.20). The set of multipliers reads

$$\Lambda = \left\{\Lambda^c, \Lambda^v_r, \Lambda^u, \Lambda^E_i, \Lambda^E_4, \Lambda^B_i, \Lambda^B_4, \Lambda^Q_k, \Lambda^\psi, \Lambda^{\psi*}, \Lambda^{JC}_k, \Lambda^S_k\right\}. \tag{3.26}$$

Calling $\mathcal{F}^c, \mathcal{F}^v_r, \mathcal{F}^u, \mathcal{F}^E_i, \mathcal{F}^E_4, \mathcal{F}^B_i, \mathcal{F}^B_4, \mathcal{F}^Q_k, \mathcal{F}^\psi, \mathcal{F}^{\psi*}, \mathcal{F}^{JC}_k, \mathcal{F}^S_k$, the left-hand sides of equations (3.2), (3.3), (3.5)–(3.9), (3.16)–(3.20), respectively, according to the second requirement of Liu's theorem, we rewrite the inequality (3.23) in the form

$$\begin{aligned}\varrho\frac{\partial S}{\partial t} + \varrho v_k S_{,k} + \Phi_{k,k} - \Big\{&\Lambda^c\mathcal{F}^c + \Lambda^v_r\mathcal{F}^v_r + \Lambda^u\mathcal{F}^u + \Lambda^E_i\mathcal{F}^E_i + \Lambda^E_4\mathcal{F}^E_4 \\ &+ \Lambda^B_i\mathcal{F}^B_i + \Lambda^B_4\mathcal{F}^B_4 + \Lambda^Q_k\mathcal{F}^Q_k + \Lambda^\psi\mathcal{F}^\psi + \Lambda^{\psi*}\mathcal{F}^{\psi*} + \Lambda^{JC}_k\mathcal{F}^{JC}_k + \Lambda^S_k\mathcal{F}^S_k\Big\} = 0.\end{aligned} \tag{3.27}$$

We introduce now the scalar (free energy density) potential F and the vector thermodynamical potential K_i [10] as follows:

$$F = U - TS, \tag{3.28}$$

$$K_k = \varrho v_k F - T\Phi_k\,. \tag{3.29}$$

The considerations of processes based on the above theorem for which those potentials hold true, strongly suggest that

$$\Lambda^u = \frac{1}{T}\,. \tag{3.30}$$

Thus the third requirement of Liu's theorem with the use of the relations

$$\varepsilon_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right), \tag{3.31}$$

$$v_{j,i} = \frac{\partial\varepsilon_{ij}}{\partial t} + w_{ij}\,, \tag{3.32}$$

where u_i denotes the elastic displacement and w_{ij} is the antisymmetric part of the velocity gradient, leads us to the following groups of results:

- *the multipliers*

$$\Lambda_r^v = 0, \qquad \Lambda_i^E = 0, \qquad \Lambda_4^E = 0, \qquad \Lambda_i^B = 0, \qquad \Lambda_4^B = 0, \tag{3.33}$$

$$\begin{aligned} &\Lambda^c = -\frac{1}{T}\mu^c, \qquad \Lambda_i^Q = -\frac{1}{T}\Pi_i^Q, \qquad \Lambda_i^{JC} = -\frac{1}{T}\Pi_i^C, \\ &\Lambda^\psi = -\frac{1}{T}\Pi^\psi, \quad \Lambda^{\psi*} = -\frac{1}{T}\Pi^{\psi*}, \qquad \Lambda_k^S = -\frac{1}{T}\Pi_k^S; \end{aligned} \tag{3.34}$$

- *the laws of state*

$$\begin{aligned} &\sigma_{ij} = \varrho\frac{\partial F}{\partial \varepsilon_{ij}}, \qquad \frac{\partial F}{\partial \varphi} = 0, \qquad \frac{\partial F}{\partial \varphi_{,k}} = 0, \qquad j_k^S = -\varrho\frac{\partial F}{\partial A_k}, \\ &S = -\frac{\partial F}{\partial T}, \qquad \frac{\partial F}{\partial T_{,i}} = 0, \qquad \mu^c = \frac{\partial F}{\partial c}; \end{aligned} \tag{3.35}$$

- *the affinities*

$$\begin{aligned} &\Pi_i^Q = \varrho\frac{\partial F}{\partial q_i}, \qquad \Pi_i^C = \varrho\frac{\partial F}{\partial j_i^c}, \qquad \Pi_i^S = \varrho\frac{\partial F}{\partial j_k^S}, \\ &\Pi^\psi = \varrho\frac{\partial F}{\partial \psi} - \left(\varrho\frac{\partial F}{\partial \psi_{'k}}\right)_{,k}, \qquad \Pi^{\psi*} = \varrho\frac{\partial F}{\partial \psi^*} - \left(\varrho\frac{\partial F}{\partial \psi^*_{'k}}\right)_{,k}; \end{aligned} \tag{3.36}$$

- *the laws of processes*

$$\begin{aligned} &\frac{\partial K_k}{\partial \varepsilon_{ij}} = 0, \quad \frac{\partial K_k}{\partial \varphi_{,i}} = 0, \quad \frac{\partial K_k}{\partial A_{i,j}} = 0, \quad \frac{\partial K_k}{\partial T_{,i}} = 0, \\ &\frac{\partial K_k}{\partial q_i} = -\delta_{ik} + \Pi_i^Q v_k, \qquad \frac{\partial K_k}{\partial \psi_{,i}} = 0, \quad \frac{\partial K_k}{\partial \psi^*_{,i}} = 0, \\ &\frac{\partial K_k}{\partial j_i^S} = \Pi_i^S v_k, \quad \frac{\partial K_k}{\partial j_i^c} = \mu^c\delta_{ik} + v_k\Pi_i^C; \end{aligned} \tag{3.37}$$

and

- *the residual inequality*

$$\begin{aligned} &-\frac{\partial K_k}{\partial \varphi}\varphi_{'k} + j_{k,k}^S\varphi + T\frac{\partial \Phi_k}{\partial A_i}A_{i,k} + T\frac{\partial \Phi_k}{\partial T}T_{,k} \\ &\qquad + T\frac{\partial \Phi_k}{\partial c}c_{,k} - \frac{\partial K_k}{\partial \psi}\psi_{,k} - \frac{\partial K_k}{\partial \psi^*}\psi^*_{,k} + j_i^N\mathcal{E}_i \\ &\qquad - \Pi_i^Q Q_i - \Pi_i^C J_i^C - \Pi_i^S J_i^S - \Pi^\psi\frac{\partial \psi}{\partial t} - \Pi^{\psi*}\frac{\partial \psi^*}{\partial t} \geq 0. \end{aligned} \tag{3.38}$$

The particular analysis of the above results shows that:

- the free energy density takes the form (cf. [6, 17])

$$F = F^N + F^S, \tag{3.39}$$

$$F^N = F^N\left(\varepsilon_{ij}, T, c, q_i, j_i^c, j_i^S\right), \tag{3.40}$$

$$F^S = F^S\left(\varepsilon_{ij}, T, c, A_i, \psi, \psi^*, \psi_{,k}, \psi_{,k}^*\right), \tag{3.41}$$

- the entropy flux after integration of relations (3.37) with the aid of (3.29) and the detailed investigations of the inequality (3.27), is as follows (cf.[6, 17]):

$$\Phi_k = \Phi_k^N + \Phi_k^S, \tag{3.42}$$

$$\Phi_k^N = \frac{1}{T}\left(q_k - \mu^c j_k^c\right), \tag{3.43}$$

$$\Phi_k^S = -\frac{1}{T}\left(j_k^S + \varrho\frac{\partial F}{\partial \psi_{,k}}\dot{\psi} + \varrho\frac{\partial F}{\partial \psi_{,k}^*}\dot{\psi}^*\right). \tag{3.44}$$

Remark that F^N and F^S as well as Φ_k^N and Φ_k^S are independent of each other.

We see that the dissipation (cf. (3.38)) due to the supercurrent comes from the following reasons:

- the changes in time and interactions of the Cooper pairs density with the fields from the set $\mathcal{C}$ (see (3.21),
- the relaxation properties of the supercurrent (cf. (3.20)),
- the quantum side of the superconductivity phenomenon.

To this end, the general extended thermodynamical model of superconducting, elastic and doped fullerenes has been completed. We see that the model extends the relations obtained in [3–9, 15–17] on the influence of impurities on conductivity properties and includes, consistently with the theory, the relaxation of the supercurrent.

If we, however, decide that the gauge can be chosen such that the scalar electrical potential vanishes (see (3.22)) [9], then we follow the experimental observations that the supercurrent exists reasonably long in time and we assume the local density of Cooper pairs to be constant (this approach is true in many practical situations where the local fluctuations in density of superelectrons in steady state are of such length and time scales that are too small to be of engineering interest [2]), the residual inequality (3.38) can be approximated by

$$T\frac{\partial \Phi_k}{\partial A_i}A_{i,k} + T\frac{\partial \Phi_k}{\partial T}T_{,k} + T\frac{\partial \Phi_k}{\partial c}c_{,k} + j_i^N\mathcal{E}_i - \Pi_i^Q Q_i - \Pi_i^C J_i^C \geq 0. \tag{3.45}$$

That situation leads to the following relations (cf. [2, 6]):

$$\varrho\frac{\partial F}{\partial \psi} - \left(\varrho\frac{\partial F}{\partial \psi_{,k}}\right)_{,k} = 0, \tag{3.46}$$

$$\varrho \frac{\partial F}{\partial \psi^*} - \left(\varrho \frac{\partial F}{\partial \psi^*_{i\,k}} \right)_{,k} = 0, \tag{3.47}$$

$$j^S_{k,k} = 0, \tag{3.48}$$

$$\frac{\partial K_k}{\partial \psi} = 0, \qquad \frac{\partial K_k}{\partial \psi^*} = 0 \tag{3.49}$$

and

$$\frac{\partial F}{\partial j^S_i} = 0. \tag{3.50}$$

The latter result indicates that when the relaxation of the supercurrent fluid is not taken into account, the classical nonequilibrium thermodynamical model is sufficient to describe a superconductor. However, the extended – like thermodynamical model is, in general, much more complete. It includes all the basic equations dealing with the physical interactions in superconducting fullerenes described in the paper, i.e. when the proper constitutive theory in particular situations is developed, we obtain

- from (3.3) – a generalized form of the equation of motion,
- from (3.5) – a generalized form of the heat conduction equation,
- from (3.2) and (3.19) – a generalized form of the mass diffusion equation,
- from (3.6) – (3.9) – a generalized form of the equation of electromagnetic field distribution,
- from (3.17) – a generalized form of the Ginzburg – Landau equation,
- from (3.20) – a generalized form of the first London equation,
- from (3.20) and (3.6) – a generalized form of the second London equation (cf. [2]) that is consistent with the Meissner effect.

Acknowledgement

The paper has been supported by the BW21-790/96 grant.

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POZNAŃ UNIVERSITY OF TECHNOLOGY,
INSTITUTE OF APPLIED MECHANICS,
ul. Piotrowo 3, 60-965 Poznań, Poland.

Received October 10, 1997.

Arch. Mech., 50, 3, pp. 509–519, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

Thermomechanics of forces driving singular point sets

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

G.A. MAUGIN (PARIS)

BY TREATING in parallel the balance of canonical momentum and the entropy equation, both at regular material points and at singular sets such as discontinuity fronts, it is shown that a consistent thermomechanics of such fronts can be constructed, especially with regard to shock waves and phase-transition fronts. Within this framework, two extreme singular cases are that of the classical shock-wave theory which relates dissipatively two states in adiabatic evolution, and that of the nondissipative phase transition which relates two generally dissipative states. In both cases, the driving force on the singular set is made to vanish yielding oversimplifications. This is obviously corrected by showing that if dissipation occurs at all, such a driving force should not be zero. It is in fact related to the details of what happens within a structured front and to the noninertial motion of such a front viewed as a quasi-particle. In passing, the role of a generating (thermodynamic) function for discontinuity fronts is exhibited.

1. Introduction

A TRUE THERMOMECHANICAL framework involves mechanical and energetical concepts on an equal footing. In that respect, the *energy-momentum* tensor due to relativists is the essential ingredient. Furthermore, on a phenomenological level where hidden microscopic rearrangement mechanisms reveal themselves in macroscopic irreversibilities, the *second law* of thermodynamics must play its proper role. This is agreed upon by all specialists of modern continuum mechanics, at least at all *regular material points*, i.e., those points where the field solution is smooth enough to allow for required operations of analysis. What is the situation regarding *singular* material points, those points where this smoothness working hypothesis fails? The answer to this question relates to the field theory of *defects*. It is observed that such "defects" move under the application of physical forces to the material body (*not* to the defect), e.g., the evolution of boundary data. Accordingly – cf. the principle of virtual power of d'Alembert – "forces" of a non-Newtonian, non-Lorentzian nature (they do *not* act per unit mass or charge) drive such defects and if this motion is irreversible, then the power expended by such "thermodynamical" forces must be related to the global dissipation in some way. The present paper aims at presenting elements of this true *thermomechanics* of defects when the extension sets of these defects are represented by lines

or surfaces. This includes "defects" such as cracks and dislocations on the one hand, and shock waves and phase-transition fronts on the other.

Such a thermodynamics was missing at the time when ESHELBY [1] introduced the notion of "force on a field singularity", and when PEACH and KOEHLER [2] proposed their celebrated force on a dislocation. Further progress was much fostered, in our opinion, by field-theoretical considerations of the Polish school of theoretical and applied mechanics (in particular ZORSKI [3, 4]), which led to the notion of *material force* (ROGULA [5]), i.e., forces which are co-vectors on the material manifold, and *not* vectors in physical space. It is the rational thermodynamics of such forces, which answers the above raised question. That is, not only is the concept of such forces useful by itself (e.g., the J-integral or the energy-release rate of fracture), but these forces acquire a true physical significance in their irreversible thermodynamics. This was only recently fully realized, essentially by the author and co-workers in a long series of works dealing with the mechanics of material rearrangements (e.g., [6, 7]). In these, it was finally acknowledged that *both canonical* balance equations of energy and momentum must be treated in parallel (as clearly indicated by the inclusive notion of "energy-momentum") while duly accounting for the second law of thermodynamics and the non-commutativity of integration and product of singular objects in the corresponding algebra. While such canonical balance laws are introduced in Sec. 2 for a sufficiently large class of materials, this noncommutativity, and the simultaneous roles of the two space-like and time-like canonical balance laws jointly with the second law, is well demonstrated on the case of fracture in Sec. 3. Section 4 presents those jump relations which are most useful in discussing the thermomechanics of two-dimensional singular sets. These include shock waves and phase-transition fronts, depending on which thermodynamical entities are continuous across them. The accompanying general formalism yields general results at such singular fronts through the notion of *generating function*. In particular, the formalism introduced is shown to offer a proper framework for treating shock waves in a consistent manner, which is missing in all theories which heretofore ignored the notion of driving force on such singular sets. Maxwell's equal area rule is also an application of the vanishing of such a driving force. Generalizations pertaining to other problems (solitonics) are mentioned by way of conclusion.

2. Balance equations at regular material points

For the sake of example, we consider materials whose free energy per unit volume of a reference configuration $\mathcal{K}_R$ reads $W = \overline{W}(\mathbf{F}, \theta, \alpha; \mathbf{X})$ with derivatives denoted:

$$\mathbf{T} = \partial\overline{W}/\partial\mathbf{F}, \qquad S = -\partial\overline{W}/\partial\theta, \qquad A = -\partial\overline{W}/\partial\alpha. \tag{2.1}$$

Here $\mathbf{F} = \nabla_R \chi$ is the direct motion gradient, if $\mathbf{x} = \chi(\mathbf{X}, t)$ is the direct smooth motion of the material body of material "particles" $\mathbf{X}$, $\theta > 0$ is the thermodynamical temperature, α represents a set of *internal* variables introduced to account for dissipation processes such as viscosity or plasticity, $\mathbf{T}$ is the first Piola–Kirchhoff stress, S is the entropy per unit volume of $\mathcal{K}_R$, and A is the thermodynamical force associated with α. The modelling considered is general enough to include many cases and not only the classical thermoelasticity of conductors (cf. [8, 9]). There is no inertia associated with the α variable. But the following results (Secs. 4 and 5) are practically unchanged if α relates to a true internal degree of freedom (compare [10]) and it is diffusive (cf. [10, 11]). Furthermore, W could depend on $\mathbf{F}$ only through one element of the multiplicative decomposition of $\mathbf{F}$, so that finite-strain plasticity is also included. We denote by ϱ_0, $\mathbf{p} = \varrho_0 \mathbf{v}$, $\mathbf{v} = \partial\chi/\partial t|_{\mathbf{X}}$, $\mathcal{K} = \varrho_0 \mathbf{v}^2/2$, $E = W + S\theta$, $\mathcal{H} = E + \mathcal{K}$, $\mathcal{L} = \mathcal{K} - W$, and $\mathbf{Q}$, respectively, the matter density at $\mathcal{K}_R$, the *linear* (physical) momentum, the physical velocity, the kinetic energy, the internal energy, "Hamiltonian" and "Lagrangian", all per unit volume at $\mathcal{K}_R$, and the material heat flux.

We assume that the *classical thermomechanics* of the material is known (e.g., in [8]) and, independently of boundary conditions, we list the classical balance equations valid at any *regular* material point $\mathbf{X}$ in the body at time t. This is done in the so-called Piola–Kirchhoff form assuming that no external body force is applied and there is no external supply of energy (this is only to place other effects more vividly in evidence):

- *Balance of mass*

$$\frac{\partial}{\partial t}\varrho_0|_{\mathbf{X}} = 0. \tag{2.2}$$

- *Balance of linear (physical) momentum*

$$\frac{\partial}{\partial t}\mathbf{p}|_{\mathbf{X}} - \operatorname{div}_R \mathbf{T} = \mathbf{0}. \tag{2.3}$$

- *Balance of energy*

$$\frac{\partial}{\partial t}\mathcal{H}|_{\mathbf{X}} - \nabla_R \cdot (\mathbf{T}\cdot\mathbf{v} - \mathbf{Q}) = \mathbf{0}. \tag{2.4}$$

Equation (2.2) means that ϱ_0 is *at most* a function of $\mathbf{X}$. If this is the case, then the material body is said to be materially inhomogeneous both *inertially* through ϱ_0 and *thermoelastically* (via the assumed explicit dependence of W on $\mathbf{X}$). The *heat equation* or, after division by θ, the *entropy* equation, reads (where it is assumed that $\mathbf{Q}$ goes to zero with $\nabla_R \theta$)

$$\left.\frac{\partial S}{\partial t}\right|_{\mathbf{X}} + \nabla_R \cdot (\mathbf{Q}/\theta) = \sigma^{\text{th}} + \sigma^{\text{intr}}, \tag{2.5}$$

wherein

$$\sigma^{\rm th} = -\theta^{-1}\mathbf{Q}\cdot\nabla_R(\ln\theta), \qquad \sigma^{\rm intr} = \theta^{-1}A\dot{\alpha}\,. \tag{2.6}$$

The second law of thermodynamics requires at any regular point $\mathbf{X}$ that the right-hand side of Eq. (2.5) be non-negative:

$$\sigma(\mathbf{X},t) := \sigma^{\rm th} + \sigma^{\rm intr} \geq 0. \tag{2.7}$$

The symbols ∇_R and div_R indicate the material nabla and the material divergence, respectively.

Three remarks are in order. First, Eqs. (2.2)–(2.4) are *strict* conservation laws, whereas it is *not* the case of (2.5). Second, $\mathbf{Q}$ and A must jointly satisfy the inequality (2.7) where $\sigma^{\rm th}$ and $\sigma^{\rm intr}$ are the *thermal* and *intrinsic* entropy sources, respectively. Finally, while (2.3) and (2.4) represent the invariance of the physical system under *physical* space-time changes (in $\mathbf{x}$ and t), we are missing the balance equation which relates to the invariance or lack of invariance under $\mathbf{X}$ changes (the space-like part of the space-time parametrization $\{\mathbf{X},t\}$). This equation has a status equivalent to that of energy in the sense that it is *canonical* and it pertains to the *whole* physical system. It is the equation of canonical momentum [6, 7] which, in the absence of dissipation, derives from the application of Noether's theorem. As dissipation is present, this equation here is obtained by operating on Eq. (2.3) and taking account of Eqs. (2.1). That is, applying $\mathbf{F}$ to the right of all terms in Eq. (2.3) and integrating by parts, we obtain the

• *Balance of canonical (material) momentum*

$$\frac{\partial}{\partial t}\mathcal{P}|_{\mathbf{X}} - \mathrm{div}_R\mathbf{b} = \mathbf{f}^{\rm inh} + \mathbf{f}^{\rm th} + \mathbf{f}^{\rm intr}, \tag{2.8}$$

wherein the canonical momentum, Eshelby stress, *material* force of inhomogeneity, *thermal* (material) force of quasi-inhomogeneity, and *intrinsic* (material) force of inhomogeneity are defined by

$$\mathcal{P} = -\mathbf{p}\cdot\mathbf{F}, \tag{2.9}$$

$$\mathbf{b} = -(\mathcal{L}1_R + \mathbf{T}\cdot\mathbf{F}), \tag{2.10}$$

$$\mathbf{f}^{\rm inh} = (\partial\mathcal{L}/\partial\mathbf{X})_{\rm expl}\,, \tag{2.11}$$

$$\mathbf{f}^{\rm th} = S\nabla_R\theta, \qquad \mathbf{f}^{\rm intr} = A\nabla_R\alpha. \tag{2.12}$$

The explicit material gradient must be here understood keeping the fields $\mathbf{v}$, $\mathbf{F}$, θ and α fixed. Equation (2.8) places in evidence three types of *material forces* at $\mathbf{X}$ as a result of true material inhomogeneities and quasi-inhomogeneities due to dissipative processes. The last two forces in (2.8) vanish only once thermodynamical equilibrium has been established. The first, $\mathbf{f}^{\rm inh}$, has nothing to do with dissipation and, therefore, has no corresponding term in the r-h-s of Eq. (2.7). It

should be noted that at all regular material points $\mathbf{X}$, Eq. (2.8) does not bring any new information, but for the properties just mentioned. The situation is altogether different at singular points as shown in Secs. 3 to 5. We note that (2.8), in general, is *not* a strict balance law although Eqs. (2.3) and (2.4) are.

3. The example of brittle fracture

Consider the case of the *pure* elasticity of materially homogeneous solids. Thus Eqs. (2.4) and (2.8), reduce to the following two *strict* conservation laws at all regular material points $\mathbf{X}$ in the body:

$$\frac{\partial \mathcal{H}}{\partial t}\Big|_{\mathbf{X}} - \nabla_R \cdot (\mathbf{T} \cdot \mathbf{v}) = 0, \tag{3.1}$$

$$\frac{\partial \mathcal{P}}{\partial t}\Big|_{\mathbf{X}} - \mathrm{div}_R \mathbf{b} = \mathbf{0}. \tag{3.2}$$

The question is, how does the field singularity at the tip of a uniformly progressing straight crack manifest, as this is a paradigmatic problem? We report the *thermomechanical* solution obtained by DASCALU and MAUGIN [12] for it constitutes what we called the *analytical mechanics of fracture*. Let the straight crack $\mathcal{C}$ of zero opening be the uniform limit of a sequence of *notches* of end radius δ. Call $\Gamma(\delta)$ the half-cylindrical front of the notch whose material points move in the limit at material velocity $\overline{\mathbf{V}}$. By integrating both (3.1) and (3.2) around the notch front and taking the limit we show that the *global* balance laws corresponding to (3.1) and (3.2) contain *source terms*, respectively the *energy release rate* (per unit thickness of the body), G, and the *material force* driving the crack tip, $\mathcal{F}$, such that

$$G = \lim_{\delta \to 0} \int_{\Gamma(\delta)} \mathcal{H}(\overline{\mathbf{V}} \cdot \mathbf{N})\, dA, \tag{3.3}$$

$$\mathcal{F} = -\lim_{\delta \to 0} \int_{\Gamma(\delta)} \left\{ \mathcal{L}\mathbf{N} - \mathcal{P}(\overline{\mathbf{V}} \cdot \mathbf{N}) \right\} dA, \tag{3.4}$$

and these two are such that we have the following *exact* result as δ goes to zero:

$$G = \overline{\mathbf{V}} \cdot \mathcal{F}, \tag{3.5}$$

while the second law requires that $G \geq 0$ (since we cannot solder back the faces of the crack, although they are mathematically indistinguishable). This example, although briefly evoked, shows that the (global) *material* force $\mathcal{F}$ driving the singularity *line* representing the crack tip, acquires a physical meaning only through the *dissipated power* that it expands in the velocity field $\overline{\mathbf{V}}$. This is also transparent in the case where the singularity set is a surface (see below).

4. Jump relations at a singular surface

Assume now that all equations of Sec. 2 are valid at all *regular* material points. To simplify (but this is not essential), we consider that in each *regular* material region, the material considered is homogeneous. Such regions, where the energy and symmetry properties can be different from one region to the next, are separated by mathematically idealized surfaces Σ, so-called *singular* or discontinuity surfaces. These may progress yielding a sudden change in the solution properties and/or abrupt structural rearrangements. The latter, according to EPSTEIN and MAUGIN [13] are governed by a driving force which necessarily involves the Eshelby stress tensor (2.10). Depending on the thermodynamical entities, that are continuous or discontinuous across Σ, we may treat in a unified framework the cases where Σ is a *shock* wave in the traditional sense or a *phase-transition front*. The first question to be answered is how do the *critical jump relations* look like? According to our comments, these are the jump relations associated with the *non*-strict conservation laws (2.5) and (2.8) as, according to the theory of weak solutions of hyperbolic systems, no problem arises concerning the jump relations associated with the strict conservation laws (2.2) through (2.4). Indeed, applying the rule to replace the operators $\partial/\partial t|_{\mathbf{X}}$ and ∇_R by $-(\overline{\mathbf{V}}\cdot\mathbf{N})\,[\cdot]$ and $\mathbf{N}[\cdot]$ where $\overline{\mathbf{V}}$ is the material velocity of points of Σ, and $\mathbf{N}$ is the unit normal to Σ oriented from the "minus" to the "plus" sign, with the convention that $[A] := A^+ - A^-$, one writes at once ($\overline{V}_N \equiv \overline{\mathbf{V}}\cdot\mathbf{N}$):

$$\overline{V}_N[\varrho_0] = 0, \tag{4.1}$$

$$\overline{V}_N[\mathbf{p}] + \mathbf{N}\cdot[\mathbf{T}] = \mathbf{0}, \tag{4.2}$$

$$\overline{V}[\mathcal{H}] + \mathbf{N}\cdot[\mathbf{T}, \mathbf{v} - \mathbf{Q}] = 0. \tag{4.3}$$

We can apply the same rule to Eqs. (2.5) and (2.8) if we add formally *unknown* source terms, i.e., we may *a priori* write down the following two jump equations:

$$\overline{V}_N[S] - \mathbf{N}\cdot[\mathbf{Q}/\theta] = \sigma_\Sigma\,, \tag{4.4}$$

$$\overline{V}[\mathcal{P}] + \mathbf{N}\cdot[\mathbf{b}] = -\mathbf{f}_\Sigma\,, \tag{4.5}$$

in which the surface source of entropy σ_Σ must be non-negative. This constitutes the statement of the second law at Σ:

$$\sigma_\Sigma \geq 0. \tag{4.6}$$

As to the *surface material* force – the *driving force on* Σ – its physical significance can be elucidated only by computing its power in the velocity field $\overline{\mathbf{V}}$ – just like in Eq. (3.5).

5. Shock waves and phase-transition fronts

Although we do not give the detailed proof here (cf. [14]), the following results hold true. Introduce at Σ the following quantities – which are continuous according to Eqs. (4.1) – (4.3):

$$m := \varrho_0 \overline{V}_N \,, \tag{5.1}$$

$$\mathcal{T}_\Sigma := m(\mathbf{p}/\varrho_0) + \mathbf{N}\cdot\mathbf{T}, \tag{5.2}$$

$$mQ_\Sigma := m(\mathcal{H}/\varrho_0) + \mathbf{N}\cdot(\mathbf{T}\cdot\mathbf{v} - \mathbf{Q}), \tag{5.3}$$

and the "generating" function $\mathfrak{M}$ by:

$$\mathfrak{M} := \theta^{-1}\{m(Q_\Sigma + (\mathcal{L}/\varrho_0)) - \mathcal{T}_\Sigma\cdot\mathbf{v}\}\,. \tag{5.4}$$

Then, for any singular surface Σ:

$$[\mathfrak{M}] = \sigma_\Sigma \geq 0 \tag{5.5}$$

and if $V_N^+ = V_N^- = \overline{V}_N$ (where $\mathbf{V} = -\mathbf{F}^{-1}\cdot\mathbf{v}$, $\mathbf{F}^{-1}$ being the inverse of $\mathbf{F}$ and $V_N = \mathbf{V}\cdot\mathbf{N}$), we have

$$P_\Sigma = \mathbf{f}_\Sigma\cdot\overline{\mathbf{V}} = [\theta\,\mathfrak{M}]. \tag{5.6}$$

That is, the scalar function $\mathfrak{M}$ defined at Σ generates *both* the surface entropy source *and* the power expended by the surface material force. Equation (5.5) generalizes to the case of deformable dissipative solids in finite strain a result of P. GERMAIN [15] in fluids. Equation (4.12) is new and clearly shows, contrary to the classical theory of shock waves, that one must consistently consider a *nonzero* driving force on a shock wave when entropy growth is required at Σ. That is, Eqs. (4.4) and (4.5) must be consistent, but the second of these is lacking in all heretofore-proposed approaches to the shock wave theory. As a matter of fact, the presence of a nonzero $\mathbf{f}_\Sigma$ at Σ is justified by considering a *structured* front across which both the quasi-inhomogeneity forces $\mathbf{f}^{\text{th}}$ and $\mathbf{f}^{\text{intr}}$ contribute, and this is paralleled by the source term σ^{th} and σ^{intr} in the entropy equation. The basic inconsistency in the classical presentation of shock-wave theory (no structured front) is that one relates through a *dissipative* front two regions supposed to be in adiabatic evolution. It follows from this that on the one hand one imposes the growth of entropy, while, on the other hand, the *driving force* vanishes identically. This driving force is none other than the *Hugoniot* functional. Indeed, expanding the trivial identity $[\mathcal{T}_\Sigma]\cdot\langle\mathbf{v}\rangle \equiv 0$ in the traditional shock-wave theory (no heat flux, no internal variables α), one obtains that

$$\text{Hugo}_{SW} := [E(\mathbf{F}, S) - \langle\mathbf{N}\cdot\mathbf{T}\rangle\cdot\mathbf{F}\cdot\mathbf{N}] \equiv 0. \tag{5.7}$$

But in our formalism this is indeed a *surface* material force which should *irreversibly* drive Σ. Unfortunately, $\text{Hugo}_{SW}\cdot\overline{V}_N \equiv 0$ for $\overline{V}_N \neq 0$, hence the

inconsistency, although Eq. (5.7) is extremely useful in discussing the position of the Hugoniot curve – which must be such that $[S] \geq 0$ – compared to isentropic curves.

The other interesting general case is that of phase-transition fronts as they may occur between phases of an allotropic material or between variants of a thermoelastic shape-memory alloy. In that case, the transition taking place at a definite temperature when the phases coexist and the variants match at Σ, the continuity of temperature, $[\theta] = 0$, holds at Σ and the *coherency* condition (no dislocation) at Σ makes that $[\mathbf{V}] = \mathbf{0}$. As a consequence of the first condition, Eqs. (4.4) and (5.6) yield the following remarkable result:

$$P_\Sigma = \mathbf{f}_\Sigma \cdot \overline{\mathbf{V}} = \theta[\mathfrak{R}] = \theta\sigma_\Sigma \geq 0. \tag{5.8}$$

As a consequence of the second condition and of Eqs. (4.2) and (4.3), it is shown that

$$P_\Sigma = f_\Sigma \overline{V}_N = \theta\sigma_\Sigma \geq 0 \tag{5.9}$$

with

$$f_\Sigma + \mathrm{Hugo}_{PT} = 0 \qquad \text{at} \quad \Sigma, \tag{5.10}$$

where f_Σ, a scalar driving force for which we need a *kinetic* equation, and the field functional Hugo_{PT}, balance one another. The latter is given by (compare to (5.7); cf. MAUGIN and TRIMARCO [16])

$$\mathrm{Hugo}_{PT} := \left[\overline{W}(\mathbf{F}, \alpha, \theta) - \langle \mathbf{N}\cdot\mathbf{T}\rangle \mathbf{F}\cdot\mathbf{N}\right]. \tag{5.11}$$

Compared to Hugo_{SW}, Hugo_{PT} is practically never zero since it must satisfy the inequality (5.9). However, one may *artificially* impose the vanishing of Hugo_{PT} for nonvanishing $\overline{V}_N$. This means a *nondissipative* phase transition although we relate through Σ the phases which are generally in nonadiabatic evolution ($\mathbf{Q} \neq \mathbf{0}$). This consideration thus is as much *singular* as the traditional shock-wave theory, but at another end of the spectrum. Indeed, the imposed vanishing of Hugo_{PT} for a still progressing Σ is shown in one dimension to yield *Maxwell's rule of equal area* [14] and, for a fluid, this condition in fact materializes in the continuity of the *chemical potential*. The relationship of chemical potential with the Eshelby stress (sometimes called chemical potential tensor) was noticed by BOWEN [17] and GRINFELD [18]. However, there is something more in the results (5.8) through (5.11): it is that no quasi-static hypothesis was used, although it is exactly *shown* that no kinetic energy can enter the final expression (5.11). This agrees with the perspicacious view of Gibbs and Duhem who indeed foresaw that only the free enthalpy must govern the local matter rearrangement represented by a phase transition. Thus only the quasi-static part of the Eshelby stress finally contributes to the Hugoniot functional Hugo_{PT} – in agreement with their vision.

6. Quasi-particle viewpoint and solitonics

Singular surfaces of mathematically zero thickness do not exist in the real physical world and they do find their justification only as limits of narrow zones of rapid, but not discontinuous, changes. Consider then that such a narrow zone Σ_δ of thickness $\delta \ll L$ where L is a macroscopic characteristic length, exists. We may look at the problem encapsulated in equations of Sec. 2 by looking at Σ_δ with a magnifying glass (so-called "zooming") so that the thickness becomes of order one. Σ_δ may locally be considered as flat and the problem is essentially one-dimensional (coordinate X orthogonal to Σ_δ). In this procedure the boundaries on both sides of Σ_δ are rejected to minus and plus infinity with field derivatives – essentially zero – outside the interval δ, in particular at $X = \pm\infty$. Henceforth we consider field solutions which are localized at Σ_δ. The "global" and canonical equations that govern the "complex" of fields along the real line are the space (along X) integrals of Eqs. (2.8) and (2.5). On account of limit conditions at infinities, these read

$$\frac{d\mathbb{P}}{dt} = \mathbb{F}, \qquad \frac{d\mathbb{S}}{dt} = \mathcal{S} \geq 0, \tag{6.1}$$

where $\mathbb{P}$ and $\mathbb{S}$ are the total canonical momentum and entropy defined by

$$\mathbb{P} = \int_{\mathbb{R}} \mathcal{P}\, dX, \qquad \mathbb{S} = \int_{\mathbb{R}} S\, dX, \tag{6.2}$$

and $\mathbb{F}$ is the driving force on Σ_δ, and $\mathcal{S}$ – the entropy source due to dissipation throughout Σ_δ:

$$\mathbb{F} = \int_{\mathbb{R}} \left(\mathbf{f}^{\text{inh}} + \mathbf{f}^{\text{th}} + \mathbf{f}^{\text{intr}}\right) dX, \qquad \mathcal{S} = \int_{\mathbb{R}} \left(\sigma^{\text{th}} + \sigma^{\text{intr}}\right) dX. \tag{6.3}$$

Here all integrals are summed over $\mathbb{R}$, but in practice over the δ interval only. Equation (6.1) may be viewed as referring to a *quasi-particle* motion where $\mathbb{P}$ relates to the whole "complex" of fields (and not only the traditional continuum motion). When $\mathbb{F} = \mathbf{0}$, the "motion" of the quasi-particle is *inertial*. In the presence of true or quasi-inhomogeneities, it is *not*. But it is only when there are quasi-inhomogeneities that $\mathbb{S}$ must simultaneously grow in time. That is, in this case the *varied* (noninertial) motion of the quasi-particle is necessarily accompanied by dissipation. If the "complex" of fields at Σ_δ moves "en bloc" with velocity $\overline{\mathbf{V}}$, (assuming then that the localized field solution is a progressive wave with $\overline{\mathbf{V}}$ slowly varying in time, then in the first approximation we have the consistency condition

$$\frac{d\mathbb{P}}{dt} = \mathbb{F}, \qquad \frac{d\mathbb{H}}{dt} = +\mathbb{F}\cdot\overline{\mathbf{V}}, \tag{6.4}$$

where $\mathbb{H}$ is the total energy. The condition $(6.4)_2$ is analogous to (3.5). If Σ_δ is a phase-transition front instead of $(6.4)_2$, we can as well write

$$\frac{d\mathbb{S}}{dt} = -\langle\theta\rangle^{-1}\mathbb{F}\cdot\overline{\mathbf{V}} \geq 0. \tag{6.5}$$

The condition is more complicated for a shock-wave when θ varies rapidly through Σ_δ.

When one studies phase-transition fronts in shape-memory alloys by means of progressive-wave fronts in the appropriate dispersive – $W = \overline{W}(\mathbf{F}, \nabla_R\mathbf{F}, \theta)$ in [19] – but nondissipative framework, one then arrives at *solitonic* solutions which correspond to an *inertial* motion of the quasi-particle representing the "complex" of fields, with zero right-hand side in both Eqs. (6.4) and (6.5). As a matter of fact, such solutions have been shown to obey the *Maxwell* rule of equal area, cf. [19] – in agreement with Sec. 5 above – with a vanishing Hugoniot driving force where the jump is taken between values at infinities in reason of the zoom operation. Thus, as we know from the soliton theory, the full equations (6.4) and (6.5) are useful in treating transient motions by means of perturbations. Whether the wave front is really a solitonic structure or a dissipative structure depends on the studied system. The nonstrict observation of the conservation of global quantities $\mathbb{P}$ and $\mathbb{H}$ in a numerical scheme may also be an indicator that this scheme is not faithful (*not* conservative), introducing then dissipation artificially (cf. Eq. (6.5)). In all, we see that the notions of *material force* and *canonical momentum* play a role at two different levels of observation of two-dimensional singular sets, whether the latter are seen as mathematical idealizations with the accompanying necessary oversimplification, or as structured fronts which generally require accounting for more detailed effects such as dissipation and dispersion. The general thermomechanics presented in Ref. [8] accounts for both. A local analysis in the last direction – but not using the notions introduced in these pages – is due to TRUSKINOWSKY [22].

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UNIVERSITE PIERRE ET MARIE CURIE
LABORATOIRE DE MODELISATION EN MECANIQUE
Tour 66, 4 place Jussieu, Case 162
75252 Paris Cedex 05, France.
e-mail: gam@ccr.jussieu.fr

Received September 19, 1997.

Arch. Mech., 50, 3, pp. 521–530, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

Pseudomomentum in relativistic continuum mechanics

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

G.A. MAUGIN (PARIS) and L. RESTUCCIA (MESSINA)

IN CLASSICAL continuum mechanics the balance or unbalance equation of *pseudomomentum* reflects the material invariance of the system under study. It relates the time derivative of pseudo-momentum and the flux of the *Eshelby stress*. It is legitimate to inquire whether this structure is conserved in a *relativistic four-dimensional* background. We examine here the relativistic definition of *pseudo/material* momentum using simultaneously variational and direct approaches (the latter using the canonical projection of space-time onto the material manifold). It appears that the truly *material entities*, just as those in a proper frame, should be the basic ones, being independent of the relativity framework used.

1. Introduction

THE NOTION of *pseudomomentum* in a continuum is so much intriguing that Sir Rudolph Peierls, a sharp observer of the physical scene, recurrently came back to that subject matter [1–3]. In nondissipative continua described in the usual Newtonian background, pseudomomentum is none other than the *canonical momentum* of *analytical continuum mechanics* [4–6]. It has thus an ontologial status which equals that of *energy*, i.e. it is the *spatial* part of a four-dimensional vectorial object or, equivalently, the mixed space-time part of a four-dimensional second-order tensor known as the canonical *energy-momentum tensor* [7]. The remarkable facts about pseudomomentum are that (i) unless the considered body is rigid, it is different from *physical momentum* (the "quantity of motion" in classical mechanics), (ii) one part of it plays a fundamental role in *crystal physics* under the name of *crystal momentum* [8], and in *electromagnetic optics* and *wavelike* phenomena under the name of *wave momentum* whether in optics or acoustics [1, 9, 10], (iii) it does play a role in the discussion of the notion of *electromagnetic momentum* in the electrodynamics of magnetized and polarized bodies [9, 11–13], and (iv) in *global form* its conservation or *non*conservation plays both a theoretical and computational role in the *dynamics of fracture* in elastic [14, 15] or inelastic [16] solids and in the *dynamics of perturbed solitonic structures* [17]. Its role in elastic solids was also recognized by other authors [18, 19]. Syntheses emphasizing the last two aspects are given in book form [20] and in two more recent review papers [21, 22].

The balance or *unbalance of pseudomomentum* of the Newtonian mechanics of continua is related to the invariance with respect to *material coordinates*, i.e. it expresses the material homogeneity or inhomogeneity of the material, while the balance of energy relates to the invariance with respect to *time*, and the balance of *physical momentum* (momentum in the *current configuration*) relates to the homogeneity of *physical space* (and *not* of the material). As shown in previous papers, all material inhomogeneities, whether of inertial, elastic or inelastic origins, are captured by the balance of pseudomomentum. Although pseudomomentum is naturally defined in a Lagrangian - Hamiltonian variational context [6, 20], it can also be given an intrinsic differential-geometrical definition (it is the natural pull-back of physical momentum to the material manifold, up to a sign, or: it is the *material covector associated, via the deformed metric, with the inverse-motion velocity*). These definitions were first given by one of the authors [6, 11]. Because of the intimate relationship between the notions of pseudomomentum and invariance, it is a natural move to look at the notion of pseudomomentum in the *relativistic* framework. In doing so we will essentially build on the approach to relativistic continuum mechanics advocated by GROT and ERINGEN [23] and MAUGIN [24, 25] - see also Chapter 16 in Ref. [26] - while recognizing our debt to pioneering works by ROGULA and KURLANDZKI [27, 28].

2. Inverse-motion description

As we know in relativistic continuum mechanics, the kinematics is best described in terms of the *inverse motion*, that is: if x^α, $\alpha = 1, 2, 3, 4, x^4$ timelike, is the actual placement of a material point X in the Riemannian physical spacetime $\mathcal{V}^4$ with metric $g_{\alpha\beta}$ of Minkowskian signature +2, then the matter deformation is described by the (here supposedly) regular mapping [23 - 26]

$$X^K = \overline{X}^K(x^\alpha), \qquad K = 1, 2, 3, \tag{2.1}$$

where X^K designate the local coordinates of the material point X on the *material manifold* $\mathcal{M}^3$, the set of *material points*. The latter has a geometry which in general is part of the solution, i.e., it is induced by the space-time metric. World lines $\mathcal{C}_X$ of material particles X in $\mathcal{V}^4$ are given by the parametrization

$$\mathcal{C}_X : x^\alpha = \overline{x}^\alpha\left(X^K, \tau\right), \tag{2.2}$$

where τ is the so-called *proper time* of X. Local spatial sections of $\mathcal{V}^4$ at $\mathbf{x} \in \mathcal{C}_X$ are defined by means of the *projector* or spatial metric

$$P_{\alpha\beta} = g_{\alpha\beta} + c^{-2}u_\alpha u_\beta = P_{\beta\alpha}, \tag{2.3}$$

a symmetric idempotent operator, where u^α is the four-velocity, a field tangent to $\mathcal{C}_X$ and normalized in such a way that $g_{\alpha\beta}u^\alpha u^\beta + c^2 = 0$, where c is the velocity

of light in vacuum. Obviously, $P_{\alpha\beta}$ and u^α satisfy the orthogonality condition $P_{\alpha\beta}u^\beta = 0$. Any space-time geometric object which admits $\mathbf{u}$ as a null vector is said to be "*essentially spatial*". The main ingredient of deformation theory is the *inverse motion gradient* $\mathbf{F}^{-1}$ defined from (2.1) by

$$\mathbf{F}^{-1} := \{\nabla_\mu \mathbf{X}\} = \left\{X^K_\mu \equiv X^K_{,\mu};\quad K = 1,2,3;\quad \mu = 1,2,3,4\right\} \tag{2.4}$$

which is such that

$$\mathbf{u}\cdot\mathbf{F}^{-1} = D_u\mathbf{X} = 0, \qquad D_u := u^\alpha\nabla_\alpha = \frac{D}{D\tau}. \tag{2.5}$$

In Eqs. (2.5) D_u denotes the invariant directional derivative or gradient in the u^α-direction.

In essence $(2.5)_1$ means that τ and the X^K are good independent time and space coordinates in the parametrization (2.2). From $\mathbf{F}^{-1}$ one constructs the following space-time invariant which acts as reciprocal deformed metric on $\mathcal{M}^3$ (T – transpose):

$$\mathbf{C}^{-1} := \mathbf{F}^{-1}.\left(\mathbf{F}^{-1}\right)^T, \qquad \text{i.e.} \qquad \mathbf{C}^{-1}{}_{KL} = X^K_\alpha X^L_\beta g^{\alpha\beta} = X^K_\alpha X^L_\beta P^{\alpha\beta}. \tag{2.6}$$

This establishes the *canonical projection* of $\mathcal{V}^4$ onto $\mathcal{M}^3$. General relativistic elastic materials were first described by means of this procedure in Ref. [24].

3. Balance equations for elastic materials

In a *nondissipative* relativistic background these balance laws consist *a priori* of the law of conservation of *mass* and *energy-momentum*. Let $\varrho_0(\mathbf{X})$ be the mass density at X on $\mathcal{M}^3$ and $\varrho(x^\alpha)$ the matter density at x^α in $\mathcal{V}^4$, where $\mathbf{X}$ and x^α are related by (2.1). These two densities are related by [26]

$$\varrho\,(x^\alpha) = \varrho_0(\mathbf{X})\ \left(\det \mathbf{C}^{-1}\right)^{1/2}. \tag{3.1}$$

For a *purely elastic* material body the other balance laws can be derived from a Hamiltonian–Lagrangian variational principle. To that purpose we consider the following Lagrangian density per unit volume of $\mathcal{V}^4$ at x^α [27]

$$\mathcal{L} = \overline{\mathcal{L}}\,(\mathbf{X}, \nabla_\mu \mathbf{X})\,, \tag{3.2}$$

where, for the sake of simplicity, we do not envisage metric-dependent effects. The Lagrangian (3.2) describes the response of elastic materials, irrespectively of their anisotropy and material homogeneity, as an explicit dependence on the "particle" X through $\mathbf{X}$ obviously indicates *material inhomogeneity*. The only restriction present in (3.2) is that elasticity manifests only through the *first*

gradient of $\mathbf{X}$, and this materializes interactions of a *local* type involving no dispersion (i.e. no characteristic length). In (3.2) according to (2.1), the X^K are the fields and the x^α are the parameters. Thus the *field equations* are given by the following evident Euler–Lagrange equations:

$$\frac{\delta \mathcal{L}}{\delta \mathbf{X}} := \left(\frac{\partial \mathcal{L}}{\partial \mathbf{X}}\right)_{\text{expl}} - \nabla_\mu \frac{\partial \mathcal{L}}{\partial (\nabla_\mu \mathbf{X})} = 0, \tag{3.3}$$

or

$$\nabla_\mu \underline{\mathfrak{S}}^\mu = \mathbf{f}^{\text{inh}}, \qquad \text{where} \quad \underline{\mathfrak{S}}^\mu := \frac{\partial \mathcal{L}}{\partial (\nabla_\mu \mathbf{X})}, \quad \mathbf{f}^{\text{inh}} := \left(\frac{\partial \mathcal{L}}{\partial \mathbf{X}}\right)_{\text{expl}} \tag{3.4}$$

For all practical purposes $\underline{\mathfrak{S}}^\mu$ is a four-vector in space-time $\mathcal{V}^4$ and $\mathbf{f}^{\text{inh}}$ is a co-vector on $\mathcal{M}^3$ (whose components in $\mathcal{V}^4$ are pure scalars!); but $\underline{\mathfrak{S}}^\mu$, just like $\nabla_\mu \mathbf{X}$ but with opposite variance, is a good example of a two-point tensor field, so that Eq. $(3.4)_1$ is indeed a co-vector equation on $\mathcal{M}^3$.

Through Noether's celebrated theorem, the variation of the *parameters* x^α of the description (3.2), yields the *conservation law of energy-momentum* as

$$\nabla_\mu T^\mu_{\cdot\nu} = 0, \tag{3.5}$$

with a *canonical* stress-energy-momentum tensor classically defined by (compare to [7], Sec. 32)

$$T^\mu_{\cdot\nu} = -\left(\mathcal{L}\delta^\mu_\nu - \nabla_\nu \mathbf{X} \cdot \frac{\partial \mathcal{L}}{\partial (\nabla_\mu \mathbf{X})}\right), \tag{3.6}$$

where the dot indicates summation over the K's of $\mathbf{X}$.

On account of (3.1) that is already in integrated form, and the fact that $\mathcal{L}$ must be at least Lorentz-invariant, there follows that

$$P_{\beta[\mu} \nabla_{\nu]} \mathbf{X} \cdot \frac{\partial \mathcal{L}}{\partial (\nabla_\beta \mathbf{X})} = 0, \tag{3.7}$$

where square brackets indicate skew-symmetrization. Equations $(3.4)_1$, and (3.5) exhaust the list of available balance equations. A natural question is whether these last two equations are independent. The answer is negative. Indeed, multiplying $(3.4)_1$ scalarly on $\mathcal{M}^3$ by $\nabla_\nu \mathbf{X}$, integrating by parts and noting that $X^K_{,\mu\nu} = X^K_{,\nu\mu}$ (remember that the X^K are just scalars in so far as space-time transformations are concerned), we obtain that

$$(\nabla_\nu \mathbf{X}) \cdot \left(\nabla_\mu \underline{\mathfrak{S}}^\mu - \mathbf{f}^{\text{inh}}\right) + (\nabla_\mu T^\mu_{\cdot\nu})_\perp = 0, \tag{3.8}$$

where the symbol $(..)_\perp$ means the space-like part obtained by full projection, i.e. in the present case

$$(\nabla_\mu T^\mu_{\cdot\nu})_\perp \equiv P_\nu^{\cdot\beta} \nabla_\mu T^\mu_{\cdot\beta}, \qquad u^\nu (\nabla_\mu T^\mu_{\cdot\nu})_\perp \equiv 0. \tag{3.9}$$

Equation (3.8) means that $(3.4)_1$ entails the spatial part of (3.5). The reciprocal statement is true although its proof is more tedious. Equation (3.8) is a relativistic dynamical statement that generalizes the Ericksen identity known for classical finite-strain elastostatics [29]. The timelike complement of (3.8) is none other than the *energy equation* which obviously reads [23]

$$u^\nu \nabla_\mu T^\mu_{.\nu} = 0, \tag{3.10}$$

so that, instead of (3.8) and (3.10) we could as well write the generalized Ericksen identity:

$$(\nabla_\nu \mathbf{X}) \cdot \left(\nabla_\mu \underline{\mathfrak{T}}^\mu - \mathbf{f}^{\text{inh}}\right) + c^{-2} u_\nu \left(u^\alpha \nabla_\mu T^\mu_{.\alpha}\right) + \nabla_\mu T^\mu_{.\nu} = 0. \tag{3.11}$$

While Eq. (3.5) is properly written in covariant form with space-time parameters and operations, we notice that the same is not true of Eq. $(3.4)_1$ on the material manifold because $\underline{\mathfrak{T}}^\mu$ still is a two-point tensor field whereas one would certainly prefer to have at hand an entirely material equation, i.e. a truly *canonical* equation fully independent of the space-time representation. That equation in classical continuum mechanics is the balance of *pseudomomentum* or *canonical material momentum* [11].

4. Balance of pseudomomentum

This equation should involve a Lagrangian density per unit volume in material space $\mathcal{M}^3$ at X and *material time* and space differentiations. Let

$$\nabla^\perp_\alpha \equiv P^{.\beta}_\alpha \nabla_\beta = \nabla_\alpha + c^{-2} u_\alpha D_u, \qquad J := \left(\det \mathbf{C}^{-1}\right)^{-1/2}. \tag{4.1}$$

Multiplying $(3.4)_1$ by J we obtain

$$J\left(\nabla^\perp_\mu + c^{-2} u_\mu D_u\right) \cdot \underline{\mathfrak{T}}^\mu = \mathbf{f}^{\text{inh}}_0, \tag{4.2}$$

where

$$\mathcal{L}_0 = J\mathcal{L}, \qquad \mathbf{f}^{\text{inh}}_0 = \left(\frac{\partial \mathcal{L}_0}{\partial \mathbf{X}}\right)_{\text{expl}}. \tag{4.3}$$

This should be the equation looked for. This goal is reached by integrating by parts and rearranging terms. We note that

$$\nabla^\perp_\mu = X^L_\mu \nabla_L, \qquad \nabla_L \equiv \partial/\partial X^L, \qquad \nabla_L \left(J X^L_\mu\right) \equiv 0. \tag{4.4}$$

On account of $(4.3)_1$ and the fact that J depends on $\mathbf{F}^{-1}$ through $\mathbf{C}^{-1}$, we let the reader prove that

$$J \nabla^\perp_\mu \cdot \underline{\mathfrak{T}}^\mu = \nabla_K b^K_{.L}, \qquad b^K_{.L} \equiv X^K_\mu \frac{\partial \mathcal{L}_0}{\partial X^L_\mu} - \mathcal{L}_0 \delta^K_L. \tag{4.5}$$

Notice that the material object **b** defined by $(4.5)_2$ is formally the material analogue of $T^{\mu}_{.\nu}$ (but the latter is not essentially spatial). This is indeed the *material energy-momentum tensor* called *Eshelby stress*. Furthermore, with the obvious condition that $u_\mu \dfrac{\partial \mathcal{L}_0}{\partial(\nabla_\mu \mathbf{X})} = 0$, we show that

$$c^{-2} J u_\mu D_u \left(\frac{\partial \mathcal{L}}{\partial \nabla_\mu X^K} \right) = -c^{-2} \left(\frac{\partial \mathcal{L}_0}{\partial \nabla_\mu X^K} - \mathcal{L}_0 x^\mu_K \right) D_u u_\mu \,, \tag{4.6}$$

where x^μ_K is such that

$$x^\mu_K = P^\mu_{.\nu} \frac{\partial x^\nu}{\partial X^K}, \qquad x^\mu_K u_\mu = 0, \qquad x^\mu_K X^K_\nu = P^\mu_{.\nu}, \qquad X^K_\nu x^\nu_L = \delta^K_L \,. \tag{4.7}$$

But

$$\frac{\partial \mathcal{L}_0}{\partial \nabla_\mu X^K} - \mathcal{L}_0 x^\mu_K = \frac{\partial \mathcal{L}_0}{\partial \nabla_\nu X^K} P^\mu_{.\nu} - \mathcal{L}_0 \delta^L_K x^\mu_L = b^L_{.K} x^\mu_L \tag{4.8}$$

as a result of $(4.7)_3$. Thus Eq. (4.2) reads in components

$$\nabla_K b^K_{.L} - c^{-2} b^K_{.L} x^\mu_K D_u u_\mu = \left(f_0^{\text{inh}} \right)_L . \tag{4.9}$$

Because of $(4.7)_2$ this can also be written as

$$\nabla_K b^K_{.L} + c^{-2} b^K_{.L} u_\mu D_u x^\mu_K = \left(f_0^{\text{inh}} \right)_L . \tag{4.10}$$

This is the fully material equation of linear momentum looked for, in which we identify the materially co-variant *inhomogeneity force* $\mathbf{f}_0^{\text{inh}}$ and the *Eshelby material stress* **b**. The material or *pseudo*-momentum, being of inertial origin, is *not* obviously present in this formulation without expliciting the Lagrangian density.

5. Explicit forms

The Lagrangian density should account for the rest and internal energies since kinetic energy is not "apparent" in the relativistic framework. For a generally anisotropic, materially inhomogeneous elastic solid, the internal energy per unit proper mass reads $\in = \overline{\in}\,(\mathbf{X}; \nabla_\mu \mathbf{X})$ or, in *objective form*, i.e. as a form-invariant expression in space-time $\mathcal{V}^4$,

$$\in = \overline{\in}\left(\mathbf{X}; \mathbf{C}^{-1}\right). \tag{5.1}$$

As a matter of fact, this is an integral of the first-order system provided by the Lorentz-invariance condition (3.7). The result is purely *material*, and is thus

invariant by all means in so far as transformations of physical space-time are concerned, that is. whether the latter is Galilean, Minkowskian or Einsteinian (i.e., accounting for general relativistic effects). Such a general invariance was perceived by pioneers of "good" relativistic continuum mechanics such as OLDROYD [30].

The Lagrangian densities $\mathcal{L}_0$ and $\mathcal{L}$ are given by

$$\begin{aligned} \mathcal{L}_0 &= -\varrho_0(\mathbf{X})c^2\left(1+\frac{\in}{c^2}\right), \\ \mathcal{L} &= -\varrho c^2\left(1+\frac{\in}{c^2}\right) = -\varrho_0(\mathbf{X})c^2\left(\det\mathbf{C}^{-1}\right)^{1/2}\left\{1+\frac{1}{c^2}\overline{\in}\left(\mathbf{X};\mathbf{C}^{-1}\right)\right\}. \end{aligned} \tag{5.2}$$

In an *inertial* frame (noted by the equality sign $\overset{*}{=}$) at the nonrelativistic limit, expression $(5.2)_1$ yields

$$\mathcal{L}_0 = \varrho_0(\mathbf{X})g_{\alpha\beta}u^\alpha u^\beta\left(1+\frac{\in}{c^2}\right) \overset{*}{=} -\varrho_0(\mathbf{X})\left(1+\frac{\in}{c^2}\right)\left(1-\beta^2\right)^{1/2}, \tag{5.3}$$

where $\beta^2 = \mathbf{v}^2/c^2$ if $\mathbf{v}$ is the physical velocity of matter. For small β this yields

$$\mathcal{L}_0 = \varrho_0(\mathbf{X})\frac{\mathbf{v}^2}{2} - \varrho_0 \in \left(\mathbf{X};\mathbf{C}^{-1}\right) = \varrho_0(\mathbf{X})\frac{\mathbf{v}^2}{2} - W\left(\mathbf{X};\mathbf{C}^{-1}\right), \tag{5.4}$$

which is a possible Lagrangian density per unit volume in the reference configuration in classical finite-strain elasticity [14, 20]. In the same approximation where

$$\begin{aligned} &g_{\alpha\beta} \overset{*}{=} \operatorname{diag}(+1,+1,+1,-1), \\ &u^\alpha \overset{*}{=} (\gamma\mathbf{v},\gamma c), \qquad i=1,2,3, \quad \gamma \equiv \left(1-\beta^2\right)^{-1/2} \end{aligned} \tag{5.5}$$

as β goes to zero we find that Eq. (2.5) reduces to

$$\mathbf{v} + \mathbf{F}_*\cdot\mathbf{V} \overset{*}{=} 0, \tag{5.6}$$

where $\mathbf{F}_*$ is the nonrelativistic direct-motion gradient and $\mathbf{V}$ is the so-called *material velocity*. With a general motion now described by either $\mathbf{x} = \chi(\mathbf{X},t)$ or $\mathbf{X} = \chi^{-1}(\mathbf{x},t)$, respectively in the direct and inverse-motion descriptions, $\mathbf{v}$, $\mathbf{F}_*$, $\mathbf{V}$, $\mathbf{F}_*^{-1}$ and $\mathbf{C}_*^{-1}$ are given by (compare [14, 20])

$$\begin{aligned} &\mathbf{v} = \left.\frac{\partial\chi}{\partial t}\right|_{\mathbf{X}}, \qquad \mathbf{F}_* = \left.\frac{\partial\chi}{\partial\mathbf{X}}\right|_t, \qquad \mathbf{V} = \left.\frac{\partial\chi^{-1}}{\partial t}\right|_{\mathbf{x}}, \\ &\mathbf{F}_* = \left.\frac{\partial\chi^{-1}}{\partial\mathbf{x}}\right|_t, \qquad \mathbf{C}_*^{-1} = \mathbf{F}_*^{-1}\left(\mathbf{F}_*^{-1}\right)^T. \end{aligned} \tag{5.7}$$

We readily check that

$$\mathbf{C}^{-1} = \mathbf{C}_*^{-1} - c^{-2}\mathbf{V}\otimes\mathbf{V}, \qquad \det\mathbf{C}^{-1} \overset{*}{=} \left(1-\beta^2\right)\det\left(\mathbf{F}_*^{-1}\right)^2 \geq 0. \tag{5.8}$$

The nonrelativistic pseudomomentum, a *material co-vector*, is usually defined by

$$\boldsymbol{\mathcal{P}} = -\varrho_0(\mathbf{X})\mathbf{F}_*^T\cdot\mathbf{v} = \varrho_0(\mathbf{X})\mathbf{C}\cdot\mathbf{V}, \tag{5.9}$$

where $\mathbf{V}$ is such that (cf. Eq. (5.6)) $\mathbf{V} = -\mathbf{F}_*^{-1}\cdot\mathbf{v}$.

We easily check that (cf. Eq. (5.8))

$$\mathbf{C} \overset{*}{=} \mathbf{C}_* + \frac{1}{\varrho_0^2 c^2}\boldsymbol{\mathcal{P}}\otimes\boldsymbol{\mathcal{P}}. \tag{5.10}$$

The closest we can come to the definition of a relativistic (material) pseudomomentum is

$$\boldsymbol{\mathcal{P}} \overset{\text{def}}{=} -\frac{1}{c^2}\mathcal{L}_0 u_\alpha \frac{\partial x^\alpha}{\partial \mathbf{X}}, \tag{5.11}$$

where x^α and $\mathcal{L}_0$ are given by $x^\alpha = \overline{x}^\alpha(\mathbf{X},\tau)$ and Eq. $(5.2)_1$. This, indeed, reduces to the classical definition $(5.9)_1$ in the nonrelativistic limit. This can be complemented by a fourth – timelike – component $\mathcal{P}_4$ such that $\mathcal{P}_4 = \varrho_0\left(c^2 + \in\right)$, i.e., the total energy density and then both this and (5.11) enter a unique four-dimensional definition ($\Delta = 1,2,3,4$)

$$\mathcal{P}_\Delta = -\frac{1}{c^2}\mathcal{L}_0 u_\alpha \frac{\partial x^\alpha}{\partial X^\Delta}, \qquad X^\Delta = \left(X^K,\tau\right), \qquad u^\alpha \equiv \frac{\partial x^\alpha}{\partial \tau}. \tag{5.12}$$

Returning now to the relativistic expression (5.2) we immediately show that

$$\frac{\partial\mathcal{L}}{\partial X_\mu^K} = -\varrho\frac{\partial\overline{\in}}{\partial\mathbf{C}^{-1}} : \frac{\partial\mathbf{C}^{-1}}{\partial X_\mu^K} + \frac{1}{2}\varrho_0\left(\det\mathbf{C}^{-1}\right)^{-3/2}\frac{\partial\left(\det\mathbf{C}^{-1}\right)}{\partial X_\mu^K}. \tag{5.13}$$

But

$$\begin{aligned}
\frac{\partial\left(\mathbf{C}^{-1}\right)^{MN}}{\partial X_\mu^K} &= \left(\delta_K^M X_\alpha^N + \delta_K^N X_\alpha^M\right)P^{\alpha\mu},\\
\frac{\partial\left(\det\mathbf{C}^{-1}\right)}{\partial X_\mu^K} &= 2\left(\det\mathbf{C}^{-1}\right)x_K^\mu,
\end{aligned} \tag{5.14}$$

from which it follows on account of $\delta_\beta^\alpha - P_{.\beta}^\alpha = -c^{-2}u^\alpha u_\beta$ that

$$T_{.\nu}^\mu = \varrho\left(1+\frac{\in}{c^2}\right)u^\mu u_\nu - t_{.\nu}^\mu, \tag{5.15}$$

wherein

$$t_{\mu\nu} = -2\varrho \frac{\partial \overline{\in}}{\partial (\mathbf{C}^{-1})^{KL}} X_\mu^K X_\nu^L = t_{\nu\mu}, \quad t_{\mu\nu} u^\nu = 0. \tag{5.16}$$

The latter quantity is the relativistic stress *per se* (an essentially spatial tensor) for a description based on the inverse motion [23, 24, 31], while the energy-momentum tensor (5.15) admits the standard space-time decomposition which, in the absence of heat flow, microstructure, and electromagnetic fields, presents no mixed space-time and time-space elements. From (5.16) we see that the spatial relativistic stress is none other than the "*push forward*" of the *covariant material stress* T_{KL} defined thermodynamically by (Note: this is *not* the second Piola–Kirchhoff stress, which is materially contravariant) $T_{KL} = -2\varrho \dfrac{\partial \overline{\in}}{\partial (\mathbf{C}^{-1})^{KL}}$.

Acknowledgment

This research was started while L.R. visited the LMM in Paris (CNR-CNRS Exchange program) and G.A.M. visited the Accademia Peloritana dei Pericolanti di Messina.

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LABORATOIRE DE MODELISATION EN MECANIQUE,
UNIVERSITE PIERRE ET MARIE CURIE, PARIS, FRANCE
e-mail: gam@ccr.jussieu.fr.
and
DIPARTIMENTO DI MATEMATICA,
UNIVERSITA DI MESSINA, MESSINA, ITALY
e-mail: lrest@dipmat.unime.it

Received October 10, 1997.

Arch. Mech., 50, 3, pp. 531–539, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

On effecting averages and changes of scale via weighting functions

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

A.I. MURDOCH (STRATHCLYDE, GLASGOW)

WEIGHTING FUNCTIONS can be used to derive continuum equations of balance from molecular considerations, and to obtain equations governing fluid flow through porous media. The methodology of such (scale-dependent) averaging is outlined, and physical implications of specific choices of weighting function are discussed.

1. Introduction

IT IS THE PURPOSE of this note to indicate a procedure by which concepts and governing equations of one description of material behaviour can be related to those of a "coarser" description of this behaviour. The methodology employs weighting functions, and is here exemplified in two contexts. The first concerns the precise derivation of continuum equations of balance for a material system from a microscopic description in which molecules are modelled as interacting point masses. The second involves fluid flow through a porous body. Starting from a small-scale description in which pores are manifest, and flows therein are governed by the Navier–Stokes equation, a corresponding equation is determined for a large-scale description (wherein all fluid-related fields are defined throughout the region occupied by fluid *and* porous body: it is at this scale that Darcy's "law" may apply).

The transition from the discrete viewpoint to its continuum counterpart is treated in Sec. 2. A discussion of the basic physics associated with different choices of weighting function is presented in Sec. 3. Porous body considerations are addressed in Sec. 4. Some applications of the results of Secs. 2 and 4 are outlined in Sec. 6.

2. Continuum relations from a discrete model

Consider a material system $\mathcal{M}$ of distinguishable molecules, modelled as a system of interacting point masses labelled P_i $(i = 1, 2, \ldots, N)$, whose masses, locations, and velocities at time t are denoted by m_i, $\mathbf{x}_i(t)$, and $\mathbf{v}_i(t)$, respectively.

The mass density distribution appropriate to choice w of weighting function is ϱ_w, where

$$\varrho_w(\mathbf{x}, t) := \sum_{i=1}^{N} m_i w(\mathbf{x}_i(t) - \mathbf{x}). \tag{2.1}$$

Here w assigns greater contributions to the sum from particles near the geometrical point $\mathbf{x}$ than those far from $\mathbf{x}$: more details will be discussed later. Holding $\mathbf{x}$ fixed,

$$\begin{aligned} \frac{\partial \varrho_w}{\partial t} = \sum_{i=1}^{N} m_i \nabla w.\mathbf{v}_i &= -\sum_{i=1}^{N} m_i \nabla_{\mathbf{x}} w.\mathbf{v}_i \\ &= -\sum_{i=1}^{N} m_i \operatorname{div}_{\mathbf{x}}\{\mathbf{v}_i w\} = -\operatorname{div} \mathbf{p}_w\,, \end{aligned} \tag{2.2}$$

where

$$\mathbf{p}_w(\mathbf{x}, t) := \sum_{i=1}^{N} m_i \mathbf{v}_i(t) w(\mathbf{x}_i(t) - \mathbf{x}). \tag{2.3}$$

Defining the corresponding velocity field $\mathbf{v}_w$ (wherever $\varrho_w \neq 0$) by

$$\mathbf{v}_w := \mathbf{p}_w / \varrho_w \tag{2.4}$$

yields, from (2.2) and (2.3), the continuity equation

$$\partial \varrho_w / \partial t + \operatorname{div} \varrho_w \mathbf{v}_w = 0. \tag{2.5}$$

In the foregoing the only restriction upon w is that it be differentiable: to ensure spatial smoothness of ϱ_w and $\mathbf{v}_w$ it should be of class C^1. To make physical sense it is necessary that

$$\int_{\text{all space}} \varrho_w = \text{total mass} = \sum_{i=1}^{N} m_i\,. \tag{2.6}$$

This requirement, in the case of $\mathcal{M}$ consisting of a single particle, mandates

$$\int_{\text{all displacements}} w = 1. \tag{2.7}$$

The normalisation condition (2.7) suffices to deliver (2.6) in general.

Linear momentum balance is obtained by considering the motion of P_i in an inertial frame. This is governed by

$$\sum_{\ell} \mathbf{f}_{i\ell} + \mathbf{b}_i = \frac{d}{dt}\{m_i \mathbf{v}_i\}\,. \tag{2.8}$$

Here $\mathbf{f}_{i\ell}$ denotes the force exerted upon P_i by P_ℓ, $\mathbf{b}_i$ the resultant force on P_i due to external agencies, and the sum is over all $\ell \neq i$. Multiplication of each term by $w(\mathbf{x}_i(t) - \mathbf{x})$ followed by summation over all i yields (see [1] for details)

$$\mathbf{f}_w + \mathbf{b}_w = \frac{\partial}{\partial t}\{\varrho_w \mathbf{v}_w\} + \operatorname{div}\{\widehat{\mathbf{D}}_w + \varrho_w \mathbf{v}_w \otimes \mathbf{v}_w\}. \tag{2.9}$$

Here

$$\mathbf{f}_w(\mathbf{x}, t) := \sum_{i=1}^{N} \sum_{\substack{\ell=1 \\ \ell \neq i}}^{N} \mathbf{f}_{i\ell}(t) w(\mathbf{x}_i(t) - \mathbf{x})\,, \tag{2.10}$$

$$\mathbf{b}_w(\mathbf{x}, t) := \sum_{i=1}^{N} \mathbf{b}_i(t) w(\mathbf{x}_i(t) - \mathbf{x})\,, \tag{2.11}$$

and

$$\widehat{\mathbf{D}}_w(\mathbf{x}, t) := \sum_{i=1}^{N} m_i \widehat{\mathbf{v}}_i(\mathbf{x}, t) \otimes \widehat{\mathbf{v}}_i(\mathbf{x}, t) w(\mathbf{x}_i(t) - \mathbf{x})\,, \tag{2.12}$$

where

$$\widehat{\mathbf{v}}_i(\mathbf{x}, t) := \mathbf{v}_i(t) - \mathbf{v}_w(\mathbf{x}, t)\,. \tag{2.13}$$

Using a theorem due to NOLL [2], the existence and explicit form of a tensor $\mathbf{T}_w^-$ such that the interaction force density

$$\mathbf{f}_w = \operatorname{div} \mathbf{T}_w^- \tag{2.14}$$

follows from very mild restriction on the decay of $\mathbf{f}_{i\ell}$ with separation of P_i, P_ℓ (satisfied quite generally by non-ionic molecules). Equations (2.9) and (2.14) yield the usual form of balance

$$\operatorname{div} \mathbf{T}_w + \mathbf{b}_w = \frac{\partial}{\partial t}\{\varrho_w \mathbf{v}_w\} + \operatorname{div}\{\varrho_w \mathbf{v}_w \otimes \mathbf{v}_w\}, \tag{2.15}$$

where the stress tensor

$$\mathbf{T}_w := \mathbf{T}_w^- - \widehat{\mathbf{D}}_w\,. \tag{2.16}$$

In particular, (2.16) demonstrates the separate contributions to stress associated with interactions ($\mathbf{T}_w^-$) and momentum transport ($-\widehat{\mathbf{D}}_w$). Further, the spatial smoothness of each of the continuum fields ϱ_w, $\mathbf{v}_w$, $\mathbf{f}_w$, $\mathbf{b}_w$, $\widehat{\mathbf{D}}_w$ and $\operatorname{div}\mathbf{T}_w^-$ is seen to be precisely the same as that of w.

Energy balance is obtained by scalar multiplication of (2.8) by $w(\mathbf{x}_i(t) - \mathbf{x})\mathbf{v}_i(t)$ followed by summation over all i. A detailed discussion is given in [1] wherein further time averaging is effected, so yielding field values in terms of local space-time averages of molecular quantities.

The foregoing may be compared with the seminal work [3] in which continuum field values were identified with space-time averages of ensemble averages (see [4] for comparison of the two approaches).

3. On the nature of the weighting function

The results obtained in Sec. 2 are only formal, since the only restrictions placed upon the weighting function were its C^1 smoothness and normalisation. Some physically sensible criteria and possible choices are now listed.

1. Defining

$$\begin{aligned} w(\mathbf{r}) &:= \frac{3}{4\pi r^3} \quad \text{if} \quad r := |\mathbf{r}| < \varepsilon, \\ w(\mathbf{r}) &:= 0 \qquad \text{if} \quad |\mathbf{r}| \geq \varepsilon \end{aligned} \tag{3.1}$$

it is clear that w is normalised, and $\varrho_w(\mathbf{x}, t)$ represents the mass of those particles lying at time t within a sphere centred at $\mathbf{x}$ with radius ε divided by the volume of this sphere. This choice is simple, intuitive, and explicitly scale-dependent. However, wherever $|\mathbf{r}| = \varepsilon$ this function is discontinuous. It is a simple matter to "mollify" w over an interval $(\varepsilon, \varepsilon + \delta)$ in such a way that w is of arbitrary given smoothness everywhere, with $\delta(> 0)$ arbitrarily small (see [1], p. 160). Accordingly the above physical interpretation of $\varrho_w(\mathbf{x}, t)$ is essentially unchanged for small enough choice of δ.

2. The spherical averaging region associated with choice (3.1) can be generalised to that of a "cell" whose geometry is appropriate to the system of interest. For example, near planar interfaces and boundaries it is useful to consider rectangular box-shaped regions with one pair of faces parallel to the interface or boundary in question. More precisely, in such case w is a mollified version of a multiple of the characteristic function for the region: the factor approximates the reciprocal of the volume of the region, is mandated by normalisation, and depends on the thickness of the mollifying envelope.

3. Values of fields ϱ_w, $\mathbf{p}_w$, $\mathbf{f}_w$ and $\mathbf{b}_w$ are biased local volume averages of molecular quantities, and may be compared with appropriate measurement values. Since actual *local* measurements reflect local space-*time* averages (no measurement is either instantaneous or localised in a region of zero volume measure), it

is time-averaged versions of these fields that are relevant. Further, different measuring devices associated with the same physical quantity are to be expected to deliver different "sampling" of molecular behaviour and as such may be identified with different weighting functions (both in space *and* time). Such considerations accord with the practical problem of calibrating different instruments which purport to measure the same quantity.

4. Averaging via weighting functions may be repeated, by defining the w-average, f_w, of a spatial field f *via*

$$f_w(\mathbf{x}) := \int_{\text{all space}} f(\mathbf{y}) w(\mathbf{y}-\mathbf{x}) d\mathbf{y} \,. \tag{3.2}$$

This accords with microscopic averages computed in Sec. 2 upon writing discrete (that is, purely microscopic) quantities in terms of distributions. For example, the microscopic mass density (at any given instant: time-dependence is suppressed)

$$\varrho_{\text{mic}}(\mathbf{x}) := \sum_{i=1}^{N} m_i \delta(\mathbf{x}_i - \mathbf{x}) \,, \tag{3.3}$$

where δ denotes the three-dimensional Dirac distribution. Clearly, from (3.2), (3.3) and (2.1),

$$(\varrho_{\text{mic}})_w = \varrho_w \,. \tag{3.4}$$

Upon repeating a w-average it is natural to compare $(f_w)_w$ with f_w. If one requires that repeated averaging yields nothing new, that is if

$$(f_w)_w = f_w \,, \tag{3.5}$$

then the form of w may be determined (see [1], p. 161). In unbounded domains the convolution format of (3.2) implies that the Fourier transform $\overline{w}(\mathbf{k})$ of w should satisfy

$$\overline{w}(\mathbf{k})^2 = \overline{w}(\mathbf{k}) \,. \tag{3.6}$$

Thus $\overline{w}(\mathbf{k}) = 0$ or 1 and the simplest (and most physical) choice is for a wave-vector "cut-off", say at $|\mathbf{k}| = \varepsilon^{-1}$ for some choice of length scale ε. That is,

$$\overline{w}(\mathbf{k}) = 1 \quad \text{if} \quad |\mathbf{k}| < \varepsilon^{-1}, \qquad \overline{w}(\mathbf{k}) = 0 \quad \text{if} \quad |\mathbf{k}| \geq \varepsilon^{-1}. \tag{3.7}$$

In such case it follows that

$$w(d) = \frac{1}{2\pi^2 d^3} \left\{ \sin\left(\frac{d}{\varepsilon}\right) - \left(\frac{d}{\varepsilon}\right) \cos\left(\frac{d}{\varepsilon}\right) \right\}, \tag{3.8}$$

where

$$d := |\mathbf{d}|\,. \tag{3.9}$$

The analogue for a bounded rectangular region of dimensions $2L_1 \times 2L_2 \times 2L_2$ yields truncated (at wavelength ε) multiple Fourier series which are delivered by

$$w(\mathbf{d}) := \frac{1}{8L_1L_2L_3} \prod_{i=1}^{3} \frac{\sin\left(\left(N_i + \frac{1}{2}\right) d_i\right)}{\sin(d_i/2)}\,, \tag{3.10}$$

where N_i is the integral part of $2L_i/\varepsilon$ and $\mathbf{d} = (d_1, d_2, d_3)$. A consequence of using (scale-dependent) weighting functions of form (3.8) or (3.10) is that averaging at scale ε_1 followed by a further averaging at scale ε_2 yields the same result as merely averaging once at the larger of the two scales.

4. Flow through a rigid porous body saturated with an incompressible fluid

Fluid flow through porous media is best described in terms of fields which are defined both in the region occupied by the fluid *and* that occupied by the porous body itself. Such an "immiscible mixture" approach (see [5]) derives from working at a scale ε_2 large compared with typical pore size and structural dimension. It is instructive to motivate the relevant equations by examining the actual flow in the pores, observed at a scale ε_1, say. The ε_2-scale equations may be obtained by averaging the (ε_1-scale) equations which govern pore flow, at least in principle. For incompressible fluid saturating pore space such a procedure is simple and elucidating.

For a Newtonian fluid, flow is governed by the Navier–Stokes equation

$$-\nabla P + \frac{\mu}{\varrho_0}\Delta\mathbf{p} + \varrho_0\mathbf{g} = \frac{\partial \mathbf{p}}{\partial t} + \frac{1}{\varrho_0}\operatorname{div}(\mathbf{p}\otimes\mathbf{p}). \tag{4.1}$$

Here P denotes pressure, μ viscosity, ϱ_0 mass density, $\mathbf{p}$ momentum density, and $\mathbf{g}$ gravitational acceleration. The w-average of any field f associated with the fluid is given by (3.2) where f is considered to be zero outside the region $\mathcal{E}_f$ occupied by fluid at scale ε_1 (more specifically, $\mathcal{E}_f$ is the support of the ε_1-scale mass density function ϱ_0). In averaging individual terms of (4.1) it is possible to relate averages of derivatives to derivatives of averages (see [6]). In particular, upon suppressing time-dependence and writing

$$\overline{f} := f_w \tag{4.2}$$

it turns out that

$$\overline{\nabla P}(\mathbf{x}) = (\nabla \overline{P})(\mathbf{x}) + \int_{\mathcal{S}(\mathbf{x})} P(\mathbf{y})\mathbf{n}(\mathbf{y})w(\mathbf{y}-\mathbf{x})\,dA_{\mathbf{y}}\,, \tag{4.3}$$

where

$$\mathcal{S}(\mathbf{x}) := \partial\mathcal{E}_f \cap \text{ support } (w(. - \mathbf{x})), \tag{4.4}$$

and $\mathbf{n}$ is that unit normal to the pore boundary $\partial\mathcal{E}_f$ directed *out* of the fluid region $\mathcal{E}_f$. If w corresponds to choice 1 of Sec. 3, then $\mathcal{S}(\mathbf{x})$ denotes that portion of the pore boundary within a sphere of radius $\varepsilon + \delta$ centred at $\mathbf{x}$. In this context averaging is often effected over so-called elementary representative volumes (see [7]) so that w corresponds to such a choice of "cell" (see choice 2 of Sec. 3). Further, noting that $\mathbf{p}$ vanishes on $\partial\mathcal{E}_f$ (this is the standard "no slip" hypothesis),

$$\overline{\Delta\mathbf{p}}(\mathbf{x}) = (\Delta\overline{\mathbf{p}})(\mathbf{x}) + \int_{\mathcal{S}(\mathbf{x})} \nabla\mathbf{p}(\mathbf{y})\mathbf{n}(\mathbf{y})w(\mathbf{y} - \mathbf{x})\, dA_{\mathbf{y}} \tag{4.5}$$

and

$$\overline{\operatorname{div}(\mathbf{p} \otimes \mathbf{p})} = (\operatorname{div}(\overline{\mathbf{p} \otimes \mathbf{p}})). \tag{4.6}$$

Finally,

$$\left\{\overline{\frac{\partial\mathbf{p}}{\partial t}}\right\} = \frac{\partial\overline{\mathbf{p}}}{\partial t} \qquad \text{and} \qquad \overline{\varrho}_0 = \varrho_0\nu, \tag{4.7}$$

where ν denotes the porosity field.

Multiplication of (4.1) (evaluated at point $\mathbf{y}$) by $w(\mathbf{y} - \mathbf{x})$ and integrating over all space yield, upon invoking results (4.3)–(4.7),

$$-\nabla\overline{P} + \frac{\mu}{\varrho_0}\Delta\overline{P} - \operatorname{div}\mathcal{D} + \mathbf{f}^{fp} + \varrho_0\nu\mathbf{g} = \frac{\partial\overline{\mathbf{p}}}{\partial t} + \operatorname{div}\left(\frac{1}{\varrho_0\nu}\overline{\mathbf{p}} \otimes \overline{\mathbf{p}}\right). \tag{4.8}$$

Here

$$\mathcal{D} := \frac{1}{\varrho_0}\overline{\mathbf{p} \otimes \mathbf{p}} - \frac{1}{\varrho_0\nu}\overline{\mathbf{p}} \otimes \overline{\mathbf{p}} \tag{4.9}$$

is the extra contribution to the pressure tensor $\overline{P}\mathbf{1}$ associated with re-scaling, and

$$\mathbf{f}^{fp} := \int_{\mathcal{S}} \left(-P\mathbf{1} + \frac{\mu}{\varrho_0}\nabla\mathbf{p}\right)\mathbf{n}w\, dA \tag{4.10}$$

denotes the force density associated with the effect of the porous body on the fluid. (It is of interest to note that if the fluid is at rest and the pressure P constant then $\mathbf{f}^{fp}$ reduces to $P\nabla\nu$.)

It is useful in this context to introduce the volume flux vector

$$\mathbf{Q} := \varrho_0^{-1}\mathbf{p}\,. \tag{4.11}$$

Writing

$$\hat{\mathbf{f}}^{fp} := -\int_S P\mathbf{n}w\,dA \tag{4.12}$$

and

$$\mu\tilde{\mathbf{f}}^{fp} := \mathbf{f}^{fp} - \hat{\mathbf{f}}^{fp}\,, \tag{4.13}$$

and making the constitutive assumption

$$\tilde{\mathbf{f}}^{fp} = -\nu\mathbf{K}^{-1}(\mathbf{V}^f - \mathbf{V}^p), \tag{4.14}$$

where

$$\mathbf{V}^f := \overline{\mathbf{p}}/\overline{\varrho} = \nu^{-1}\mathbf{Q}$$

denotes the ε_2-scale fluid velocity field and $\mathbf{V}^p$ the corresponding porous body velocity field, (4.8) becomes

$$\begin{aligned}\operatorname{div}(-\overline{P}\mathbf{1} + \mathcal{D}) + \mu\Delta\mathbf{Q} + \hat{\mathbf{f}}^{fp} - \mu\mathbf{K}^{-1}\mathbf{Q} + \varrho_0\nu\mathbf{g} \\ = \varrho_0\left(\frac{\partial\mathbf{Q}}{\partial t} + \operatorname{div}\left(\frac{1}{\nu}\mathbf{Q}\otimes\mathbf{Q}\right)\right).\end{aligned} \tag{4.15}$$

Here the rigid body has been considered stationary ($\mathbf{V}^p = \mathbf{0}$) and $\mathbf{K}$ denotes the permeability tensor. For steady, uniform, uniaxial flow through an isotropic ($\mathbf{K} = k\mathbf{1}$) homogeneous (k and ν constant) body, (4.15) reduces to

$$\operatorname{div}(-\overline{P}\mathbf{1} - \mathcal{D}) + \hat{\mathbf{f}}^{fp} - \frac{\mu}{k}\mathbf{Q} + \varrho_0\nu\mathbf{g} = \mathbf{0}. \tag{4.16}$$

If $\mathcal{D} = \hat{P}\mathbf{1}$, and $\hat{\mathbf{f}}^{fp}$ and $\varrho_0\nu\mathbf{g}$ are neglected, then (4.16) reduces to Darcy's "Law"

$$\mathbf{\Pi} = -\frac{\mu}{k}\mathbf{Q}\,, \tag{4.17}$$

where $\mathbf{\Pi}$ denotes the pressure gradient $\nabla(\overline{P} + \hat{P})$.

5. Applications

The discussion of Sec. 2, when extended to take account of a further time averaging (at scale Δ, say: see [1], p.171) enables the notion of "reproducible macroscopic behaviour" at a specific pair of length-time scales to be made precise [8]. Further, such considerations form the basis of a Statistical Mechanics

approach [8, 9] to non-equilibrium macroscopically-reproducible behaviour via the definition of a "macroscopic state" at a given length scale, together with projection operator methodology.

The averaging procedure for a porous body outlined in Sec. 4 draws attention to the existence of a highly inhomogeneous interfacial region located at the boundary of the body, and facilitates detailed analysis of uniaxial flow over and within a rectangular slab of porous material subjected to a constant, externally applied, pressure gradient. Such a study elucidates the status of the *ad hoc* slip boundary condition employed for such flows introduced in [10]: see [6].

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DEPARTMENT OF MATHEMATICS,
UNIVERSITY OF STRATHCLYDE - GLASGOW,
26, Richmond Street, Glasgow G1 1XH, Scotland.

Received October 6, 1997.

Arch. Mech., 50, 3, pp. 541–547, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

Objectivity and frame indifference, revisited

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

W. MUSCHIK (BERLIN)

BECAUSE ONE HAS to distinguish between changing the observer and changing the state of motion of materials, objectivity and material frame indifference are redefined: Objectivity denotes a special tensor property in case of changing the observer, whereas material frame indifference is characterized by quantities being independent of different states of motion of the material. To describe these different states of motion of the material, an arbitrary standard frame of reference and a Constitutive Family is introduced. We prove that the constitutive map is isotropic in the state variables, if these and the material properties are objective.

1. Introduction

OBJECTIVITY AND/OR FRAME-INDIFFERENCE is one of the five "principles" governing constitutive equations in Rational Continuum Theories [1]. Although there is a flood of publications in the field [2 – 11] (only some of them can be mentioned here) and nearly all aspects of these two items are discussed in detail, one can see that during a meeting, experienced scientists suddenly begin to discourse controversially on "objectivity". This only can mean that questions around objectivity are not answered so satisfactorily that a common agreement could exist. The aim of the paper is to demonstrate that no vagueness remains, if we properly distinguish between two different situations. In the first situation, one material is described by various observers; in the second one, two differently moving materials are described by the same observer. If the two differently moving materials have additionally the property that they are identical, if resting with respect to each other, then the question arises, whether they are also identical when they are moving with respect to each other. As we will see, in general the answer is "no", provided they belong to the same Constitutive Family.

2. Changing frames

As it is well known [12], in non-relativistic theory the change of frame $\mathsf{B} \to \mathsf{B}^*$

is achieved locally by an Euclidean transformation of the position coordinates [1]

$$\mathbf{x}^* = \mathbf{Q}\cdot(\mathbf{x} - \mathbf{c}). \tag{2.1}$$

Here we denote an arbitrary, but fixed B^* as a *standard frame of reference*, whereas B is the chosen frame. This Euclidean change of frame is described by the orthogonal time-dependent transformation $\mathbf{Q}(t)$ [2]

$$\widetilde{\mathbf{Q}}\cdot\mathbf{Q} = \mathbf{Q}\cdot\widetilde{\mathbf{Q}} = \mathbf{1}, \qquad \det\mathbf{Q} = 1, \tag{2.2}$$

and by the components of the difference vector between the origins of the frames $\mathbf{c}(t)$.

The material velocity transforms by changing the frame

$$\mathbf{v}^* = \mathbf{Q}\cdot\mathbf{V} = \mathbf{Q}\cdot(\mathbf{v} + \mathbf{v}^{\mathrm{rel}}) =: \mathbf{Q}\cdot(\mathbf{v} - \dot{\mathbf{c}} + \boldsymbol{\Omega}\cdot(\mathbf{x} - \mathbf{c})). \tag{2.3}$$

Here $\mathbf{v}^{\mathrm{rel}}$ is the relative velocitiy between the two frames [3] which decomposes into the translational part $-\dot{\mathbf{c}}$ and the rotational part $\boldsymbol{\Omega}\cdot(\mathbf{x} - \mathbf{c})$ by use of the skew-symmetric spin matrix:

$$\boldsymbol{\Omega} := \widetilde{\mathbf{Q}}\cdot\dot{\mathbf{Q}} = -\widetilde{\boldsymbol{\Omega}}. \tag{2.4}$$

The relative velocity $\mathbf{v}^{\mathrm{rel}}$ depends only on quantities characterizing the relative motion of the two frames considered, whereas the material velocity $\mathbf{v}$ is independent of the relative motion of both the frames. In non-relativistic theories time and also the mass density are *frame-independent*

$$t^* = t, \qquad \varrho^* = \varrho, \tag{2.5}$$

whereas according to (2.3) the material velocity is *frame-dependent.*

A balance equation in an arbitrary frame B has the form

$$\partial_t(\varrho\Psi) + \nabla\cdot(\varrho\mathbf{v}\Psi + \boldsymbol{\Phi}) + \Sigma = 0. \tag{2.6}$$

Because no frame (observer) is distinguished, balance equations are *frame-invariant*, that means, they have the same shape in all frames. Thus we have according to (2.6) in B^*

$$\partial_t^*(\varrho^*\Psi^*) + \nabla^*\cdot(\varrho^*\mathbf{v}^*\Psi^* + \boldsymbol{\Phi}^*) + \Sigma^* = 0, \tag{2.7}$$

and the question arises, how the field quantities Ψ, $\boldsymbol{\Phi}$, and Σ transform. In general they transform as the material velocity (2.3) does,

$$\Psi^* = \Psi + \Psi^{\mathrm{rel}}, \qquad \boldsymbol{\Phi}^* = \mathbf{Q}\cdot(\boldsymbol{\Phi} + \boldsymbol{\Phi}^{\mathrm{rel}}), \qquad \Sigma^* = \Sigma + \Sigma^{\mathrm{rel}}, \tag{2.8}$$

[1] We write the equations for the coordinates in a symbolic way: $\mathbf{x}$ is the column of the position coordinates.

[2] Note: $\mathbf{Q}(t)$ is a proper orthogonal matrix.

[3] The notion "relative velocity" is often used in another context. Here it denotes the relative velocity between the standard frame of reference B^* and the chosen frame B.

or if the balance (2.6) has its range in R^3, we have the transformations

$$\Psi^* = \mathbf{Q}\cdot[\Psi + \Psi^{\mathrm{rel}}], \qquad \Phi^* = \mathbf{Q}\cdot[\Phi + \Phi^{\mathrm{rel}}]\cdot\tilde{\mathbf{Q}}, \qquad \Sigma^* = \mathbf{Q}\cdot[\Sigma + \Sigma^{\mathrm{rel}}]. \tag{2.9}$$

In the standard frame of reference, the relative part of all quantities is identically zero by definition

$$\Psi^{\mathrm{rel}*} \equiv 0, \qquad \Phi^{\mathrm{rel}*} \equiv \mathbf{0}, \qquad \Sigma^{\mathrm{rel}*} \equiv 0. \tag{2.10}$$

Quantities whose relative parts vanish in all frames transform according to (2.8) or (2.9) as tensor components. This gives rise to the

DEFINITION. *Quantities whose relative parts vanish in all frames are called objective.*

3. Derivatives

We consider a function of arbitrary range

$$f(\mathbf{x}^*, t) = f(\mathbf{Q}\cdot(\mathbf{x} - \mathbf{c}), t), \tag{3.1}$$

taking (2.1) into account. Its gradient is

$$\nabla f(\mathbf{x}^*, t) = \nabla^* f(\mathbf{x}^*, t)\cdot\mathbf{Q}. \tag{3.2}$$

Thus we have proved the

□ PROPOSITION.

$$\nabla = \tilde{\mathbf{Q}}\cdot\nabla^* = \nabla^*\cdot\mathbf{Q}. \tag{3.3}$$

□

There are two time derivatives belonging to different frames

$$\text{in } \mathsf{B}^* : \quad \left.\frac{\partial}{\partial t}\right|_{\mathbf{x}^*} \equiv \partial_t{}^*, \tag{3.4}$$

$$\text{in } \mathsf{B} : \quad \left.\frac{\partial}{\partial t}\right|_{\mathbf{x}} \equiv \partial_t. \tag{3.5}$$

We now can prove the

□ PROPOSITION. The transformation equation of the partial time derivative is

$$\partial_t{}^* = \partial_t - \mathbf{v}^{\mathrm{rel}}\cdot\nabla \tag{3.6}$$

for arbitrary components in its domain.

For proving this proposition we obtain by the chain rule

$$\partial_t f(\mathbf{x}^*, t) = [\partial_t{}^* + \partial_t\mathbf{x}^*\cdot\nabla^*]\, f(\mathbf{Q}\cdot(\mathbf{x} - \mathbf{c}), t). \tag{3.7}$$

According to (2.1), relation

$$\partial_t \mathbf{x}^* = \dot{\mathbf{Q}} \cdot (\mathbf{x} - \mathbf{c}) - \mathbf{Q} \cdot \dot{\mathbf{c}} \tag{3.8}$$

is valid. By use of (2.4) and (2.3) we obtain

$$\partial_t \mathbf{x}^* = \mathbf{Q} \cdot \mathbf{v}^{\mathrm{rel}} \tag{3.9}$$

by which Eq. (3.7) results in the transformation equation (3.6) we are looking for, if Eq. (3.3) was taken into account. □

According to (3.6) the partial time derivative is non-objective, because its relative part is not identically equal zero

$$\partial_t{}^{\mathrm{rel}} \equiv -\mathbf{v}^{\mathrm{rel}} \cdot \nabla. \tag{3.10}$$

The balance equations (2.7) and (2.6) are often written down by means of the material time derivative

DEFINITION. *The frame-invariantly defined material time derivative is*

$$\frac{d^*}{dt} := \partial_t{}^* + \mathbf{v}^* \cdot \nabla^*, \qquad \frac{d}{dt} := \partial_t + \mathbf{v} \cdot \nabla. \tag{3.11}$$

We now prove the

□ PROPOSITION. The material time derivative is frame-independent, and therefore objective.

By (3.6) we obtain from $(3.11)_1$

$$\frac{d^*}{dt} = \partial_t - \mathbf{v}^{\mathrm{rel}} \cdot \nabla + \mathbf{v}^* \cdot \nabla^*. \tag{3.12}$$

Taking (2.3) and (3.3) into account, Eq. (3.11) yields the proposition

$$\frac{d^*}{dt} = \partial_t + \mathbf{v} \cdot \nabla = \frac{d}{dt}. \tag{3.13}$$

□

The frame independence of the material time derivative needs an interpretation. For that purpose we introduce the so-called local rest frame for which we have locally (at point $\mathbf{x}^0$) $\mathbf{v}^0(\mathbf{x}^0(t), t) = \mathbf{0}$. In this rest frame B^0 we obtain for the material time derivative $(3.11)_2$

$$\frac{d^0}{dt} = \partial_t{}^0, \tag{3.14}$$

what means, that in this frame the material time derivative describes the explicit temporal change in the rest frame. Because of (3.13), the material time derivative in an arbitrary frame B describes this explicit time rate in the rest frame, too.

If we introduce the frame-invariant *material spin matrix*

$$\boldsymbol{\omega}(\mathbf{x},t) := \frac{1}{2}[\nabla\mathbf{v} - (\nabla\mathbf{v})\tilde{}], \tag{3.15}$$

we can prove the following well-known

□ PROPOSITION.

$$\boldsymbol{\omega}^*(\mathbf{x}^*,t) = \mathbf{Q}\cdot[\boldsymbol{\omega}(\mathbf{x},t) + \boldsymbol{\Omega}]\cdot\tilde{\mathbf{Q}}, \tag{3.16}$$

$$\frac{d}{dt}^* a^* = \frac{d}{dt}(a + a^{\mathrm{rel}}), \tag{3.17}$$

$$\frac{d}{dt}^* \mathbf{a}^* - \boldsymbol{\omega}^*\cdot\mathbf{a}^* = \mathbf{Q}\cdot\left[\frac{d}{dt}(\mathbf{a} + \mathbf{a}^{\mathrm{rel}}) - \boldsymbol{\omega}\cdot(\mathbf{a} + \mathbf{a}^{\mathrm{rel}})\right], \tag{3.18}$$

$$\begin{aligned}\frac{d}{dt}^* \mathbf{a}^* - \boldsymbol{\omega}^*\cdot\mathbf{a}^* + \mathbf{a}^*\cdot\boldsymbol{\omega}^* \\ = \mathbf{Q}\cdot\left[\frac{d}{dt}(\mathbf{a} + \mathbf{a}^{\mathrm{rel}}) - \boldsymbol{\omega}\cdot(\mathbf{a} + \mathbf{a}^{\mathrm{rel}}) + (\mathbf{a} + \mathbf{a}^{\mathrm{rel}})\cdot\boldsymbol{\omega}\right]\cdot\tilde{\mathbf{Q}}.\end{aligned} \tag{3.19}$$

□

Here we can see from (3.18) that also for an objective $\mathbf{a}$ its material time derivative is not objective in general, although the material time derivative itself is an objective operator according to (3.13). Now we have to take constitutive equations into account.

4. Material frame indifference

We now consider three frames: the standard frame of reference B^*, an arbitrary frame B, and the *local co-rotational rest frame* B^0 which is fixed at a material point of position $\mathbf{x}^0(t)$

$$\text{in } \mathsf{B}^0: \quad \mathbf{v}^0(\mathbf{x}^0(t),t) = \mathbf{0}, \qquad \boldsymbol{\omega}^0(\mathbf{x}^0(t),t) = \mathbf{0}. \tag{4.1}$$

We need B^0 for describing the motion of the material with respect to the standard frame of reference. If we introduce an abstract state space spanned by a set of variables z, these variables will transform by an abstract linear mapping B (because it operates on tensor components of different orders included in z) depending on the relative motion of both the frames with respect to each other

$$z^* = B(z + z^{\mathrm{rel}}) = B^0(z^0 + z^{0\mathrm{rel}}). \tag{4.2}$$

Here B describes the change of frames $\mathsf{B} \to \mathsf{B}^*$, and B^0 that of $\mathsf{B}^0 \to \mathsf{B}^*$.

There is no doubt about the validity of the following statement:

I. *Constitutive properties do not depend on the relative motion of frames.*

Two observers in different frames, B and B*, investigating the same material observe the same constitutive properties. This trite statement should not be confused with the second statement.

II. *Constitutive properties do not depend on the motion of the material with respect to the standard frame of reference.*

Experience shows that this statement is wrong: Materials perform their motion with respect to the standard frame of reference B*, and therefore the constitutive properties depend on B^0. Hence we introduce the *Constitutive Family*

$$M(\mathbf{x},t) = \mathcal{M}(z(\mathbf{x},t);\square^*), \qquad \square^* \equiv \mathcal{F}[\mathbf{Q}^0(t),\mathbf{c}^0(t)]. \tag{4.3}$$

The material properties M are generated by the constitutive map $\mathcal{M}$ which is defined on the state space spanned by the z. The family parameter is the functional $\mathcal{F}$ which describes the influence of motion of the material. If this functional is of differential type, we have

$$\square^* = F[\mathbf{Q}^0,\mathbf{c}^0,\boldsymbol{\Omega}^0,\dot{\mathbf{c}}^0,\dot{\boldsymbol{\Omega}}^0,\ddot{\mathbf{c}}^0,\ldots]. \tag{4.4}$$

Thus different observers describe the same material in a special state of motion by

$$M(\mathbf{x},t) = \mathcal{M}(z(\mathbf{x},t);\square^*), \tag{4.5}$$

$$M^*(\mathbf{x}^*,t) = \mathcal{M}^*(z^*(\mathbf{x}^*,t);\square^*) \qquad M^0(\mathbf{x}^0,t) = \mathcal{M}^0(z^0(\mathbf{x}^0,t);\square^*). \tag{4.6}$$

Here it seems that to each frame belongs its own constitutive family, although the different observers see the same material. In this case we cannot define what identical materials are. Therefore we formulate the

Principle of material frame-indifference:

i. Because observers are not distinguished, the constitutive map $\mathcal{M}(\bullet;\sharp)$ describing one constitutive family is frame-invariant

$$\mathcal{M}(\bullet;\sharp) = \mathcal{M}^*(\bullet;\sharp) = \mathcal{M}^0(\bullet;\sharp) = \ldots . \tag{4.7}$$

ii. Uniform motions of the material with respect to the standard frame of reference do not influence constitutive properties. Consequently the domain of (4.4) is

$$\square^* = F[\boldsymbol{\Omega}^0,\dot{\boldsymbol{\Omega}}^0,\ddot{\mathbf{c}}^0,\ldots]. \tag{4.8}$$

We now prove the following

□ PROPOSITION. If the state variables z and the constitutive properties M are objective quantities, the constitutive map $\mathcal{M}$ is isotropic in the state variables.

From $(4.6)_1$ we obtain taking (4.7) into account

$$M^* = \mathcal{M}(z^*;\square^*), \tag{4.9}$$

and application of the transformation properties (4.2) yields

$$B(M + M^{\mathrm{rel}}) = \mathcal{M}(B(z + z^{\mathrm{rel}}); \square^*). \tag{4.10}$$

From this and (4.5) we obtain

$$M + M^{\mathrm{rel}} = B^{-1}\mathcal{M}(B(z + z^{\mathrm{rel}}); \square^*) = \mathcal{M}(z; \square^*) + M^{\mathrm{rel}}. \tag{4.11}$$

If the state variables z and the constitutive properties M are objective quantities, we obtain

$$\mathcal{M}(z; \square^*) = B^{-1}\mathcal{M}(Bz; \square^*), \tag{4.12}$$

which is the maintained isotropy of $\mathcal{M}$. □

Consequently all representation theorems of isotropic functions are valid for the Constitutive Family.

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INSTITUT FÜR THEORETISCHE PHYSIK,
TECHNISCHE UNIVERSITÄT BERLIN

Hardenbergstr. 36, D-10623 Berlin, Germany.
e-mail: womu0433@itp0.physik.tu-berlin.de

Received October 1, 1997.

Arch. Mech., 50, 3, pp. 549–558, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

Random field models and scaling laws of heterogenous media

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

M. OSTOJA-STARZEWSKI (ATLANTA)

IN MANY PROBLEMS of solid mechanics (e.g., stochastic finite elements, statistical fracture mechanics) there is a need for resolution of dependent fields over scales not infinitely larger than the microscale. This task may be accomplished through a "meso-scale window" which becomes the classical Representative Volume Element (RVE) in the infinite limit relative to the microscale. It turns out that the material properties at such a mesoscale cannot be uniquely approximated by a random field of stiffness/compliance with locally isotropic realizations, but, rather, two random continuum fields with locally anisotropic realizations, corresponding respectively to Dirichlet and Neumann boundary conditions on the meso-scale, need to be introduced to bound the material response from above and from below. We discuss statistical characteristics of these two mesoscale random fields, including their spatial correlation structure, for anti-plane elastic response of random two-phase composites with Voronoi geometry at the percolation point. Particular attention is given to the scaling of effective responses obtained from both conditions, which sheds light on the minimum acceptable size of an RVE.

1. Does there exist a locally isotropic, inhomogeneous elastic continuum?

EVERY SOLID MATERIAL possess a certain microstructure, whose complexity is very often characterized by a geometric and physical randomness of basic constituents – typical examples are polycrystals, composites, fibrous, cellular, and granular media. In studying mechanics of such materials one typically introduces an approximating continuum model which relies on a so-called Representative Volume Element (RVE). The constitutive properties – tensor $C^{\text{eff}}_{ijkl} \equiv \mathbf{C}^{\text{eff}}$ – of the RVE are usually being calculated either by a method of bounds (e.g., of Hashin–Shtrikman type) or by a less rigorous, but sometimes more convenient, effective medium theory (e.g., a self-consistent model); excellent reviews of these topics are provided in [1, 2, 3, 4]. The resulting constitutive response is deterministic, as it is tacitly assumed that the typical scales of variability of macroscopic stress, strain, and displacement fields are much larger than the RVE size.

Aside from this classical category of studies in micromechanics, there has been developed for the past two decades a subject area of Stochastic Finite Elements (SFE) [5, 6, 7], which aims at the inclusion of microscale material variability in the solution of boundary value problems set on scales much larger than the length

scale d of the microstructure. In SFE the microstructural variability is accounted for by simply assuming perturbations C'_{ijkl} to be present in the Hooke's law

$$\begin{aligned} \sigma_{ij} &= C_{ijkl}(\mathbf{x},\omega)\varepsilon_{kl}\,, \qquad \mathbf{x}\in\mathbf{B}, \quad \omega\in\Omega, \\ C_{ijkl}(\mathbf{x},\omega) &= \langle C_{ijkl}\rangle + C'_{ijkl}(\mathbf{x},\omega). \end{aligned} \tag{1.1}$$

In other words, C_{ijkl} is taken as a random field over the material domain $\mathbf{B}$; here ω denotes a realization from a sample space Ω. In fact, typically a locally isotropic continuum is being assumed

$$C_{ijkl}(\mathbf{x},\omega) = \lambda(\mathbf{x},\omega)\delta_{ij}\delta_{kl} + \mu(\mathbf{x},\omega)(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \tag{1.2}$$

where λ and μ are the Lamé constants. Let us note here that the Statistical Fracture Mechanics [8] is another, yet related, area whose analyses often require random field models.

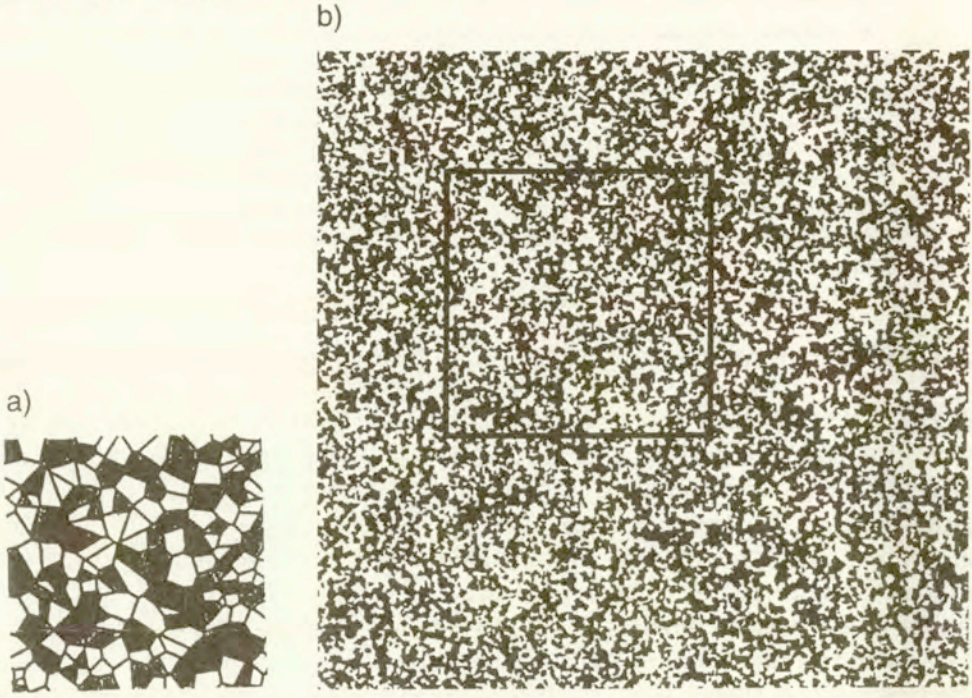

FIG. 1. A close-up of a two-phase material with a Voronoi mosaic microgeometry is shown in (a), and a larger sample with 250,000 grains at volume fraction 50% is depicted in (b), where an arbitrary window of length scale $L \times L$ is drawn. There are, on average, ten pixels per one Voronoi cell in (b).

The above considerations lead us to a basic issue of the dependence of effective Hookeś law on the size L of a so-called *window*, such as shown in Fig. 1. Here we

introduce a nondimensional parameter, relative to the grain size d,

$$\sigma = \frac{L}{d} \tag{1.3}$$

to quantify this scale dependence.

It can easily be inferred from Fig. 1 that fluctuations are present for any finite window, but as its size tends to infinity, they die out to zero – this is the classical, deterministic, continuum limit $\delta \to \infty$, in which the RVE possesses a statistical representation of the microstructure with all the typical microheterogeneities. Below this limit we have a random field problem: $C_{ijkl}(\mathbf{x}, \omega, \delta)$ has to be described statistically. The question is: how do the statistics of effective moduli behave as a function of δ? Furthermore, as shown in our previous papers [9, 10, 11, 12] and discussed in Sec. 2 below, associated with the scale dependence of $C_{ijkl}(\mathbf{x}, \omega, \delta)$, there is an interesting issue of non-uniqueness of the effective constitutive response, and, in order to bound the latter rigorously, one can choose either essential or natural boundary conditions. In fact, according to the Hill's prescription [13] the relations between volume average stress and strain become the same in the $\delta \to \infty$ limit regardless of which of these two conditions have been used. Let us note that this is different from a methodology due to DRUGAN and WILLIS [14].

We note here that the problem of determination of the RVE received considerable attention in the field of porous materials [15]. In the terminology of that reference, our window would be called an Arbitrary Volume Element, the volume being equivalent to a window's area in two dimensions $(2 - D)$. However, as shown in [12], connectivity of a soft phase versus a stiff one plays a very important role in the approach to the RVE: a matrix with rigid inclusions approaches the RVE limit quite rapidly ($\delta < 10$), while a matrix with very soft (hole-type) inclusions requires windows of the order of several hundred hole diameters to get there. This result motivates the setting of our present study in two-phase Voronoi mosaics, where, by varying the volume fraction of one phase versus another, we can go from a situation of a disconnected stiff phase embedded in a matrix of a soft one, through a system of percolation of both phases, up to a situation of a soft phase being disconnected in a matrix of a stiff one. In this paper we discuss scale dependence of effective moduli and their statistics in the most challenging regime: percolation point.

2. Scale-dependent hierarchies of bounds on effective moduli

In this section we focus on $2 - D$, two-phase microstructures of linear elastic materials in antiplane shear. The microstructural geometry is specified by a Voronoi mosaic in which each cell is being occupied by either phase 1 or 2 according to a probability equal to the global volume fraction, which is chosen at

50%, Fig. 1. This is the percolation point because the dual Delaunay network is six-coordinated on average (i.e., each Voronoi cell has a mean of six neighbors).

The Hooke's law of either phase (1 or 2) is given by

$$\sigma_i = C_{ij}\varepsilon_j, \quad i,j = 1,2, \qquad C_{ij} = C^{(1)}\delta_{ij} \quad \text{or} \quad C^{(2)}\delta_{ij}\,, \tag{2.1}$$

where, for simplicity of notation, we denote

$$\sigma_i \equiv \sigma_{i3}\,, \qquad \varepsilon_i \equiv \varepsilon_{i3}\,, \qquad i,j = 1,2. \tag{2.2}$$

On the microscale, the governing equation of this piecewise-constant material is

$$C\left(\frac{\partial^2 u}{\partial x_1} + \frac{\partial^2 u}{\partial x_2}\right) = 0, \qquad C = C^{(1)} \text{ or } C^{(2)}, \qquad u \equiv u_3\,. \tag{2.3}$$

The isotropy of both stiffness tensors $C^{(1)}$ and $C^{(2)}$ in (2.3) leads to a so-called *contrast* $\alpha \equiv C^{(2)}/C^{(1)}$, sometimes also called a *stiffness mismatch*; without loss of generality we assume $\alpha \geq 1$. Figure 1 depicts just one realization $\mathbf{B}(\omega)$ of a *random medium*, which, as is commonly done in mechanics of random media, is taken as a set $\mathbf{B} = \{\mathbf{B}(\omega);\ \omega \in \Omega\}$.

Let us note that there are several other physical problems equivalent to anti-plane shear by virtue of well known mathematical analogies – for example, in-plane conductivity. Also, the microstructure chosen here may be applied to model a range of different materials – examples are offered by duplex steels [16] for a finite α, or porous materials [15] for an extreme $\alpha = 0$ or ∞.

The effective moduli for a finite window domain of scale δ sampled in our material can be defined in several ways. Here we choose an approach based on an interpretation of a Hooke's law as one in which either a uniform strain ε_j^0 or a uniform stress σ_j^0 is prescribed. In the first case, we should choose essential (or displacement, Dirichlet) boundary conditions while in the second case, we should choose natural (or traction, Neumann) boundary conditions. The first setup is

$$\overline{\sigma}_i = C^e_{ij}\varepsilon^0_j \qquad \text{under} \qquad u(\mathbf{x}) = \varepsilon^0_j L_j \quad \forall\, \mathbf{x} \in \partial\mathbf{B}\,, \tag{2.4}$$

where $\overline{\sigma}_{ij}$ id the resulting mean (volume average) stress, and which leads to an effective stiffness $\mathbf{C}^e_\delta$. The second setup is

$$\overline{\varepsilon}_i = S^n_{ij}\sigma^0_j \qquad \text{under} \qquad t(\mathbf{x}) = \sigma^0_j n_j(\mathbf{x}) \quad \forall\, \mathbf{x} \in \partial\mathbf{B}\,, \tag{2.5}$$

where $\overline{\varepsilon}_{ij}$ is the resulting mean (volume average) strain, and leads to an effective compliance $\mathbf{S}^n_\delta$. Determination of either tensor, $\mathbf{C}^e_\delta$ or $\mathbf{S}^n_\delta$, requires three tests.

For any realization $\mathbf{B}(\omega)$, a window's response on the mesoscale (δ finite) is, under these definitions, nonunique – because $C^e_{ij} \neq (S^n_{ij})^{-1}$ almost surely – and anisotropic. Thus, the answer to the question posed by the title of Sec. 1

is negative. However, considering the ergodicity of the Poisson point process underlying our two-phase microstructure, it can be shown from the variational principles [11, 17, 18], that the ensemble averages of these two tensors provide, with the increasing scale δ, an ever tighter pair of bounds on $\mathbf{C}^{\text{eff}}$

$$\begin{aligned}(2.6)\qquad \mathbf{C}^R \equiv (\mathbf{S}^R)^{-1} \equiv \langle \mathbf{S}_1^n \rangle^{-1} \leq \langle \mathbf{S}_{\delta'}^n \rangle^{-1} \leq \langle \mathbf{S}_{\delta}^n \rangle^{-1} \\ \leq \mathbf{C}^{\text{eff}} \leq \langle \mathbf{C}_{\delta}^e \rangle \leq \langle \mathbf{C}_{\delta'}^e \rangle \leq \langle \mathbf{C}_1^e \rangle \equiv \mathbf{C}^V \qquad \forall\, \delta' < \delta.\end{aligned}$$

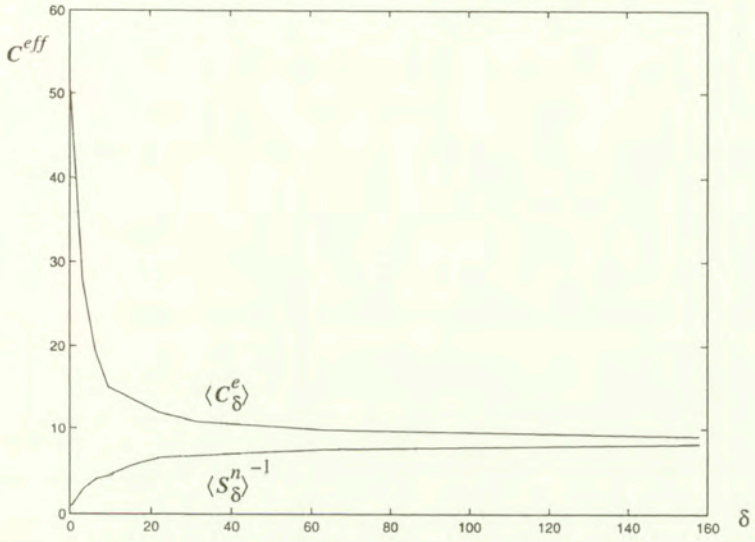

FIG. 2. Hierarchies of bounds on effective anti-plane moduli $\mathbf{C}_\delta^e$ and $\mathbf{S}_\delta^n$ of the two-phase microstructure of Fig. 1 at $C^{(1)} = 1$ and contrast $\alpha = 100$.

In Fig. 2 we show this hierarchy for our two-phase Voronoi composite at contrast $\alpha = 100$ at 50% volume fraction of either phase. Although it is the percolation point for this system – the most challenging regime in random systems – the scale (i.e., δ) and contrast (i.e., α) dependence of both tensors follow, with very high accuracy, the laws first found for $2 - D$ Bernoulli lattices [11], namely

$$(2.7)\qquad \langle \mathbf{C}_\delta^e \rangle = a_0 + a_1 \exp\left(a_2 \delta^{-a_3 \alpha}\right), \qquad \langle \mathbf{S}_\delta^n \rangle = b_0 + b_1 \exp\left(b_2 \delta^{-b_3 \alpha}\right).$$

Indeed, the contrast dependence in (2.7) has been verified for $\alpha = 10, 10^2, 10^3$, and 10^4.

The probability distributions of $\mathbf{C}_\delta^e$ and $\mathbf{S}_\delta^n$ that are involved in the hierarchy (2.6) are now assessed in terms of the statistics of their traces and radii of the corresponding Mohr's circles; the radius is, of course, defined by $R \equiv C_{12,\max} = \sqrt{(C_{11} - C_{22})^2/4 + C_{12}^2}$. Figures 3 and 4 display, for five scales δ, these statistics for tensors $\mathbf{C}_\delta^e$ and $\mathbf{S}_\delta^n$, respectively. They have been obtained by solving, through

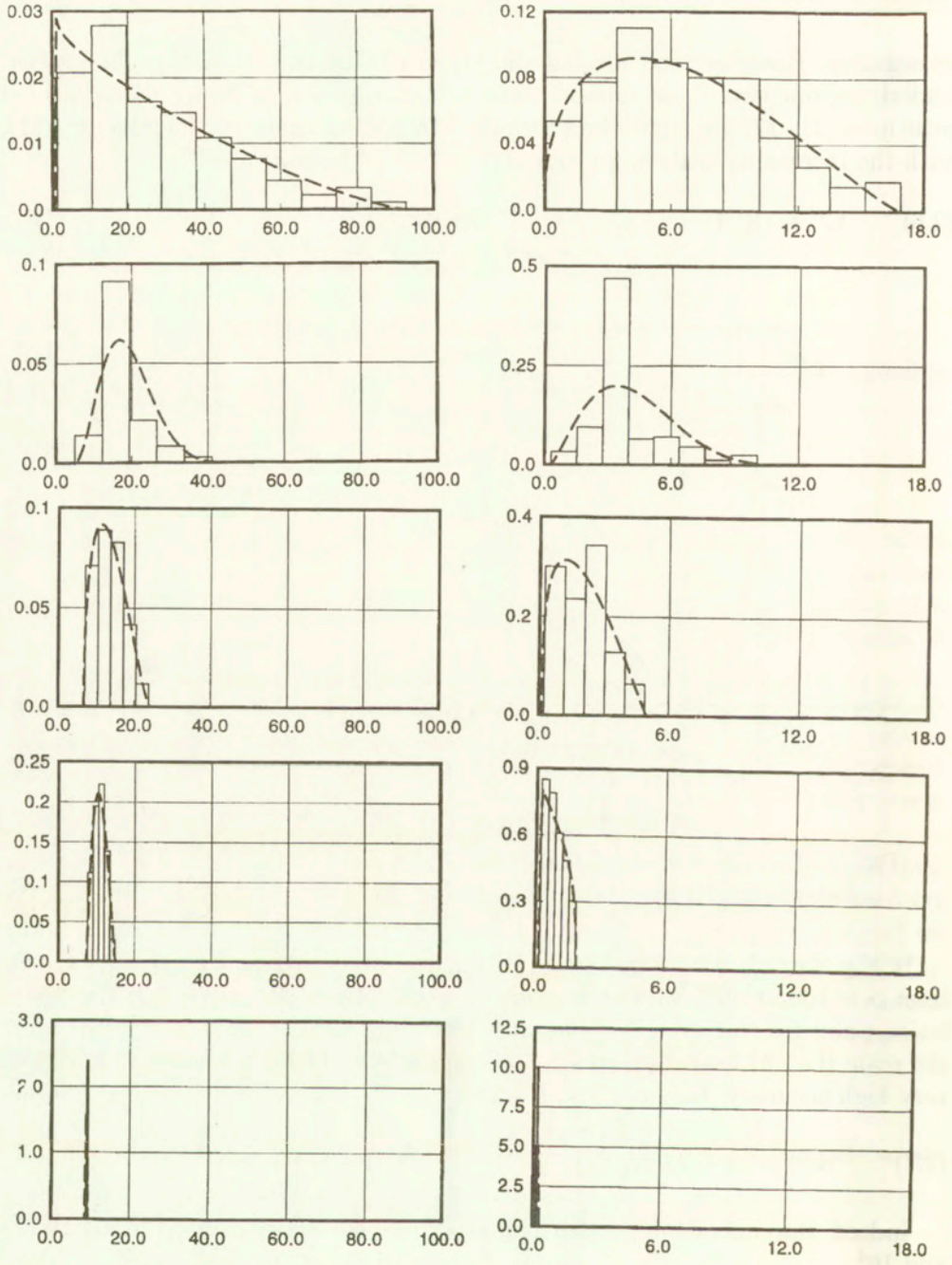

FIG. 3. The histograms and beta function probability fits to $\operatorname{tr} \mathbf{C}_\delta^\varepsilon$ (left column) and R (right column) as functions of the window scale $\delta = 3.16,\ 6.32,\ 15.8,\ 31.6$, and 158 under displacement boundary condition of the two-phase microstructure of Fig. 1 at volume fraction 50%, $C^{(1)} = 1$, and contrast $\alpha = 100$.

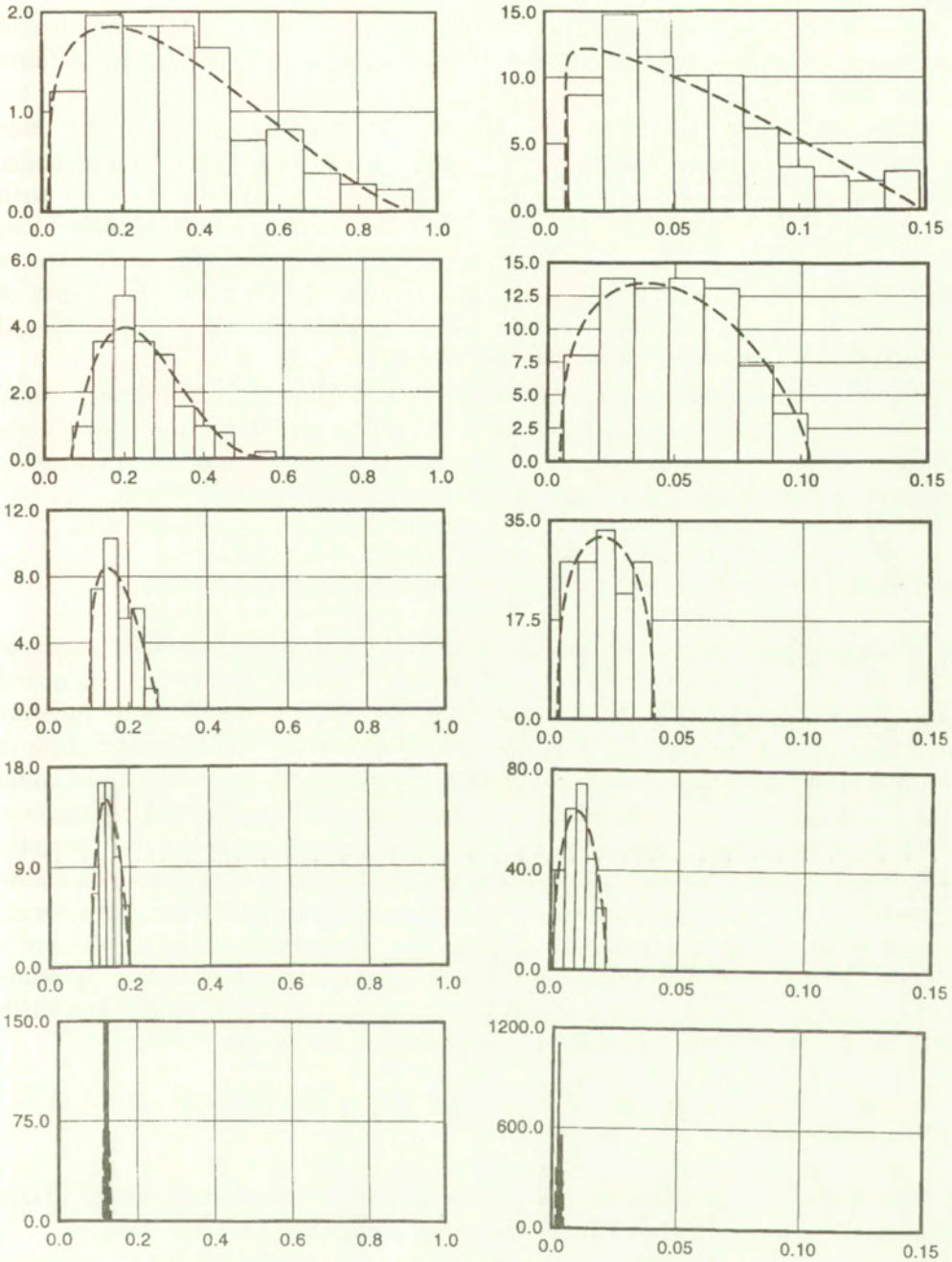

FIG. 4. The histograms and beta function probability fits to $\mathrm{tr}\,\mathbf{S}_\delta^\epsilon$ (left column) and R (right column) as functions of the window scale $\delta = 3.16,\ 6.32,\ 15.8,\ 31.6$, and 158 under traction boundary condition of the two-phase microstructure of Fig. 1 at volume fraction 50%, $C^{(1)} = 1$, and contrast $\alpha = 100$.

a computational mechanics method, boundary value problems for a number of two-phase Voronoi composites $\mathbf{B}(\omega)$ of the set $\mathbf{B}$, all being generated in a Monte Carlo sense.

Note that while the traces have asymmetric distributions, their character is very similar for both tensors. The Mohr's circles' radii have even stronger skewness, and their coefficient of variation (COV) is practically constant with the changing scale: COV $\cong 0.5 \pm 0.05$; this holds again for both tensors. Also shown in Figs. 3 and 4 are Beta function probability density fits to the traces and radii, which, as discussed in [12], are very satisfactory for other types of composites as well. This latter reference also gives a discussion of the spatial correlation structure of random fields $\mathbf{C}^e_\delta$ and $\mathbf{S}^n_\delta$.

These results provide a stepping stone for a stochastic finite element study of macroscopic response of a material with such a microstructure [19], where, following the approach developed earlier [20, 21], we recognize our meso-scale window to play the role of a single finite element.

3. Closure

It should finally be noted that there are other ways to define effective meso-scale responses. First of all, besides (2.4) and (2.5) one could consider mixed (displacement-traction) boundary conditions [22], which would result in some intermediate response. Next, by appropriately modifying the microstructure in the boundary zone through an introduction of a meso-scale periodicity, one could look at the displacement-periodic and traction-periodic conditions. A comparison of all the above cases, in the setting of matrix-inclusion composites, has recently been conducted in [23]. Other possible approaches include a homogenization formulation, and nonclassical (e.g., nonlocal) models. In particular, considering the presence of the grain-type microstructure, we face a question whether a classical or a micropolar continuum is more appropriate. A forthcoming study [24] outlines the determination of effective micropolar moduli, which thus sheds light on a heretofore enigmatic Cosserat characteristic length.

Acknowledgment

Support of this research by the National Science Foundation under grants MSS-9202772 and CMS-9713764 is gratefully acknowledged.

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INSTITUTE OF PAPER SCIENCE AND TECHNOLOGY,
AND GEORGIA INSTITUTE OF TECHNOLOGY
Atlanta, GA 30318-5794, U.S.A.
e-mail: martin.ostoja@ipst.edu

Received October 2, 1997.

Arch. Mech., 50, 3, pp. 559–566, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

Nonlinear dynamics of the alignment tensor in the presence of electric fields

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

C. PAPENFUSS (BERLIN)

IN THE MESOSCOPIC theory field quantities are introduced, which depend not only on position and time, but also on an additional orientational variable, the microscopic director. The orientation distribution function (ODF) gives the fraction of particles of a particular orientation. An equation of motion for the second order alignment tensor, including the influence of electromagnetic fields and of spatial inhomogeneities, is derived. The starting point are the mesoscopic balance equations of mass and of angular momentum. A constitutive equation on the mesoscopic level is discussed. The two balance equations together with the constitutive equation yield an equation of motion for the ODF. This finally leads to a nonlinear partial differential equation for the alignment tensor, which involves also the fourth and the sixth moment of the ODF.

Notations

ϱ mass density,
$\underline{v}$ material velocity,
$\underline{\underline{t}}$ stress tensor,
$\underline{f}$ acceleration of external forces,
$\underline{s}$ specific density of internal angular momentum,
$\underline{\underline{\Pi}}$ couple stresses,
$\underline{g}$ couple forces,
f orientation distribution function.

1. Introduction

THE DYNAMICS of the orientational order in liquid crystals under the influence of electromagnetic fields is interesting from the practical as well as from the theoretical point of view. The most important application is the switching of the preferred orientation in liquid crystalline devices. There are other experiments, where a rotating electric field is applied to a thin free-standing film [3]. The formation of dynamical orientation patterns is observed. In these orientation patterns the orientational order is spatially inhomogenuous. This importance of spatial gradients has not been taken into account in previous papers [9, 5] and will be considered now.

The orientational order in liquid crystals is described by the orientation distribution function or approximately, by the alignment tensor of second order. The aim of the present paper is a derivation of a differential equation for the orientation distribution function (ODF) and from there, the derivation of a differential equation for the alignment tensor. The starting point is the mesoscopic theory of liquid crystals.

Up to now, the theoretical work on the dynamics of the orientational order has been based on a Fokker–Planck-equation for the orientation distribution function [6, 7, 4]. This equation is motivated by physical arguments, but has not been derived from the basic principles. On the other hand, the mesoscopic balance of mass yields an equation of motion for the orientation distribution function (ODF). However this is not a closed equation, as long as the field of orientation change velocity and the higher order alignment tensors are not given. In the present paper, an equation for the ODF is derived on the grounds of the mesoscopic theory.

2. Mesoscopic concept

Liquid crystals consist of non-spherical particles. Here it is assumed that the particles are rotationally symmetric, with the axis of rotation called microscopic director $\underline{n}$. In all liquid crystalline phases the microscopic directors exhibit a long-range orientational order, but no (three-dimensional) positional order. The orientational order can be described by introducing an orientation distribution function (ODF) (see Fig. 1).

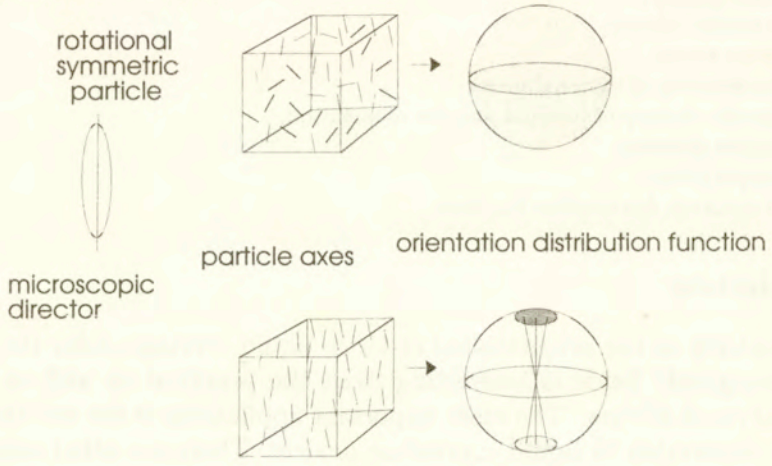

FIG. 1.

The axes of the rotationally symmetric particles are the miroscopic directors. Their orientations are distributed at random in the isotropic phase, and they are more or less parallel in the liquid crystalline phases. This corresponds to

an isotropic orientation distribution function on the unit sphere, or an ODF concentrated around one direction, respectively. If the orientation distribution function is rotationally symmetric, the axis of rotational symmetry is called the macroscopic director $\underline{d}$.

This distribution function is defined on the so-called nematic space. The nematic space is spanned by positions $\underline{x}$, orientations $\underline{n}$, and time t. $\underline{x}$ and $\underline{n}$ determine the configuration of the rotationally symmetric particle. In all liquid crystalline phases the ODF is anisotropic, whereas in the isotropic phase it is a homogenuous distribution on the unit sphere. In the liquid crystalline phase the ODF can be uniaxial or biaxial. In the nematic phase it is observed experimentally in most cases to be uniaxial. For uniaxial orientation distribution functions there exists an axis of rotational symmetry called macroscopic director $\underline{d}$. The anisotropic moments of the ODF are called alignment tensors. They are defined as

$$a^{(k)} := \int_{S^2} f(\underline{x}, \underline{n}, t) \underbrace{\overline{\underline{n} \dots \underline{n}}}_{k} d^2 n \,, \tag{2.1}$$

where $\overline{\dots}$ denotes the symmetric irreducible part of a tensor. Because of the symmetry of the ODF $f(-\underline{n}) = f(\underline{n})$, only even order alignment tensors are nonzero. If the ODF is uniaxial, the alignment tensors can be expressed in terms of the order parameters $S^{(k)}$ and the macroscopic director:

$$a^{(k)} = S^{(k)} \underbrace{\overline{\underline{d} \dots \underline{d}}}_{k} \tag{2.2}$$

for symmetry reasons, and analogously for the even-order moments which are not traceless:

$$\int_{S^2} f(\underline{x}, \underline{n}, t) \underbrace{\underline{n} \dots \underline{n}}_{k} d^2 n = \sigma^{(k)} \underbrace{\underline{d} \dots \underline{d}}_{k} \,. \tag{2.3}$$

The second order parameter S is the Maier–Saupe order parameter.

The idea of the mesoscopic theory is to define fields on a higher-dimensional domain, in contrast to the Ericksen–Leslie theory, which introduces an additional macroscopic field (the macroscopic director $\underline{d}$). So-called mesoscopic fields are introduced, which are fields of physical quantities defined on the nematic space, i.e. depending not only on position and time, but also on the microscopic director (the orientation). For instance, the mesoscopic mass density $\widehat{\varrho}(\underline{x}, \underline{n}, t)$ is the mass density of particles of the particular orientation $\underline{n}$. Mesoscopic fields are denoted by a mark $\widehat{\ }$. Macroscopic fields are obtained from the mesoscopic ones by avaraging with the ODF. The ODF gives the fraction of particles of orientation $\underline{n}$:

$$f(\underline{x}, \underline{n}, t) = \frac{\widehat{\varrho}(\underline{x}, \underline{n}, t)}{\varrho(\underline{x}, t)} \,. \tag{2.4}$$

For the mesoscopic quantities, the balance equations have been derived [1, 2]. From the mesoscopic balance of mass one obtains for the ODF in the case of an incompressible fluid:

$$\frac{\partial f}{\partial t} + \underline{\hat{v}} \cdot \nabla f + \nabla_n \cdot (\underline{u} f) = 0. \tag{2.5}$$

$\underline{\hat{v}}$ is the material velocity of particles of orientation $\underline{n}$. $\underline{u}$ is the orientation change velocity. It is tangential to the unit sphere. ∇_n denotes the covariant derivative with respect to the orientation variable. The last term on the left-hand side of Eq. (2.5) is the flux in orientation space. It expresses the fact that the fraction of particles of orientation $\underline{n}$ changes if the particles change their orientation (see Fig. 2). The orientation change velocity $\underline{u}$ is tangential to the unit sphere.

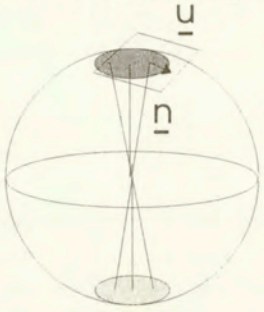

FIG. 2.

3. Balance of spin and simplifications

The mesoscopic balance of spin reads:

$$\frac{\partial \widehat{\varrho \underline{s}}}{\partial t} + \nabla \cdot \left(\widehat{\varrho \underline{v} \underline{s}} - \left(\underline{n} \times \underline{\underline{\hat{\Pi}}} \right)^T \right) + \nabla_n \cdot (\widehat{\varrho \underline{u} \underline{s}}) = \underline{\underline{\epsilon}} : \underline{\underline{\hat{t}}} + \widehat{\varrho \underline{n}} \times \underline{\hat{g}}. \tag{3.1}$$

The symbols are: $\underline{\hat{s}}$: mesoscopic specific spin density, $\underline{\underline{\hat{\Pi}}}$: couple stresses ($\nabla \cdot \underline{\underline{\hat{\Pi}}}$ are short-range forces acting on the orientation), $\underline{\underline{\hat{t}}}$: mesoscopic stress tensor, $\underline{\hat{g}}$: couple forces (long-range forces acting on the orientation). Equation (3.1) shows that the antisymmetric part of the stress tensor produces the spin.

3.1. Approximations

In contrast to the previous work [9], the system is not assumed to be uniform. The following simplifications are made:

1. The spin is stationary: $\dfrac{\partial \underline{\hat{s}}}{\partial t} = 0$.

2. There is no material flux: $\underline{\hat{v}} \equiv 0$. In the case of freestanding liquid crystalline films in a rotating electric field, there are experimental hints that there is no flow of material [3].

Then the spin balance (3.1) simplifies to

$$\hat{\varrho}\underline{u}\cdot\nabla_n\underline{\hat{s}} = \underline{\underline{\epsilon}} : \underline{\hat{t}} + \hat{\varrho}\underline{n}\times\underline{\hat{g}} + \nabla\cdot\left(\underline{n}\times\underline{\underline{\hat{\Pi}}}\right)^T ; \tag{3.2}$$

$\underline{\hat{t}}$, $\underline{\underline{\hat{\Pi}}}$ and $\underline{\hat{g}}$ are constitutive quantities. They depend on the variables in the state space (see below) in a material-dependent manner. From Eq. (3.2) we see that $\underline{\underline{\epsilon}} : \underline{\hat{t}} + \hat{\varrho}\underline{n}\times\underline{\hat{g}} + \nabla\cdot\left(\underline{n}\times\underline{\underline{\hat{\Pi}}}\right)^T$ vanishes if $\nabla_n\underline{\hat{s}} = 0$. Therefore we can write down a constitutive equation of the form

$$\underline{\underline{\epsilon}} : \underline{\hat{t}} + \hat{\varrho}\underline{n}\times\underline{\hat{g}} + \nabla\cdot\left(\underline{n}\times\underline{\underline{\Pi}}\right)^T = \hat{\varrho}\underline{\hat{G}}\cdot\nabla_n\underline{\hat{s}}\,. \tag{3.3}$$

The orientation change velocity $\underline{u}$ is a solution of the stationary spin balance (3.2) if

$$\underline{u} = \underline{\underline{P}}\cdot\underline{\hat{G}}, \qquad \underline{\underline{P}} = \underline{\underline{\delta}} - \underline{n}\underline{n}\,. \tag{3.4}$$

It has been taken into account that $\underline{u}$ is orthogonal to $\underline{n}$, with the projector $\underline{\underline{P}}$ onto the space orthogonal to $\underline{n}$ (see Eq. (3.4)), because $\underline{u} = \dot{\underline{n}}$, and $\underline{n}$ is a unit vector.

For the mesoscopic quantity $\underline{\hat{G}}$ we make a constitutive assumption.

4. Constitutive equations

In order to make a constitutive assumption it is necessary to fix the domain of the constitutive functions, i.e. to choose the state space. The state space has to be a mesoscopic one, because we are dealing with mesoscopic constitutive functions. It also has to include spatial gradients, because orientation patterns are inhomogenuous in space. The electric field $\underline{E}$ is also included. It is chosen here as

$$Z = \left(\hat{\varrho}, T, \underline{E}, \underline{a}, \nabla\underline{a}, \nabla\nabla\underline{a}, \frac{\nabla\hat{\varrho}}{\hat{\varrho}}, \frac{\nabla\nabla\hat{\varrho}}{\hat{\varrho}}, \frac{\nabla_n\hat{\varrho}}{\hat{\varrho}}, \underline{n}\right), \tag{4.1}$$

here T is the temperature. It includes macroscopic $(T, \underline{E}, \underline{a}, \nabla\underline{a}, \nabla\nabla\underline{a})$ and mesoscopic variables $\left(\hat{\varrho}, \frac{\nabla\hat{\varrho}}{\hat{\varrho}}, \frac{\nabla\nabla\hat{\varrho}}{\hat{\varrho}}, \frac{\nabla_n\hat{\varrho}}{\hat{\varrho}}, \underline{n}\right)$. Especially the macroscopic quantity, the second order alignment tensor $\underline{a}$, has been included in the state space. This inclusion of an integral quantity is necessary, because the action on particles of one orientation depends not only on particles of similiar orientations, but also on particles of very different orientations.

Then a representation theorem for $\underline{\hat{G}}$, linear in all derivatives and quadratic in $\underline{E}$, gives:

$$\begin{aligned}\underline{u} = \underline{\underline{P}}\cdot\underline{\hat{G}} = \beta_3\nabla_n\ln\hat{\varrho} + \underline{\underline{P}}\cdot\Big(&\beta_5\underline{a} + \beta_6\underline{a}\cdot\underline{a} + \beta_9\underline{a}\cdot\underline{n}\underline{n}\cdot\underline{a} + \beta_7\underline{E}\underline{E} \\ &+ \beta_8\underline{n}\underline{n} : \nabla\nabla\underline{a} + \beta_{10}\frac{\nabla\nabla\hat{\varrho}}{\hat{\varrho}} + \beta_{11}\underline{n}\cdot\nabla\nabla\underline{a}\cdot\underline{n} + \beta_{12}\underline{n}\underline{n} : \underline{\underline{a}}\underline{a}\Big)\cdot\underline{n}\,.\end{aligned} \tag{4.2}$$

Here it has been taken into account that the orientation change velocity must be an even function of $\underline{n}$

$$\underline{u}(-\underline{n}) = -\underline{u}(\underline{n}) . \tag{4.3}$$

The coefficients β_j are functions of the macroscopic mass density $\varrho(\underline{x}, t)$ and the temperature $T(\underline{x}, t)$.

5. The equations of motion for the orientation distribution function and for the second order alignment tensor

The second tensorial irreducible moment of Eq. (2.5) reads

$$\frac{\partial}{\partial t} \int_{S^2} f \, \overline{\underline{n}\underline{n}} \, d^2n + \underline{v} \cdot \nabla \int_{S^2} f \, \overline{\underline{n}\underline{n}} \, d^2n + \int_{S^2} \overline{\underline{n}\underline{n}} \, \nabla_n \cdot (f\underline{u}) d^2n = 0 . \tag{5.1}$$

The first two terms are derivatives of the alignment tensor. The third term is integrated by parts using the Gauss theorem on the unit sphere. The resulting equation reads:

$$\frac{\partial \underline{\underline{a}}}{\partial t} + \underline{v} \cdot \nabla \underline{\underline{a}} = \frac{d\underline{\underline{a}}}{dt} = \int_{S^2} f\underline{u} \cdot \nabla_n (\underline{n}\underline{n}) d^2n . \tag{5.2}$$

In our case we have $\underline{v} \equiv 0$. Then inserting Eq. (4.2) and integrating the first term by parts, we obtain:

$$\begin{aligned} \frac{\partial \underline{\underline{a}}}{\partial t} = {} & 6\beta_3 \underline{\underline{a}} + 2\beta_{10} \left(\nabla\nabla \cdot \underline{\underline{a}} \right)^{\text{symm}} + \left(\left(\underline{\underline{a}} + \frac{1}{3} \underline{\underline{\delta}} \right) \cdot \underline{\underline{A}} \right)^{\text{symm}} \\ & - 2 \left(\underline{\underline{A}} + \beta_{10} \nabla\nabla \right) : \int_{S^2} \underline{n}\underline{n}\underline{n}\underline{n} f d^2n \\ & + 2 \left(\underline{\underline{\underline{B}}} : \cdot \int_{S^2} \underline{n}\underline{n}\underline{n}\underline{n} f d^2n \right)^{\text{symm}} \\ & - 2 \left((\beta_8 + \beta_{11}) \nabla\nabla \underline{\underline{a}} + \beta_{12} \underline{a}\underline{a} \right) :: \int_{S^2} \underline{n}\underline{n}\underline{n}\underline{n}\underline{n}\underline{n} f d^2n , \end{aligned} \tag{5.3}$$

where $(\ldots)^{\text{symm}}$ denotes the symmetric part of a tensor, and we have introduced $\left(\nabla\nabla \underline{\underline{a}} \right)^T_{ijkl} := \nabla_k \nabla_l a_{ij}$. It has been taken into account that

$$\nabla_n \underline{n} = \underline{\underline{P}} = \underline{\underline{\delta}} - \underline{n}\underline{n} , \tag{5.4}$$

and we have introduced the abbreviations

$$\underline{\underline{A}} := \beta_5 \underline{\underline{a}} + \beta_6 \underline{\underline{a}} \cdot \underline{\underline{a}} + \beta_7 \underline{\underline{E}}\underline{\underline{E}} , \tag{5.5}$$

$$\underline{\underline{\underline{B}}} = \left(\beta_8 \left(\nabla\nabla \underline{\underline{a}} \right)^T + \beta_{11} \nabla\nabla \underline{\underline{a}} + \beta_{12} \underline{\underline{a}}\underline{\underline{a}} \right) . \tag{5.6}$$

The higher moments $\int_{S^2} \underline{nnnn} f d^2n$ and $\int_{S^2} \underline{nnnnnn} f d^2n$ can be expressed by the second order one using the closure relation, which can be derived using the principle of maximum entropy [8]. This derivation of a closure relation will be published elsewhere.

6. Conclusions

Starting with the orientational balances, we have derived a Fokker–Planck type differential equation for the orientation distribution function (ODF). The special form of this equation was obtained under several assumptions mentioned in Subsec. 3.1. Because the second order alignment tensor, which is the second moment of the orientation distribution function, enters this equation, the equation for the distribution function is an integro-differential equation. Taking the second moment of this equation, a nonlinear partial differential equation for the second order alignment tensor is obtained. The orientation distribution function is hardly experimentally accessible, and the second order alignment tensor is the most important quantity from the experimental point of view. The fourth and the sixth moment of the ODF enter the equation for the second order alignment tensor. Closure relations expressing these higher moments in terms of the second one can be derived by applying the principle of maximum entropy on the phase space. The entropy is maximized under the constraints that the phase space averages of the fields of mass density, internal energy density, spin density and second order aligmnent tensor are prescribed at every $\underline{x}$ and t.

In most cases the ODF is uniaxial and the alignment tensor can be expressed by the scalar order parameter S and the macroscopic director $\underline{d}$. For this uniaxial case, coupled differential equations for S and $\underline{d}$ can be derived.

Acknowledgments

Many helpful discussions with W. MUSCHIK and H. EHRENTRAUT are gratefully acknowledged. The work has been supported financially by Draloric Company (D-95100 Selb), the European Union (grant ERBCHRXCT920007) and the Sfb 335 "Anisotrope Fluide".

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INSTITUT FÜR THEORETISCHE PHYSIK,
TECHNISCHE UNIVERSITÄT BERLIN
Hardenbergstr. 36, D-10623 Berlin, Germany.

Received November 19, 1997.

Arch. Mech., 50, 3, pp. 567–575, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

On defective crystallography

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

G.P. PARRY (NOTTINGHAM)

SUPPOSE that a solid crystal derives from a perfect (Bravais) lattice of atoms, so that the set of rearrangements of the points of this lattice provides symmetries of the crystal. In the elasticity theory appropriate to such a crystal, it is traditional to assert that the corresponding strain energy density function has invariance properties related to a (proper) subset of these symmetries. Here I discuss similar issues in the context of the continuum mechanics of smoothly defective crystals, focusing on planar distributions of defects.

1. Introduction

I DISCUSS issues related to material symmetry for defective crystals. Experience with perfect crystals shows that choosing an appropriate symmetry group for constitutive functions that govern the mechanics is a subtle procedure. To be specific, one usually chooses a point group of orthogonal transformations as symmetry group for the strain energy function (say) of a cubic crystal in continuum mechanics, even though this is not the full group of symmetries of a cubic lattice, and even though a cubic lattice is not a continuum. So it is natural to try to understand the issues related to the choice of symmetry group first of all in the context of perfect crystals, before proceeding to the defective case, and I outline relevant concepts in Sec. 2 of the paper. Aside from the purely pragmatic reason that calculations based on the point group symmetries perform reasonably well in linear elasticity theories, there is just one logical reason that I know to prefer these groups. That reason derives from a calculation of FONSECA [6], which shows that

- for a strain energy function w with symmetry group corresponding to the full set of rearrangements of a cubic lattice,
- with A the class of Lipshitz deformations $\mathbf{u}$ defined on a region Ω satisfying homogeneous boundary condition $\mathbf{u} = F\mathbf{x}$, $F \in M^+_{3\times 3}$, $\mathbf{x} \in \partial\Omega$,

$$\inf_A \int_\Omega w(\nabla \mathbf{u}) = |\Omega|\, \phi(\det F) \tag{1.1}$$

for some $\phi : \mathbb{R}^+ \to \mathbb{R}$ (see also CHIPOT [2]). This implies, loosely, that a perfect crystal cannot sustain shear stresses in equilibrium, and it is a rigorous result

which one must somehow reconcile with the fact that the shear strength of real crystals is nonzero. Various options present themselves for consideration:

- no real crystal is perfect, but if for the sake of argument we suppose that some real crystal is perfect,
- equilibria do not correspond to infima of an energy functional of the form given above, but if equilibria do correspond to such an infimum,
- the choice of symmetry of group for the energy function is incorrect.

In this paper, responding in part to these three options:

- In Sec. 2, I describe aspects of perfect crystal symmetry, concentrating on two-dimensional crystals, for the sake of simplicity;
- In Sec. 3, I introduce geometric variables which categorize crystals which are not perfect, but which are *defective*, and focus on special cases where the defectiveness of the crystals is uniform;
- For *planar* defective crystals, in Sec. 4, I discuss the construction of discrete sets of points which are compatible with the continuum description of the crystal, and derive some symmetries of these sets of points. Then I suggest that some of these symmetries should be taken over to the continuum model. It turns out that relevant symmetries are determined by the dislocation density tensor, so that the symmetries depend on position only to the extent that the dislocation density depends on position.

2. Perfect crystal symmetry

Let

$$\Lambda(\mathbf{v}_a) = \left\{\mathbf{x} \in \mathbb{R}^2;\ \ \mathbf{x} = m_a\mathbf{v}_a,\ \ m_1, m_2 \in \mathcal{Z}\right\} \tag{2.1}$$

be a real 2-dimensional lattice with the two basis vectors $\mathbf{v}_1$, $\mathbf{v}_2$ linearly independent. Note that $\Lambda(\mathbf{v}_a) = \Lambda(\mathbf{v}'_0)$ if and only if

$$\mathbf{v}'_a = m_{ab}\mathbf{v}_b\,, \tag{2.2}$$

where (m_{ab}) is a matrix of integers with $|\det(m_{ab})| = 1$. If one regards the points of $\Lambda(\mathbf{v}_a)$ as embedded in a continuum, then any deformation of the continuum, with deformation gradient denoted F, which has the property that

$$F\mathbf{v}_a = \mathbf{v}'_a\,, \tag{2.3}$$

maps the lattice onto itself, in the sense that if $x \equiv m_a\mathbf{v}_a \in \Lambda(\mathbf{v}_a)$, then

$$F\mathbf{x} = F(m_a\mathbf{v}_a) = m_a(F\mathbf{v}_a) = m_a\mathbf{v}'_a \in \Lambda(\mathbf{v}'_a) \equiv \Lambda(\mathbf{v}_a). \tag{2.4}$$

So there is an infinite number of deformations which rearrange the discrete points of the lattice $\Lambda(\mathbf{v}_a)$.

The apparatus of traditional crystallography is directed at the classification of subgroups of the set of rearrangements of the points of $\Lambda(\mathbf{v}_a)$. Specifically, one considers those rearrangements (m_{ab}) such that

$$F\mathbf{v}_a = m_{ab}\mathbf{v}_b\,, \tag{2.5}$$

where F is orthogonal. If $\{\mathbf{v}_a\}$ is given, the orthogonal transformations that satisfy (2.5), for some (m_{ab}) of the appropriate form, make up the *point group* of $\Lambda(\mathbf{v}_a)$, and the rearrangements that satisfy (2.5) for some orthogonal F make up the *lattice group* of $\Lambda(\mathbf{v}_a)$ (see ERICKSEN [5], PARRY [16], ZANZOTTO [19]).

If one deals, in nonlinear elasticity, with strain energy density functions of the form $\tilde{w}(\mathbf{v}_a)$ and accepts that the individual atoms which correspond to the points of $\Lambda(\mathbf{v}_a)$ are indistinguishable, then it is reasonable to require that

$$\tilde{w}(\mathbf{v}'_a) = \tilde{w}(\mathbf{v}_a), \tag{2.6}$$

whenever (2.2) holds. In addition, it is common to assume that there exist fixed vectors $\mathbf{V}_a$ such that

$$\mathbf{v}_a = T\mathbf{V}_a\,, \tag{2.7}$$

where T is the macroscopic deformation gradient which governs the behaviour of material line elements relative to an appropriate reference configuration. This is called the Cauchy–Born hypothesis (see ZANZOTTO [20] for comments on this hypothesis). With (2.6) and (2.7), define $w(T)$ by

$$w(T) = \tilde{w}(\mathbf{v}_a). \tag{2.8}$$

Then the symmetry property (2.6) gives

$$\begin{aligned} w(T) = \tilde{w}(\mathbf{v}_a) = \tilde{w}(m_{ab}\mathbf{v}_b) = \tilde{w}(m_{ab}T\mathbf{V}_b) = \tilde{w}(Tm_{ab}\mathbf{V}_b) \\ = \tilde{w}(TS\mathbf{V}_b) = w(TS), \end{aligned} \tag{2.9}$$

if one writes, following (2.5),

$$S\mathbf{V}_b = m_{ab}\mathbf{V}_b\,. \tag{2.10}$$

One might call the orthogonal S which satisfy (2.10) elements of the point group of the reference lattice $\Lambda(\mathbf{V}_a)$, so the symmetries of the corresponding strain energy density include those given by $w(T) = w(TS)$, with S in this point group, as in (2.9). However there is no logical reason, *a priori*, to exclude those non-orthogonal solutions S of (2.10) which correspond to the symmetry property (2.6) (but recall Fonseca's calculation) and concentrate just on the relevant point group.

Finally, classical theorems of invariant theory (GREEN and ADKINS [8], WEYL [18]) give representations of the solutions $w(\cdot)$ of (2.9) for an arbitrary point

group. Solutions $\tilde{w}(\cdot)$ of (2.6), on the other hand, are constructed by finding a fundamental domain $\mathcal{D}$ with the properties that

(i) if $\{\mathbf{v}_a\} \in \mathcal{D}$, then there is no other point of $\mathcal{D}$ which has the form $\{m_{ab}\mathbf{v}_b\}$,
(ii) each $\{\mathbf{v}'_a\}$ may be written as $\{m_{ab}\mathbf{v}_b\}$ with $\{\mathbf{v}_b\} \in \mathcal{D}$.

There are various ways of constructing such a domain $\mathcal{D}$;

• PARRY [13] and PITTERI [17] give (equivalent) geometric and analytic methods of finding $\mathcal{D}$.

• One can conveniently rephrase the problem in complex form, see PARRY [16]. This method has various other advantages, too.

• CONWAY and SLOANE [3] give arithmetical ways of solving the problem.

3. Defective crystals

In this section I replace the basis vectors $\{\mathbf{v}_a\}$ which generate the perfect Bravais lattice $\Lambda(\mathbf{v}_a)$ by *lattice vector fields* $\{\mathbf{d}_a(\cdot)\}$ which are imagined to characterize the internal structure of the crystal, see DAVINI and PARRY [4], PARRY [14], FONSECA and PARRY [7].

A *state* Σ of the crystal consists of three lattice vector fields $\mathbf{d}_1(\mathbf{x})$, $\mathbf{d}_2(\mathbf{x})$, $\mathbf{d}_3(\mathbf{x})$ defined at each point $\mathbf{x}$ of a region Ω, thus

$$\Sigma = \{\mathbf{d}_a(\cdot), \quad a = 1,2,3; \Omega\}. \tag{3.1}$$

For brevity I write henceforward $\Sigma = \{\mathbf{d}_a(\cdot), \Omega\}$. It is assumed that $\mathbf{d}_1(\mathbf{x})\cdot\mathbf{d}_2(\mathbf{x})\wedge\mathbf{d}_3(\mathbf{x}) \neq 0$, for all $\mathbf{x} \in \Omega$, so there exist *dual lattice vector fields* $\mathbf{d}^1(\mathbf{x}), \mathbf{d}^2(\mathbf{x}), \mathbf{d}^3(\mathbf{x})$ with the property that $\mathbf{d}^a(\mathbf{x})\cdot\mathbf{d}_b(\mathbf{x}) = \delta^a_b$. Two states $\Sigma = \{\mathbf{d}_a(\cdot), \Omega\}$, $\Sigma^* = \{\mathbf{d}^*_a(\cdot), \Omega^*\}$ are *elastically related* to each other if there exists an invertible smooth mapping $\mathbf{u} : \Omega \to \Omega^* = \mathbf{u}(\Omega)$ such that

$$\begin{aligned} \mathbf{d}^*_a(\mathbf{u}(\mathbf{x})) &= \nabla\mathbf{u}(\mathbf{x})\mathbf{d}_a(\mathbf{x}), \qquad \text{or} \\ \mathbf{d}^{a*}(\mathbf{u}(\mathbf{x})) &= [\nabla\mathbf{u}(\mathbf{x})]^{-T}\mathbf{d}^a(\mathbf{x}), \qquad a = 1,2,3, \quad \mathbf{x} \in \Omega. \end{aligned} \tag{3.2}$$

It is evident from (3.2) that the Burgers integral $\oint_C \mathbf{d}^a(\mathbf{x})\cdot\mathbf{dx}$, C a contour, is an *elastic invariant integral*, in the sense that

$$\oint_{\mathbf{u}(C)=C^*} \mathbf{d}^{a*}(\mathbf{y})\cdot\mathbf{dy} = \oint_C \mathbf{d}^a(\mathbf{x})\cdot\mathbf{dx} \tag{3.3}$$

if Σ and Σ^* are elastically related to each other. It is shown in [4] that there is an infinite number of elastic invariant integrals, and that there is a finite functional basis for the corresponding set of densities. Central to the proof of these results is the notion of a (real-valued) *scalar* defined on a state $\Sigma = \{\mathbf{d}_a(\cdot), \Omega\}$. Thus

$$\mu_\Sigma(\mathbf{x}) \equiv \mu(\mathbf{x}, \mathbf{d}_a(\mathbf{x}), \quad \nabla\mathbf{d}_a(\mathbf{x}), \quad \nabla^2\mathbf{d}_a(\mathbf{x}), \quad \ldots) \tag{3.4}$$

is a *scalar* if wherever Σ and Σ^* are elastically related to each other, then

$$\mu_\Sigma(\mathbf{x}) = \mu_{\Sigma^*}(\mathbf{u}(\mathbf{x})). \tag{3.5}$$

From (3.5) one can regard the scalars as some kind of internal variables for plasticity theory, since they are transported unchanged in any elastic deformation. The prototypical examples of such a function $\mu_\Sigma(\cdot)$ are the nine functions

$$\frac{\mathbf{d}^a \cdot \nabla \wedge \mathbf{d}^b}{\det\{\mathbf{d}^a\}} \equiv \frac{S^{ab}}{n} \tag{3.6}$$

which are lattice components of the dislocation density tensor, cf. KONDO, BILBY, KRÖNER [9, 1, 10, 11]. (In (3.6), I *define* $S^{ab} = \mathbf{d}^a \cdot \nabla \wedge \mathbf{d}^b$, $n = \det\{\mathbf{d}^a\} = \mathbf{d}^1 \cdot \mathbf{d}^2 \wedge \mathbf{d}^3$). From (3.2) and (3.5) it is clear that $\oint_C \mu_\Sigma(x)\mathbf{d}^a(\mathbf{x}) \cdot \mathbf{dx}$ is also an elastic invariant integral, one can also easily show that $\int_V \mu_\Sigma(\mathbf{x}) n \, dV$ is an elastic invariant integral.

Slips and rearrangements enter this theory if one enquires how two different given states are connected when all the elastic invariant integrals match in the two states. It is clear that if the two states are elastically related, then these integrals match; the point is that there are other changes of state which preserve the integrals which are *not* elastic deformations. It is shown in PARRY [14] that these changes of state can be interpreted as *slip* in surfaces (say) where lattice vector fields are constant. Also there is some compatibility requirement on states that allow slip (partial integrability). Again in [14] it is shown that if there is a non-elastic change of state, from $\Sigma = \{\mathbf{d}_a(\cdot), \Omega\}$ to $\Sigma' = \{\mathbf{d}'_a(\cdot), \Omega\}$, preserving the integral invariants, then

$$\nabla \wedge (\mathbf{d}^a - \mathbf{d}^{a\prime}) = 0, \qquad \nu n = \nu' n', \qquad \nabla\nu \wedge (\mathbf{d}^a - \mathbf{d}^{a\prime}) = 0, \tag{3.7}$$

whenever

$$\nu \in \mathcal{F} \equiv \left\{ 1, \frac{S^{ab}}{n}(\cdot), \ (\mathbf{d}_c \cdot \nabla)\frac{S^{ab}}{n}(\cdot); \ a, b, c = 1, 2, 3 \right\}. \tag{3.8}$$

In fact these last equations (3.7) are *necessary and sufficient* that *all* integral invariants match in the two states Σ, Σ'. I do not discuss the derivation of these equations here, nor the requirement that Σ, Σ' are defined over the same region Ω (this is not a restriction, in fact). In [15] I use a theorem of Cartan, in a form quoted by OLVER [12], to derive abstract properties of states Σ which are such that (3.7) has a nontrivial solution for Σ' (that is, a solution with $\Sigma' \neq \Sigma$). I choose to display the relevant properties of such states, here, only in the particular case where the nine scalars S^{ab}/n are *constant* throughout Ω.

THEOREM 1. *States Σ such that* (3.7) *has a solution $\Sigma' \neq \Sigma$ are locally diffeomorphic to a state Σ^{mc} which has the structure of a (local) Lie group with structure constants $\varepsilon_{ijk}(S^{\ell k}/n)$.*

NOTES

1. States $\Sigma = \{\mathbf{d}_a(\cdot), \Omega\}$, $\Sigma^{mc} = \{\mathbf{D}_a(\cdot), \Omega^{mc}\}$ are locally diffeomorphic if and only if for each $\mathbf{x}_0 \in \Omega$ there exists a neighbourhood $N_{\mathbf{x}_0}$ of $\mathbf{x}_0$ in Ω and a diffeomorphism $\mathbf{u}_{\mathbf{x}_0} : N_{\mathbf{x}_0} \to \mathbf{u}_{\mathbf{x}_0}(N_{\mathbf{x}_0})$ such that $\mathbf{D}_a(\mathbf{u}_{\mathbf{x}_0}(\mathbf{x})) = \nabla \mathbf{u}_{\mathbf{x}_0}(\mathbf{x})\mathbf{d}_a(\mathbf{x})$, $\mathbf{x} \in N_{\mathbf{x}_0}$.

2. I say that Σ^{mc} has the structure of a (local) Lie group $\mathcal{G}$ with structure constants $\varepsilon_{ijk}(S^{\ell k}/n)$ if and only if

$$\mathbf{D}_a(\zeta(\mathbf{X}, \mathbf{Y})) = \nabla_{\mathbf{X}} \zeta(\mathbf{X}, \mathbf{Y}) \mathbf{D}_a(\mathbf{X}), \qquad \mathbf{Y} \in \Omega^{mc}, \tag{3.9}$$

where ζ is the composition function for $\mathcal{G}$, so that if $g(X)$, $g(Y)$ are group elements corresponding to the parametrization by points $\mathbf{X} \in \Omega^{mc}$, then $g(\zeta(\mathbf{X}, \mathbf{Y})) = g(\mathbf{X})g(\mathbf{Y})$. If one fixes $\mathbf{Y}$ in (3.9) and puts $\zeta(\mathbf{X}, \mathbf{Y}) \equiv \mathbf{u}_{\mathbf{Y}}(\mathbf{X})$, then (3.9) becomes

$$\mathbf{D}_a(\mathbf{u}_{\mathbf{Y}}(\mathbf{X})) = \nabla_{\mathbf{X}} \mathbf{u}_{\mathbf{Y}}(\mathbf{X}) \mathbf{D}_a(\mathbf{X}), \tag{3.10}$$

so that Σ^{mc} is locally diffeomorphic to *itself*. This result could be derived from [4]; what is new here is the identification of the local elastic deformation which takes Σ^{mc} to itself as the composition function for $\mathcal{G}$. States which allow slip, then, have the Lie group structure given by (3.9). The corresponding dual vector fields $\mathbf{D}^a(\mathbf{x})$ are called left-invariant in the Lie group literature, they are the Maurer–Cartan fields (forms) on the group.

4. Symmetry of crystals with planar distributions of defects

Now I focus on the particular case where

$$\mathbf{d}_1 = \mathbf{d}_1(x_1, x_2), \qquad \mathbf{d}_2 = \mathbf{d}_2(x_1, x_2), \qquad \mathbf{d}_3 = \mathbf{e}_3 . \tag{4.1}$$

In this case only two of the components of the dislocation density may be nonzero and they are

$$S^{31}/n = -\lambda, \qquad S^{32}/n = \mu. \tag{4.2}$$

I assume that λ and μ are constant (so that the theorem of Sec. 3 applies), and I show elsewhere that there is no loss of generality (so far as the subsequent discussion is concerned) in assuming that

$$\mathbf{d}_1 = \mathbf{e}_1 + \mu \mathbf{x}, \qquad \mathbf{d}_2 = \mathbf{e}_2 + \lambda \mathbf{x}. \tag{4.3}$$

To decide on the symmetry of relevant constitutive functions, I ask if there are any sets of points naturally associated with these vector fields. One might have the view that if there is an "atom" of the crystal at the point $\mathbf{x}$, then there must also be an atom at the point $\mathbf{x} + \mathbf{d}_a(\mathbf{x})$ (by virtue of an interpretation of the vectors $\mathbf{d}_a$ as vectors joining "nearest neighbour" atoms, perhaps). However

this notion does not have appropriate invariance properties, in general, and it is better to assert that if there is an atom at $\mathbf{x}$, then there is also an atom at $\mathbf{x}_a$ where $\mathbf{x}_a$ is defined by

$$\dot{\mathbf{y}} = \mathbf{d}_a(\mathbf{y}), \qquad \mathbf{y}(0) = \mathbf{x}, \qquad \mathbf{y}(t_a) = \mathbf{x}_a\,, \tag{4.4}$$

where the numbers t_1, t_2, t_3 are to be prescribed. A set of points which is consistent with this interpretation of the vector fields should have the properties:

(i) iterations (4.4) of points in the set remain in the set,

(ii) there is a (nonzero) minimum distance between points in the set.

The numbers $\{t_a\}$ determine whether or not these properties are satisfied. I give results just for the simple case where

$$\mu t_1 = \lambda t_2 = \ln 2, \qquad t_3 = 1 \tag{4.5}$$

(more general results will be given elsewhere). In this case, from (4.4), notice that $\dot{\mathbf{y}} = \mathbf{d}_1(\mathbf{y}) = \mathbf{e}_1 + \mu\mathbf{y}$ may be written as $(\mathbf{y} + \mu^{-1}\mathbf{e}_1)^{\cdot} = \mu(\mathbf{y} + \mu^{-1}\mathbf{e}_1)$, so $\mathbf{y} + \mu^{-1}\mathbf{e}_1 = e^{\mu t}(\mathbf{x} + \mu^{-1}\mathbf{e}_1)$. Thus $(\mathbf{x}_1 + \mu^{-1}\mathbf{e}_1) = 2(\mathbf{x} + \mu^{-1}\mathbf{e}_1)$ and in the same way $\mathbf{x}_2 + \lambda^{-1}\mathbf{e}_2 = 2(\mathbf{x} + \lambda^{-1}\mathbf{e}_2)$. Then, one can show that the set of points

$$S(\mathbf{x}) = \left\{\mathbf{y} : \mathbf{y} = 2^m\left(\mathbf{x} + \frac{\mathbf{e}_1}{\mu}\right) + n\left(\frac{\mathbf{e}_1}{\mu} - \frac{\mathbf{e}_2}{\lambda}\right) - \frac{\mathbf{e}_1}{\mu}, \quad m \in \mathcal{Z}^+, \quad n \in \mathcal{Z}\right\}, \tag{4.6}$$

has properties (i) and (ii) above, and so the rearrangements of $S(\mathbf{x})$ are of interest. Note that $S(\mathbf{x})$ can be rewritten as

$$S(\mathbf{x}) = \left\{\mathbf{y} : \mathbf{y} = 2^m\frac{\mathbf{d}_1(x)}{\mu} + n\left(\frac{\mathbf{d}_1(\mathbf{x})}{\mu} - \frac{\mathbf{d}_2(\mathbf{x})}{\lambda}\right) - \frac{\mathbf{e}_1}{\mu}, \quad m \in \mathcal{Z}^+, \quad n = \mathcal{Z}\right\}. \tag{4.7}$$

Let

$$\tilde{\mathbf{d}}_1 = \mathbf{d}_1 + \mu\boldsymbol{\nu}, \qquad \tilde{\mathbf{d}}_2 = \mathbf{d}_2 + \lambda\boldsymbol{\nu}, \qquad \boldsymbol{\nu} = \frac{\mathbf{d}_1}{\mu} - \frac{\mathbf{d}_2}{\lambda}, \qquad \tilde{\boldsymbol{\nu}} = \frac{\tilde{\mathbf{d}}_1}{\mu} - \frac{\tilde{\mathbf{d}}_2}{\lambda} \quad (\equiv \boldsymbol{\nu}).$$

Then $S(\mathbf{x})$ can also be recast as

$$S(\mathbf{x}) = \left\{\mathbf{y} : \mathbf{y} = 2^m\frac{\tilde{\mathbf{d}}_1(\mathbf{x})}{\mu_1} + n\tilde{\boldsymbol{\nu}} - \frac{\mathbf{e}_1}{\mu}, \quad m \in \mathcal{Z}^+, \quad n \in \mathcal{Z}\right\}, \tag{4.8}$$

so that the mapping $\mathbf{d}_a \to \tilde{\mathbf{d}}_a$ gives a rearrangement of $S(\mathbf{x})$, But $\tilde{\mathbf{d}}_a = \gamma_{ab}\mathbf{d}_b$, where

$$(\gamma_{ab}) = \begin{pmatrix} 2 & -\mu/\lambda & 0 \\ \lambda/\mu & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{4.9}$$

Recalling (4.2), one sees that this symmetry of the set of points $S(\mathbf{x})$ depends on the dislocation density tensor.

If, now, one seeks to identify symmetries of an objective strain energy density function

$$w = w(\mathbf{d}^a \cdot \mathbf{d}^b, \ S^{ab}/n), \tag{4.10}$$

which have the form $\mathbf{d}_a \to \gamma_{ab}\mathbf{d}_b \equiv \tilde{\mathbf{d}}_b$, notice first of all that $\tilde{\mathbf{d}}^a = (\gamma^{-T})^{ab}\mathbf{d}^b$, so that $\tilde{S}^{ab} = (\gamma^{-\top})^{ab}S^{cd}(\gamma^{-1})^{db}$ and $\tilde{n} = (\det\gamma)^{-1}n$. The point of view that has been taken in this paper suggests that the *particular* mapping corresponding to (4.9) be taken as a symmetry of the energy density, as it preserves a relevant set of points. But for this particular mapping, and for the particular dislocation density (4.2) one calculates that

$$\tilde{S}^{ab}/\tilde{n} = S^{ab}/n, \tag{4.11}$$

so that the symmetry derived by consideration of the rearrangements of the discrete set of points preserves the (continuum) dislocation density tensor (moreover, the symmetry is independent of the point $\mathbf{x}$ which parameterizes $S(\mathbf{x})$). Finally, one deduces that the energy density must, at least, satisfy

$$w\left(\mathbf{d}^a \cdot \mathbf{d}^b, \ S^{ab}/n\right) = w\left(\tilde{\mathbf{d}}^a \cdot \tilde{\mathbf{d}}^b, \ S^{ab}/n\right), \tag{4.12}$$

where $\tilde{\mathbf{d}}^a = (\gamma^{-\top})^{ab}\mathbf{d}^b$ and (γ) is given by (4.9), which generalizes (2.6) to the case of a defective crystal.

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DEPARTMENT OF THEORETICAL MECHANICS,
UNIVERSITY OF NOTTINGHAM
Nottingham NG7 2RD, UK.

Received September 8, 1997.

Arch. Mech., 50, 3, pp. 577–597, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

A theory of the elastic-viscoplastic Cosserat continuum

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

C. SANSOUR (DARMSTADT)

BASED on the multiplicative decomposition of the stretch tensor and the additive decomposition of the second Cosserat deformation tensor into elastic and inelastic parts, a theory of the elastic-viscoplastic Cosserat continuum is formulated. It is stressed that the rotation field is to be treated as a kinematical variable which can not be decomposed into elastic and inelastic parts. A thorough discussion of the configuration space by relying on basic concepts of Lie groups is provided and the field equations are derived from a variational statement. The flow rules are specified by means of the postulate of maximum dissipation paralleling some developments of the classical theory.

1. Introduction

THE COSSERAT continuum belongs to the class of the so-called generalized continua where, in addition to the displacement field, further fields are considered which specify the micro-structure of the continuum under consideration. In the case of the Cosserat continuum, it is a rotation field which is considered to be independent of displacements. Accordingly, to every point of the continuum, a displacement vector and a rotation tensor (an element of the special orthogonal group) are attached. Since the work of ERICKSEN and TRUESDELL [1] and ERINGEN and KAFADAR [2], the Cosserat continuum attracted the interest of many researchers. Specifically within the shell theory, the philosophy of the Cosserat continuum proved to be very helpful (GREEN *et al.* [3], COHEN and DE SILVA [4], NAGHDI [5], ZHILIN [6], SANSOUR and BEDNARCZYK [7]). In three dimensions, the interest in the Cosserat continuum is increasing since the observation that already the geometric linear Cosserat continuum can prevent ill-conditioning of the field equations within classical elasto-plasticity. Specifically the loss of ellipticity of the governing equations and the observation of mesh-dependence of the finite element solutions can be circumvented if the formulation is a Cosserat-based one (see MÜHLHAUS [8], DE BORST [9], STEINMANN [10]). Hence, the formulation of the elasto-plastic Cosserat continuum can be understood as a regularization method. The so-called internal length needed for such a regularization corresponds to the micro-structure of the continuum which is provided by the Cosserat continuum in a completely natural way.

Early geometrically linear formulations of the elasto-plastic Cosserat continuum are due to LIPPMANN [11] and BESDO [12]. Recently, using different assumptions, geometrically exact formulations have been given by SIEVERT [13] and STEINMANN [14]. The reader is also referred to a recent review article by LIPPMANN [15] where experimental observations in conjunction with the plastic spin are discussed and further references can be found.

The aim of the paper is to give a formulation of the geometrically exact elastic-viscoplastic Cosserat Continuum. A fundamental aspect of the formulation is the crucial understanding that the rotations constitute a kinematical field which, together with the displacements, defines the configuration space. A basic feature of kinematical variables is the existence of field equations corresponding to them (the Euler–Lagrange equations of an appropriate functional) and, correspondingly, the fact that they can not be decomposed into elastic and inelastic parts. Exactly this statement stands in contradistinction to some attempts to develop the theory by means of a decomposition of the rotation field itself (see e.g. STEINMANN [14]).

Another aspect relates to the choice of the strain measures which have to be decomposed in an appropriate way in elastic and inelastic parts. The theory is based on the decomposition of the first and second Cosserat deformation tensors. The decomposition is multiplicative for the first Cosserat deformation tensor (the stretch tensor), and is additive for the second one.

The paper is organized as follows. In Sec. 2, fundamentals of the Cosserat continuum are presented. We focus on the structure of the configuration space and basics of Lie groups are incorporated in the discussion. Specifically the relations between variations and time derivatives within the orthogonal group is discussed. In Sec. 3 the elastic-viscoplastic Cosserat continuum is presented. First the assumed decompositions are introduced and possible derivation of the field equations from a variational statement is discussed. Finally, the flow rules are specified by making use of the postulate of maximum dissipation. Although this postulate does not constitute a physical law, it is helpful due to the lack of sufficient experimental data needed for the formulation of alternative evolution equations. The paper closes with conclusions. In the Appendix, the linearization of the field equations is treated. Hereby the structure of the configuration space is further discussed focusing on the rule of a Killing metric defined on it.

2. Kinematics

2.1. Preliminaries

Let $\mathbb{R}$ denote the real numbers. With a set $\mathcal{B} \subset \mathbb{R}^3$ we define a material body as a three-dimensional manifold. The map $\boldsymbol{\varphi}(t) : \mathcal{B} \to \mathbb{R}^3$ is an embedding depending on a time-like parameter $t \in \mathbb{R}$. Hereby, $\boldsymbol{\varphi}_0 = \boldsymbol{\varphi}(t = t_0)$ defines a reference configuration which we use to identify the material points. Accordingly,

we choose φ_0 to be the identity map. Writing $\mathcal{B}$ for $\varphi_0\mathcal{B}$ and $\mathcal{B}_t$ for $\varphi(t)\mathcal{B}$ we get $\varphi(t) : \mathcal{B} \to \mathcal{B}_t$. For $\mathbf{X} \in \mathcal{B}$ and $\mathbf{x} \in \mathcal{B}_t$ we have $\mathbf{x}(t) = \varphi(\mathbf{X}, t)$ and $\mathbf{X}(t) = \varphi^{-1}(\mathbf{x}, t)$.

We consider ϑ^i, $i = 1, 2, 3$, as coordinate charts in $\mathcal{B}$ which we choose to be attached to the body (convected). The tangent spaces of $\mathcal{B}$ and $\mathcal{B}_t$ are denoted by $\mathcal{T}\mathcal{B}$ and $\mathcal{T}\mathcal{B}_t$, respectively. Accordingly, the covariant base vectors are

$$\mathbf{G}_i = \frac{\partial \mathbf{X}}{\partial \vartheta^i} \qquad \text{with} \qquad \mathbf{G}_i \in \mathcal{T}\mathcal{B}, \tag{2.1}$$

and

$$\mathbf{g}_i = \frac{\partial \mathbf{x}}{\partial \vartheta^i} \qquad \text{with} \qquad \mathbf{g}_i \in \mathcal{T}\mathcal{B}_t\,. \tag{2.2}$$

The Riemannian metric in either configuration is denoted by $\mathbf{G}$, $\mathbf{g}$ respectively, their components are given by $G_{ij} = \mathbf{G}_i \cdot \mathbf{G}_j$ and $g_{ij} = \mathbf{g}_i \cdot \mathbf{g}_j$, where scalar products of vectors are denoted by a dot. The corresponding determinants of the metrics are denoted by G and g, their inverse as usual by G^{ij} and g^{ij}, respectively. Further we denote the basic skew-symmetric three-dimensional Levi-Civita tensor (permutation tensor) by e_{ijk} where we have $e_{ijk} = e^{ijk}$ by its Euclidean structure. Further we define $\varepsilon_{ijk} := \sqrt{G}\, e_{ijk}$, $\varepsilon^{ijk} := 1/\sqrt{G}\, e^{ijk}$, and later on make use of the absolute notation $\boldsymbol{\epsilon} \equiv \varepsilon^{ijk}\mathbf{G}_i \otimes \mathbf{G}_j \otimes \mathbf{G}_k$.

In addition to the base system $\mathbf{G}_i$ we consider a Cartesian frame denoted by $\mathbf{e}_i$, $i = 1, 2, 3$ and define, for later use, the matrices

$$c_{ij} = \mathbf{G}_i \cdot \mathbf{e}_j \tag{2.3}$$

which relate the two base systems to one another since we have $\mathbf{G}_i = c_{ij}\mathbf{e}_j$ and $\mathbf{e}_i = c_{ij}\mathbf{G}^j$.

The Cosserat continuum is characterized by a rotation field understood as independent of φ. To every point in $\mathcal{B}$ we attach a tensor $\mathbf{R} \in SO(3)$, where $SO(3)$ denotes the special orthogonal group, parameterised with the help of the exponential map as follows (CHOQUET *et al.* [16], DUBROVIN *et al.* [17]):

$$\mathbf{R} = \exp(\mathbf{A}) = \mathbf{1} + \mathbf{A} + \frac{\mathbf{A}^2}{2!} + \frac{\mathbf{A}^3}{3!} + \cdots = \mathbf{1} + \frac{\sin|\boldsymbol{\alpha}|}{|\boldsymbol{\alpha}|}\mathbf{A} + \frac{1 - \cos|\boldsymbol{\alpha}|}{|\boldsymbol{\alpha}|^2}\mathbf{A}^2, \tag{2.4}$$

with the skew-symmetric tensor $\mathbf{A} = -\mathbf{A}^T$, the axial vector of which is denoted by $\boldsymbol{\alpha}$. Accordingly we have $\mathbf{R}\,\boldsymbol{\alpha} = \boldsymbol{\alpha}$. Using the permutation tensor one may write directly

$$\boldsymbol{\alpha} = -\frac{1}{2}\boldsymbol{\epsilon} : \mathbf{A}. \tag{2.5}$$

Here a double contraction is denoted by (:) (for two second order tensors $\mathbf{A}$, $\mathbf{B}$ the relation holds $\mathbf{A} : \mathbf{B} = \operatorname{tr}(\mathbf{A}\,\mathbf{B}^T)$ with tr denoting the trace operation). The fact that $\boldsymbol{\epsilon}$ is a three-dimensional tensor reveals the product $\boldsymbol{\epsilon} : \mathbf{A}$ to be a vector.

2.2. Strain measures

The deformation gradient is the tangent of the map $\varphi : \mathcal{T}\varphi \equiv \mathbf{F}$ with $\mathcal{T}\varphi : \mathcal{TB} \to \mathcal{TB}_t$, or $\mathbf{F} : \mathbf{G}_i \to \mathbf{g}_i$. It is given as the tensor product

$$\mathbf{F} = \mathbf{g}_i \otimes \mathbf{G}^i. \tag{2.6}$$

By introducing the displacement field $\mathbf{u} = \mathbf{x} - \mathbf{X}$ and denoting partial derivatives by a comma, we get from (2.1) and (2.2)

$$\mathbf{g}_i = \mathbf{G}_i + \mathbf{u}_{,i} \tag{2.7}$$

and from (2.6)

$$\mathbf{F} = (\mathbf{G}_i + \mathbf{u}_{,i}) \otimes \mathbf{G}^i. \tag{2.8}$$

By the relation

$$\mathbf{R}\,\mathbf{R}^T = \mathbf{1} \tag{2.9}$$

we have

$$\mathbf{R}^T\mathbf{R}_{,i} + \mathbf{R}^T_{,i}\mathbf{R} = \mathbf{0}. \tag{2.10}$$

The relation shows that the products $\mathbf{R}^T\mathbf{R}_{,i}$ are skew-symmetric. We denote the corresponding axial vectors by $\mathbf{k}_i$. Between $\boldsymbol{\alpha}$ and $\mathbf{k}_i$ the relation holds (see e.g. PIETRASZKIEWICZ and BADUR [18])

$$\mathbf{k}_i = \frac{\sin|\boldsymbol{\alpha}|}{|\boldsymbol{\alpha}|}\boldsymbol{\alpha}_{,i} + \frac{1-\cos|\boldsymbol{\alpha}|}{|\boldsymbol{\alpha}|^2}\boldsymbol{\alpha}_{,i} \times \boldsymbol{\alpha} + \left(\frac{1}{|\boldsymbol{\alpha}|} - \frac{\sin|\boldsymbol{\alpha}|}{|\boldsymbol{\alpha}|^2}\right)\frac{(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha}_{,i})}{|\boldsymbol{\alpha}|}\boldsymbol{\alpha}. \tag{2.11}$$

The strain measures we are considering are the first Cosserat deformation tensor (ERINGEN and KAFADAR [2], HJALMARS [19])

$$\mathbf{U} := \mathbf{R}^T\mathbf{F} \tag{2.12}$$

and the second Cosserat deformation tensor

$$\mathbf{K} := \mathbf{k}_i \otimes \mathbf{G}^i. \tag{2.13}$$

Alternatively, $\mathbf{K}$ may be written down in terms of the rotation tensor directly as

$$\mathbf{K} = -\frac{1}{2}\boldsymbol{\epsilon} : \mathbf{R}^T\mathbf{R}_{,i} \otimes \mathbf{G}^i. \tag{2.14}$$

For the sake of completeness we include explicit expressions for the strain measures where it is convenient to underline the following decompositions

$$\mathbf{U} = U_{ji}\mathbf{G}^i \otimes \mathbf{G}^j, \qquad \mathbf{K} = K_{ji}\mathbf{G}^i \otimes \mathbf{G}^j, \tag{2.15}$$

$$\mathbf{u} = u_k\mathbf{e}_k\,, \qquad \boldsymbol{\alpha} = \alpha_k\mathbf{e}_k\,. \tag{2.16}$$

With (2.4), (2.8), (2.11)–(2.16) we get the following expressions for the strain measures

$$U_{rs} = G_{rs} + c_{sk}\, u_{k,r} + (c_{rk} + u_{k,r})c_{sj} \times \left[\frac{\sin|\boldsymbol{\alpha}|}{|\boldsymbol{\alpha}|} e_{ijk}\,\alpha_i + \frac{1-\cos|\boldsymbol{\alpha}|}{|\boldsymbol{\alpha}|^2}\,(\alpha_k\alpha_j - \alpha_i\alpha_i\delta_{jk})\right], \tag{2.17}$$

$$K_{rs} = c_{sk}\left(\frac{\sin|\boldsymbol{\alpha}|}{|\boldsymbol{\alpha}|}\alpha_{k,r} + \frac{1-\cos|\boldsymbol{\alpha}|}{|\boldsymbol{\alpha}|^2} e_{ijk}\alpha_{i,r}\alpha_j + \frac{|\boldsymbol{\alpha}| - \sin|\boldsymbol{\alpha}|}{|\boldsymbol{\alpha}|^2}|\boldsymbol{\alpha}|_{,r}\alpha_k\right). \tag{2.18}$$

2.3. Rates and variations

The deformation of the Cosserat continuum is completely described in terms of the pair $(\mathbf{u}, \mathbf{R})$ attached to every point of the continuum. This motivates the definition of the configuration space as the set $\mathcal{C}$ consisting of all admissible configurations of the body $\mathcal{B}$. A precise definition of it is given by

$$\mathcal{C}(\mathcal{B}) = \{\mathcal{U} = (\mathbf{u}, \mathbf{R}) \mid \mathcal{U} : \mathcal{B} \longrightarrow \mathbb{R}^3 \times SO(3)\} \tag{2.19}$$

with $\mathbf{R} = \exp(\mathbf{A})$ and $\mathbf{A} = -\mathbf{A}^T$.

The deformation gradient $\mathbf{F}$ and the rotation tensor $\mathbf{R}$ define fields over $\mathbf{X}$. Pointwise, they take values parameterized by the real time t or by a time-like parameter where the set of all admissible values of $\mathbf{F}$ and $\mathbf{R}$, related to one and the same particle, constitute a Lie group. In fact, it proves to be very fruitful to understand $\mathbf{F}$ as well as $\mathbf{R}$ as elements of a Lie group. This becomes crucial in conjunction with the linearization process where variations or time derivatives should be understood as vectors in the tangent space of an appropriate Lie group. First let $\mathcal{G}$ be a linear Lie group. Of special interest for us is the group of invertable matrices with positive determinants $GL^+(3)$ since we have $\mathbf{F} \in GL^+(3)$ and the special orthogonal group $SO(3)$ where we have $\mathbf{R} \in SO(3)$. We consider a curve in $\mathcal{G}$. By the very definition of a group, the identity $\mathbf{1}$ is an element of $\mathcal{G}$. Any element $\mathbf{Z} \in \mathcal{G}$ in the neighbourhood of the identity can be reached by the exponential map according to

$$\mathbf{Z} = \exp(\mathbf{b}) = \mathbf{1} + \mathbf{b} + \frac{\mathbf{b}^2}{2!} + \frac{\mathbf{b}^3}{3!} + \cdots, \tag{2.20}$$

where $\mathbf{b}$ is an element of the Lie algebra which defines the tangent space of $\mathcal{G}$ at the identity. In the case of $GL^+(3)$, the Lie algebra, which is denoted by $gl^+(3)$, consists of quadratic matrices. In the case of $SO(3)$, the Lie algebra is denoted by $so(3)$ and consists of skew-symmetric matrices.

Consider now any $\mathbf{Z} \in \mathcal{G}$. A curve in $\mathcal{G}$ parametrized by t and going through $\mathbf{Z}$ at $t = t_0$ is given by the one-parameter subgroup

$$\mathcal{V}(t) = [\exp((t - t_0)\widehat{\mathbf{b}})\mathbf{Z}]. \tag{2.21}$$

$\widehat{\mathbf{b}}$ is then an element of the corresponding Lie algebra of the group. Tangent vector fields in $\mathcal{G}$ are given by means of derivation with respect to the time-like parameter t. Explicitly we have

$$D\mathbf{Z} = \frac{D}{Dt}\mathcal{V}_{|t=t_0} = \frac{D}{Dt}[\exp((t-t_0)\widehat{\mathbf{b}})\mathbf{Z}]_{|t=t_0} = \widehat{\mathbf{b}}\,\mathbf{Z}. \tag{2.22}$$

$\widehat{\mathbf{b}}\mathbf{Z}$ is understood as a tangent vector in $\mathcal{G}$; a right invariant tangent vector, strictly spoken. The above tangents have been derived by considering the so-called left action of the group. Alternatively, a curve in $\mathcal{G}$ and a corresponding derivative with respect to t can be defined by means of a right group action according to

$$D\mathbf{Z} = \frac{D}{Dt}\mathcal{V}_{|t=t_0} = \frac{D}{Dt}[\mathbf{Z}\exp((t-t_0)\mathbf{b})]_{|t=t_0} = \mathbf{Z}\,\mathbf{b}. \tag{2.23}$$

Here, $\mathbf{Z}\,\mathbf{b}$ is a left invariant tangent vector. The relation holds

$$\mathbf{b} = \mathbf{Z}^{-1}\widehat{\mathbf{b}}\,\mathbf{Z}. \tag{2.24}$$

We apply now these concepts directly to $\mathbf{F}$ and $\mathbf{R}$ by understanding them as elements of the Lie groups $GL^+(3)$ and $SO(3)$, respectively. One has

$$\dot{\mathbf{F}} = \mathbf{l}\mathbf{F} \tag{2.25}$$

with $\mathbf{l}$ as the left rate, and

$$\dot{\mathbf{F}} = \mathbf{F}\mathbf{L} \tag{2.26}$$

with $\mathbf{L}$ as the right rate. In terms of continuum mechanics, $\mathbf{l}$ is the rate defined at the actual configuration whereas $\mathbf{L}$ is its material counterpart. From (2.25) and (2.26) we get directly

$$\mathbf{L} = \mathbf{F}^{-1}\mathbf{l}\mathbf{F}. \tag{2.27}$$

In the same spirit we have

$$\dot{\mathbf{R}} = \widehat{\boldsymbol{\Omega}}\,\mathbf{R} \tag{2.28}$$

with $\widehat{\boldsymbol{\Omega}} \in so(3)$ (that is $\widehat{\boldsymbol{\Omega}}$ is skew-symmetric) as the left rate, and

$$\dot{\mathbf{R}} = \mathbf{R}\,\boldsymbol{\Omega} \tag{2.29}$$

with $\boldsymbol{\Omega}$ as the corresponding right rate. Here again we have

$$\boldsymbol{\Omega} = \mathbf{R}^T\widehat{\boldsymbol{\Omega}}\,\mathbf{R}. \tag{2.30}$$

Further, it is useful to consider the material rate related to $\mathbf{l}$ by means of a rotation. From (2.12), (2.25) and (2.29) we conclude

$$\mathbf{l} = \mathbf{R}\,\widehat{\mathbf{L}}\,\mathbf{R}^T, \qquad \widehat{\mathbf{L}} = \dot{\mathbf{U}}\,\mathbf{U}^{-1} + \boldsymbol{\Omega}. \tag{2.31}$$

Instead of the time derivatives we can consider variations in the same way. These are explicitly needed for the rotation space. We consider for this purpose again the configuration space consisting of the pairs $(\mathbf{u}, \mathbf{R})$ considered as a Cartesian product. The space is understood as a Lie group where for two elements $(\mathbf{u}, \mathbf{R})$ and $(\mathbf{w}, \mathbf{Q})$ the group operation is defined by the direct product, namely $(\mathbf{u}, \mathbf{R}) \circ (\mathbf{w}, \mathbf{Q}) = (\mathbf{u} + \mathbf{w}, \mathbf{QR})$. To derive variational formulas we rely on the above concepts and consider the neighbourhood of an element say $\mathcal{U} = (\mathbf{u}, \mathbf{R})$. Again a curve $\mathcal{V}(s)$ in $\mathcal{C}$ passing through $\mathcal{U} = (\mathbf{u}, \mathbf{R})$ with $\mathcal{V}(s = s_0) = \mathcal{U}$ is given as the one-parameter subgroup

$$\mathcal{V}(s) = [\mathbf{u} + (s - s_0)\hat{\mathbf{u}}, \exp((s - s_0)\widehat{\mathbf{W}})\mathbf{R}]. \tag{2.32}$$

The variation now is defined as the tangent at $\mathcal{U}$ which is given by the derivation with respect to the parameter s

$$D\mathcal{U} = \frac{D}{Ds}\mathcal{V}_{|s=s_0} = \frac{D}{Dt}[\mathbf{u} + (s - s_0)\hat{\mathbf{u}}, \exp((s - s_0)\widehat{\mathbf{W}})\mathbf{R}]_{|s=s_0} \tag{2.33}$$

$$= (\hat{\mathbf{u}}, \widehat{\mathbf{W}}\,\mathbf{R}) \qquad \text{with} \quad \widehat{\mathbf{W}} \in so(3).$$

The pair $(\hat{\mathbf{u}}, \widehat{\mathbf{W}}) = \delta\mathcal{U}$ defines the infinitesimal deformation to be superimposed on a given admissible state. That is, with (2.33) a neighbourhood of $\mathcal{U}$ is given as

$$(\mathbf{u}, \mathbf{R}) \circ (\hat{\mathbf{u}}, \widehat{\mathbf{W}}) = (\mathbf{u} + \hat{\mathbf{u}}, \widehat{\mathbf{W}}\,\mathbf{R}). \tag{2.34}$$

To make it more convenient we make use of the notation

$$\delta\mathbf{R} = \widehat{\mathbf{W}}\,\mathbf{R}. \tag{2.35}$$

The crucial point now is the fact that $\delta\mathbf{R}$ is to be understood as a tangent vector in the space $SO(3)$. This fact will play a dominant role when taking the linearization of these vectors, that is considering the second variations, issues to be addressed later on. Already by considering the time derivatives we have seen that one can define two derivatives, a left one and a right one. Here again and completely in the same way, one can define a variation on the basis of the right group action as

$$\delta\mathbf{R} = \mathbf{R}\,\mathbf{W}. \tag{2.36}$$

Comparison of (2.35) with (2.36) gives

$$\mathbf{W} = \mathbf{R}^T\widehat{\mathbf{W}}\,\mathbf{R}. \tag{2.37}$$

Here again, $\widehat{\mathbf{W}}$ is the variation defined at the actual configuration whereas $\mathbf{W}$ is that defined at the reference one.

Having established the time derivatives as well as the variations of $\mathbf{R}$, a relation can be constructed between the variations of the time derivatives and the

time derivatives of the variations. We excercise these aspects by considering the material rates only. By considering the equality

$$(\delta\mathbf{R})^{\cdot} = \delta\dot{\mathbf{R}} \tag{2.38}$$

and by making use of (2.29) and (2.36), we get

$$\dot{\mathbf{R}}\,\mathbf{W} + \mathbf{R}\dot{\mathbf{W}} = \mathbf{R}\,\mathbf{W}\,\boldsymbol{\Omega} + \mathbf{R}\delta\boldsymbol{\Omega} \tag{2.39}$$

or

$$\delta\boldsymbol{\Omega} = \boldsymbol{\Omega}\,\mathbf{W} - \mathbf{W}\,\boldsymbol{\Omega} + \dot{\mathbf{W}}. \tag{2.40}$$

In terms of the axial vectors $\boldsymbol{\omega}$ and $\mathbf{w}$ of $\boldsymbol{\Omega}$ and $\mathbf{W}$, respectively, we have the relation

$$\delta\boldsymbol{\omega} = \boldsymbol{\omega} \times \mathbf{w} + \dot{\mathbf{w}}. \tag{2.41}$$

For a complete discussion we need relations for the time derivatives and the first variations of the strain measures. A useful equation relating the variation of $\mathbf{k}_i$ to $\mathbf{w}$, the axial vector of $\mathbf{W}$ and to its derivative, is obtained by making use of (2.13), (2.14) and (2.36). After some algebraic manipulations, which we omit for the sake of shortness, we get

$$\delta\mathbf{k}_i = \mathbf{w}_{,i} + \mathbf{k}_i \times \mathbf{w}. \tag{2.42}$$

A similar relation holds for the time derivatives

$$\dot{\mathbf{k}}_i = \boldsymbol{\omega}_{,i} + \mathbf{k}_i \times \boldsymbol{\omega}. \tag{2.43}$$

3. The elastic-viscoplastic Cosserat continuum

3.1. Stress tensors, equilibrium equations and external power

Let $\boldsymbol{\sigma}$ be the Cauchy stress tensor. We define the moment tensor (the couple stress tensor) $\boldsymbol{\gamma}$ which is expected to fulfill the Cauchy lemma with respect to external moments. For a field of external moments $\mathbf{m}_s$ acting on $\partial\mathcal{B}_{t_s}$, the boundary of $\mathcal{B}_t$ with prescribed tractions, and with $\boldsymbol{\nu}$ being the actual normal vector at that boundary, we have

$$\mathbf{m}_s = \boldsymbol{\gamma}\,\boldsymbol{\nu}. \tag{3.1}$$

The equilibrium equations read (ERINGEN and KAFADAR [2])

$$\frac{D}{Dt}\int\limits_{\mathcal{B}_t} \varrho\dot{\mathbf{u}}\,dv = \int\limits_{\mathcal{B}_t} \mathbf{f}\,dv + \int\limits_{\partial\mathcal{B}_{t_s}} \mathbf{f}_s\,da, \tag{3.2}$$

$$\frac{D}{Dt}\int\limits_{\mathcal{B}_t} \varrho(\mathbf{x}\times\dot{\mathbf{u}} + \hat{\boldsymbol{\Theta}}\,\hat{\boldsymbol{\omega}})dv = \int\limits_{\mathcal{B}_t} (\mathbf{x}\times\mathbf{f} + \mathbf{m})dv + \int\limits_{\partial\mathcal{B}_{t_s}} (\mathbf{x}\times\mathbf{f}_s + \mathbf{m}_s)da. \tag{3.3}$$

Here, $\mathbf{f}$, $\mathbf{f}_s$ mean external forces acting in the field and at the boundary, $\mathbf{m}$, $\mathbf{m}_s$ are the corresponding external moments, $\widehat{\Theta}$ is the rotational inertia, dv and da are the volume and area elements. By straightforward calculations the above equations can be localized leading to the following field equations:

$$\varrho \ddot{\mathbf{u}} = \operatorname{div} \boldsymbol{\sigma} + \mathbf{f}, \tag{3.4}$$

$$\varrho \frac{D}{Dt}(\widehat{\Theta}\,\widehat{\boldsymbol{\omega}}) = -\boldsymbol{\epsilon} : \boldsymbol{\sigma} + \operatorname{div} \boldsymbol{\gamma} + \mathbf{m}, \tag{3.5}$$

where div means the divergence operation at the actual configuration. To recast the above equations in a material setting, we define by the following isometric material stress and moment tensors

$$\boldsymbol{\Sigma} = \frac{\varrho_{\mathrm{ref}}}{\varrho} \mathbf{R}^T \boldsymbol{\sigma}\, \mathbf{R}, \qquad \boldsymbol{\Gamma} = \frac{\varrho_{\mathrm{ref}}}{\varrho} \mathbf{R}^T \boldsymbol{\gamma}\, \mathbf{R}, \qquad \mathbf{M} = \mathbf{R}^T \mathbf{m}. \tag{3.6}$$

The equilibrium equations have then the alternative material form

$$\varrho_{\mathrm{ref}} \ddot{\mathbf{u}} = \operatorname{Div} \mathbf{R}\, \boldsymbol{\Sigma}\, \mathbf{U}^{-T} + \mathbf{f}, \tag{3.7}$$

$$\varrho_{\mathrm{ref}} (\Theta\, \dot{\boldsymbol{\omega}} + \boldsymbol{\omega} \times \Theta\, \boldsymbol{\omega}) = -\boldsymbol{\epsilon} : \boldsymbol{\Sigma} + \mathbf{R}^T \operatorname{Div} \mathbf{R}\, \boldsymbol{\Gamma}\, \mathbf{U}^{-1} + \mathbf{M}, \tag{3.8}$$

where Div means the divergence operator at the reference configuration and we have $\Theta = \mathbf{R}^T \widehat{\Theta} \mathbf{R}$. In deriving the left-hand side of (3.8), use is made of the relation $\widehat{\Theta}\, \widehat{\boldsymbol{\omega}} = \mathbf{R}\, \Theta \boldsymbol{\omega}$. Note further that Θ is assumed to be constant.

The boundary conditions hold

$$\mathbf{R}\, \boldsymbol{\Sigma}\, \mathbf{U}^{T-1} \mathbf{G}^i \mu_i = \mathbf{f}_s, \qquad \boldsymbol{\Gamma}\, \mathbf{U}^{-1} \mathbf{G}^i \mu_i = \mathbf{M}_s \qquad \text{on} \quad \partial \mathcal{B}_s, \tag{3.9}$$

where μ_i are the components of the normal vector at the reference configuration. The validity of (3.7) and (3.8) is proved in Sec. 3.2 by deriving them from a variational statement.

Dealing with dissipation later on, we need the following expression for the mechanical power $\mathcal{P}$ which is derived straightforwardly under the assumption that the equilibrium equations hold

$$\mathcal{P} = \int_{\mathcal{B}_t} \left[\boldsymbol{\sigma} : \mathbf{l} + \boldsymbol{\gamma} : (\widehat{\boldsymbol{\omega}}_{,i} \otimes \mathbf{g}^i) \right] dv. \tag{3.10}$$

Making use of the material rates as given in (2.27) or (2.31) as well as of (2.6), (2.12), (2.43), and (3.6), the above relation can be rewritten in the form

$$\mathcal{P} = \int_{\mathcal{B}} (\boldsymbol{\Sigma} : \dot{\widehat{\mathbf{L}}} + \boldsymbol{\Gamma}\, \mathbf{U}^{-1} : \dot{\mathbf{k}}_i \otimes \mathbf{G}^i)\, dV, \tag{3.11}$$

or alternatively in the form

$$\mathcal{P} = \int_{\mathcal{B}} (\boldsymbol{\Xi} : \mathbf{L} + \boldsymbol{\Gamma}\,\mathbf{U}^{-1} : \dot{\mathbf{k}}_i \otimes \mathbf{G}^i)\, dV. \tag{3.12}$$

Here we have

$$\boldsymbol{\Xi} = \frac{\varrho_{\mathrm{ref}}}{\varrho} \mathbf{F}^{-1} \boldsymbol{\sigma}\, \mathbf{F} \tag{3.13}$$

which is nothing but the mixed variant pull-back of the Kirchhoff stress tensor.

3.2. Multiplicative-additive split of the strain measures

A first step in formulating elasto-viscoplasticity will be an adequate split of the strain measures in elastic and inelastic parts. Starting with $\mathbf{U}$ we note that this strain measure is not symmetric. From its physical meaning it may itself be understood as an element of the group $GL^+(3)$ for which multiplicative products are a natural operation defining the group action. Accordingly two possible splits can be considered. First

$$\mathbf{U} = \mathbf{U}^p \mathbf{U}^e, \tag{3.14}$$

where $\mathbf{U}^p$ stands for the inelastic part of the stretch tensor and, correspondingly, $\mathbf{U}^e$ stands for the elastic part. Alternatively, the decomposition

$$\mathbf{U} = \overline{\mathbf{U}}^e \overline{\mathbf{U}}^p \tag{3.15}$$

may be considered as well. By the use of a "bar", the different decompositions are distinguished.

As a next step we consider the decomposition of the second Cosserat deformation tensor $\mathbf{K}$. Two observations are helpful. First, the deformation gradient $\mathbf{F}$ or the stretch tensor $\mathbf{U}$ can be understood as elements of a matrix group acting on the tangent space at the identity. This is reflected also in their physical meaning by stretching (for $\mathbf{F}$ also rotating) the tangent space. For such an action, a multiplicative decomposition is a natural choice. Such a mathematical or physical meaning is not assigned to the tensor $\mathbf{K}$. Second, from its very definition, (Eq. (2.13)), the tensor $\mathbf{K}$ is equivalent to the three vectors $\mathbf{k}_i$ for which an additive decomposition is, due to lack of any motivation for a mutiplicative decomposition, an appropriate operation. Accordingly we consider the following decomposition

$$\mathbf{K} = \mathbf{K}^e + \mathbf{K}^p. \tag{3.16}$$

Moreover, the couple stresses are assumed to be small in comparison with the macroscopic stress tensor $\boldsymbol{\Sigma}$ which gives a further justification for the additive decomposition of $\mathbf{K}$.

We consider now the rates of the above decompositions, specifically the rates of $\mathbf{U}$ and $\mathbf{U}^p$. From (2.31) we conclude that the material rate corresponding to $\dot{\mathbf{U}}\,\mathbf{U}^{-1}$ is of special interest. By the first decomposition one has

$$\dot{\mathbf{U}} = \dot{\mathbf{U}}^p\mathbf{U}^e + \mathbf{U}^p\dot{\mathbf{U}}^e \tag{3.17}$$

and

$$\dot{\mathbf{U}}\,\mathbf{U}^{-1} = \dot{\mathbf{U}}^p\mathbf{U}^{p^{-1}} + \mathbf{U}^p\dot{\mathbf{U}}^e\mathbf{U}^{e^{-1}}\mathbf{U}^{p^{-1}}. \tag{3.18}$$

From this equation we infer that it is useful to use a left rate for $\mathbf{U}^p$ and a right one for $\mathbf{U}^e$ according to

$$\dot{\mathbf{U}}^p = \mathbf{L}^p\,\mathbf{U}^p, \qquad \dot{\mathbf{U}}^e = \mathbf{U}^e\mathbf{L}^e, \tag{3.19}$$

which inserted in (3.18) give

$$\dot{\mathbf{U}}\,\mathbf{U}^{-1} = \mathbf{L}^p + \mathbf{U}\,\mathbf{L}^e\mathbf{U}^{-1}. \tag{3.20}$$

In the case of the second decomposition (3.15) one has

$$\dot{\mathbf{U}}\,\mathbf{U}^{-1} = \overline{\mathbf{U}}^e\dot{\overline{\mathbf{U}}}^p\overline{\mathbf{U}}^{p^{-1}}\overline{\mathbf{U}}^{e^{-1}} + \dot{\overline{\mathbf{U}}}^e\overline{\mathbf{U}}^{e^{-1}}. \tag{3.21}$$

From this relation it follows that it is more appropriate to choose a right rate for $\overline{\mathbf{U}}^p$ and a left rate for $\overline{\mathbf{U}}^e$ according to

$$\dot{\overline{\mathbf{U}}}^p = \overline{\mathbf{U}}^p\overline{\mathbf{L}}^p, \qquad \dot{\overline{\mathbf{U}}}^e = \overline{\mathbf{L}}^e\overline{\mathbf{U}}^e. \tag{3.22}$$

Correspondingly we have

$$\dot{\mathbf{U}}\,\mathbf{U}^{-1} = \overline{\mathbf{U}}\,\overline{\mathbf{L}}^p\overline{\mathbf{U}}^{-1} + \overline{\mathbf{L}}^e \tag{3.23}$$

as the counterpart of (3.20).

The rate of the second Cosserat deformation tensor is directly given by

$$\dot{\mathbf{K}} = \dot{\mathbf{K}}^e + \dot{\mathbf{K}}^p. \tag{3.24}$$

With the rates of deformation at hand we can proceed to discuss the frame of the theory.

3.3. The weak form of the equilibrium equations

The theory is completely determined by two functions: the internal energy function and the flow rule. The internal energy function is assumed to depend on the elastic strain tensors as well as on further internal variables which we

collect in the vector $\mathbf{q}$. Hence we define $\psi(\mathbf{U}^e, \mathbf{K}^e, \mathbf{q})$ as the free energy under consideration.

Under these assumptions, the equilibrium equations (3.7) and (3.8) can be derived as Euler–Lagrange equations of an appropriate action. Note that even in a purely elastic response, a Hamiltonian can not be formulated. The last statement is due to the fact that, even in the case of constant external moments, an external potential does not exist since the variation of the rotation vector itself does not constitute the work conjugate of an external moment. These issues are discussed in detail in SANSOUR and BEDNARCZYK [7] to which the reader is referred. The statements stand in contradistinction to the formulation of a variational principle for the Cosserat continuum (see SACZUK [20]).

Pointwise the kinetic energy is defined by

$$T = \frac{1}{2}\varrho_{\text{ref}}(\dot{\mathbf{u}}\cdot\dot{\mathbf{u}} + \boldsymbol{\Theta}\,\boldsymbol{\omega}\cdot\boldsymbol{\omega}). \tag{3.25}$$

Note that the last term can be rewritten by means of spatial quantities as $1/2\hat{\boldsymbol{\Theta}}\,\hat{\boldsymbol{\omega}}\cdot\hat{\boldsymbol{\omega}}$.

Now we consider the following functional:

$$\delta\int_{t_0}^{t_1}\int_{B} T\,dV\,dt - \int_{t_0}^{t_1}\left[\int_{\mathcal{B}}(\mathbf{n}:\delta\mathbf{U} + \mathbf{m}:\delta\mathbf{K})\,dV - \int_{\mathcal{B}}\mathbf{f}\cdot\delta\mathbf{u}\,dV - \int_{\partial\mathcal{B}}\mathbf{f}_s\cdot\delta\mathbf{u}\,dA - \int_{\mathcal{B}}\mathbf{M}\cdot\mathbf{w}\,dV - \int_{\partial\mathcal{B}}\mathbf{M}_s\cdot\mathbf{w}\,dA\right]dt = 0. \tag{3.26}$$

The assumption of the existence of a free energy function is equivalent to the assumption that the relations hold

$$\mathbf{n} = \varrho_{\text{ref}}\frac{\partial\psi}{\partial\mathbf{U}}, \qquad \mathbf{m} = \varrho_{\text{ref}}\frac{\partial\psi}{\partial\mathbf{K}}.$$

Since ψ is a function of $\mathbf{U}^e$, $\mathbf{K}^e$ and via the latter a function of $\mathbf{U}$, $\mathbf{K}$, we conclude

$$\int_{\mathcal{B}}(\mathbf{n}:\delta\mathbf{U} + \mathbf{m}:\delta\mathbf{K})\,dV = \int_{\mathcal{B}}\varrho_{\text{ref}}\left(\frac{\partial\psi_{\text{int}}(\mathbf{U}^e,\mathbf{K}^e)}{\partial\mathbf{U}^e}:\mathbf{U}^{p^{-1}}\delta\mathbf{U} + \frac{\partial\psi_{\text{int}}(\mathbf{U}^e,\mathbf{K}^e)}{\partial\mathbf{K}^e}:\delta\mathbf{K}\right)dV. \tag{3.27}$$

Using (2.12), (2.13), and (2.42) we have

$$\delta\mathbf{U} = \delta\mathbf{R}^T\mathbf{F} + \mathbf{R}^T\delta\mathbf{F} = \delta\mathbf{R}^T\mathbf{R}\,\mathbf{U} + \mathbf{R}^T\delta\mathbf{F}, \tag{3.28}$$

$$\delta\mathbf{K} = \delta\mathbf{k}_i\otimes\mathbf{G}^i = (\mathbf{w}_{,i} + \mathbf{k}_i\times\mathbf{w})\otimes\mathbf{G}^i. \tag{3.29}$$

Correspondingly, we use (2.41), (3.25) to get

$$\begin{aligned} \delta T &= \varrho_{\mathrm{ref}} \left(\dot{\mathbf{u}} \cdot \delta \dot{\mathbf{u}} + \boldsymbol{\Theta}\, \boldsymbol{\omega} \cdot \delta \boldsymbol{\omega} \right), \\ &= \varrho_{\mathrm{ref}} \left[\dot{\mathbf{u}} \cdot \delta \dot{\mathbf{u}} + \boldsymbol{\Theta}\, \boldsymbol{\omega} \cdot \left(\dot{\mathbf{w}} + \boldsymbol{\omega} \times \mathbf{w} \right) \right]. \end{aligned} \tag{3.30}$$

From the latter relation the essence of Sec. 4 and its great value, especially of relation (2.41), becomes apparent.

By introducing (3.27)–(3.30) in (3.26) and after some manipulations we arrive at

$$\begin{aligned} \int_{t_0}^{t_1} \Bigg[\int_{\mathcal{B}} \varrho_{\mathrm{ref}} \left[\dot{\mathbf{u}} \cdot \delta \dot{\mathbf{u}} + \boldsymbol{\Theta}\, \boldsymbol{\omega} \cdot \left(\dot{\mathbf{w}} + \boldsymbol{\omega} \times \mathbf{w} \right) \right] dV \\ - \int_{\mathcal{B}} \varrho_{\mathrm{ref}} \mathbf{R}\, \mathbf{U}^{p-T} \frac{\partial \psi_{\mathrm{int}}(\mathbf{U}^e, \mathbf{K}^e)}{\partial \mathbf{U}^e} \mathbf{G}^i \cdot \delta \mathbf{u}_{,i}\, dV \\ - \int_{\mathcal{B}} \varrho_{\mathrm{ref}} \left(-\mathbf{U}^{p-T} \frac{\partial \psi_{\mathrm{int}}(\mathbf{U}^e, \mathbf{K}^e)}{\partial \mathbf{U}^e} \mathbf{U}^T : \mathbf{W} + \frac{\partial \psi_{\mathrm{int}}(\mathbf{U}^e, \mathbf{K}^e)}{\partial \mathbf{K}^e} \mathbf{G}^i \cdot \left(\mathbf{w}_{,i} + \mathbf{k}_i \times \mathbf{w} \right) \right) dV \\ + \int_{\mathcal{B}} \mathbf{f} \cdot \delta \mathbf{u}\, dV + \int_{\partial \mathcal{B}} \mathbf{f}_s \cdot \delta \mathbf{u}\, dA + \int_{\mathcal{B}} \mathbf{M} \cdot \mathbf{w}\, dV + \int_{\partial \mathcal{B}} \mathbf{M}_s \cdot \mathbf{w}\, dA \Bigg] dt = 0. \end{aligned} \tag{3.31}$$

Note that (2.36) has been used and that $\mathbf{w}$ is the axial vector of the skew- symmetric tensor $\mathbf{W}$. Standard regularity assumptions with respect to time together with the fact that the variations vanish at $t = t_0$ and $t = t_1$, lead to

$$\begin{aligned} \int_{\mathcal{B}} \varrho_{\mathrm{ref}} \left[\ddot{\mathbf{u}} \cdot \delta \mathbf{u} + \left(\boldsymbol{\Theta}\, \dot{\boldsymbol{\omega}} - \boldsymbol{\Theta}\, \boldsymbol{\omega} \times \boldsymbol{\omega} \right) \cdot \mathbf{w} \right] dV \\ + \int_{\mathcal{B}} \varrho_{\mathrm{ref}} \mathbf{R}\, \mathbf{U}^{p-T} \frac{\partial \psi_{\mathrm{int}}(\mathbf{U}^e, \mathbf{K}^e)}{\partial \mathbf{U}^e} \mathbf{G}^i \cdot \delta \mathbf{u}_{,i}\, dV \\ + \int_{\mathcal{B}} \varrho_{\mathrm{ref}} \left(-\mathbf{U}^{p-T} \frac{\partial \psi_{\mathrm{int}}(\mathbf{U}^e, \mathbf{K}^e)}{\partial \mathbf{U}^e} \mathbf{U}^T : \mathbf{W} + \frac{\partial \psi_{\mathrm{int}}(\mathbf{U}^e, \mathbf{K}^e)}{\partial \mathbf{K}^e} \mathbf{G}^i \cdot \left(\mathbf{w}_{,i} + \mathbf{k}_i \times \mathbf{w} \right) \right) dV \\ - \int_{\mathcal{B}} \mathbf{f} \cdot \delta \mathbf{u}\, dV - \int_{\partial \mathcal{B}} \mathbf{f}_s \cdot \delta \mathbf{u}\, dA - \int_{\mathcal{B}} \mathbf{M} \cdot \mathbf{w}\, dV - \int_{\partial \mathcal{B}} \mathbf{M}_s \cdot \mathbf{w}\, dA = 0. \end{aligned} \tag{3.32}$$

The last equation splits into the two equations

$$\begin{aligned} \int_{\mathcal{B}} \varrho_{\mathrm{ref}} \ddot{\mathbf{u}} \cdot \delta \mathbf{u} = \int_{\mathcal{B}} \mathbf{f} \cdot \delta \mathbf{u}\, dV + \int_{\partial \mathcal{B}} \mathbf{f}_s \cdot \delta \mathbf{u}\, dA \\ - \int_{\mathcal{B}} \varrho_{\mathrm{ref}} \mathbf{R}\, \mathbf{U}^{p-T} \frac{\partial \psi_{\mathrm{int}}(\mathbf{U}^e, \mathbf{K}^e)}{\partial \mathbf{U}^e} \mathbf{G}^i \cdot \delta \mathbf{u}_{,i}, \end{aligned} \tag{3.33}$$

$$\int_{\mathcal{B}} \varrho_{\text{ref}} \left(\boldsymbol{\Theta}\, \dot{\boldsymbol{\omega}} + \boldsymbol{\omega} \times \boldsymbol{\Theta}\, \boldsymbol{\omega} \right) \cdot \mathbf{w}\, dV = \int_{\mathcal{B}} \mathbf{M} \cdot \mathbf{w}\, dV + \int_{\partial \mathcal{B}} \mathbf{M}_s \cdot \mathbf{w}\, dA$$

$$- \int_{\mathcal{B}} \varrho_{\text{ref}} \left(-\mathbf{U}^{p^{-T}} \frac{\partial \psi_{\text{int}}(\mathbf{U}^e, \mathbf{K}^e)}{\partial \mathbf{U}^e} \mathbf{U}^T : \mathbf{W} + \frac{\partial \psi_{\text{int}}(\mathbf{U}^e, \mathbf{K}^e)}{\partial \mathbf{K}^e} \mathbf{G}^i \cdot (\mathbf{w}_{,i} + \mathbf{k}_i \times \mathbf{w}) \right) dV, \tag{3.34}$$

which can be recognized as the weak form of the field equations (3.7), (3.8) if the identifications are made

$$\boldsymbol{\Sigma} = \varrho_{\text{ref}} \frac{\partial \psi(\mathbf{U}^e, \mathbf{K}^e)}{\partial \mathbf{U}} \mathbf{U}^T = \varrho_{\text{ref}} \mathbf{U}^{p^{-T}} \frac{\partial \psi(\mathbf{U}^e, \mathbf{K}^e)}{\partial \mathbf{U}^e} \mathbf{U}^T, \tag{3.35}$$

$$\boldsymbol{\Gamma} = \varrho_{\text{ref}} \frac{\partial \psi(\mathbf{U}^e, \mathbf{K}^e)}{\partial \mathbf{K}} \mathbf{U}^T = \varrho_{\text{ref}} \frac{\partial \psi(\mathbf{U}^e, \mathbf{K}^e)}{\partial \mathbf{K}^e} \mathbf{U}^T. \tag{3.36}$$

These identifications are justified on the basis of the principle of positive dissipation to be discussed in the next section.

Clearly, the recovery of the field equations (3.7) and (3.8) as Euler–Lagrange equations necessitates some algebraic operations which we have omitted for the sake of brevity. Note also that standard regularity assumptions of the involved fields are assumed to hold.

3.4. Positive dissipation and flow rules

We proceed further and formulate the principle of positive dissipation

$$\int_{\mathcal{B}} \mathcal{D}\, dV = \mathcal{W} - \int_{\mathcal{B}} \varrho_{\text{ref}} \dot{\psi}_{\text{int}}\, dV > 0. \tag{3.37}$$

In the above expression $\mathcal{D}$ means the dissipation function and $\mathcal{W}$ is the difference between the mechanical power and the rate of the kinetic energy. It is defined by

$$\mathcal{W} = \mathcal{P} - \int_{\mathcal{B}} \dot{T}\, dV = \int_{\mathcal{B}} (\mathbf{f} \cdot \dot{\mathbf{u}} + \mathbf{M} \cdot \boldsymbol{\omega})\, dV + \int_{\partial \mathcal{B}} (\mathbf{f}_s \cdot \dot{\mathbf{u}} + \mathbf{M}_s \cdot \boldsymbol{\omega})\, dA - \int_{\mathcal{B}} \dot{T}\, dV. \tag{3.38}$$

Assuming that the equilibrium equations hold, it is straightforward to show that the mechanical power reduces to the forms given in (3.10), (3.11) or (3.12).

Making use of (3.11) as well as of

$$\int_{\mathcal{B}} \varrho_{\text{ref}} \dot{\psi}(\mathbf{U}^e, \mathbf{K}^e, \mathbf{q}) = \int_{\mathcal{B}} \varrho_{\text{ref}} \left(\frac{\partial \psi}{\partial \mathbf{U}^e} : \dot{\mathbf{U}}^e + \varrho_{\text{ref}} \frac{\partial \psi}{\partial \mathbf{K}^e} : \dot{\mathbf{K}}^e + \varrho_{\text{ref}} \frac{\partial \psi}{\partial \mathbf{q}} \cdot \dot{\mathbf{q}} \right) dV \tag{3.39}$$

$$= \int_{\mathcal{B}} \varrho_{\text{ref}} \left[\mathbf{U}^{p^{-T}} \frac{\partial \psi}{\partial \mathbf{U}^e} \mathbf{U}^T : (\dot{\mathbf{U}}\, \mathbf{U}^{-1} - \dot{\mathbf{U}}^p \mathbf{U}^{p^{-1}}) \right.$$

$$\left. + \frac{\partial \psi}{\partial \mathbf{K}^e} : (\dot{\mathbf{K}} - \dot{\mathbf{K}}^p) + \frac{\partial \psi}{\partial \mathbf{q}} \cdot \dot{\mathbf{q}} \right] dV,$$

where the decomposition (3.14) is underlined, and assuming that the equilibrium equations hold along with the standard thermomechanical arguments, the principle of positive dissipation results in the constitutive relations

$$\boldsymbol{\Sigma} = \varrho_{\text{ref}} \mathbf{U}^{p^{-T}} \frac{\partial \psi(\mathbf{U}^e, \mathbf{K}^e, \mathbf{q})}{\partial \mathbf{U}^e} \mathbf{U}^T, \tag{3.40}$$

$$\boldsymbol{\Xi} = \varrho_{\text{ref}} \mathbf{U}^{e^T} \frac{\partial \psi(\mathbf{U}^e, \mathbf{K}^e, \mathbf{q})}{\partial \mathbf{U}^e}, \tag{3.41}$$

$$\boldsymbol{\Gamma} = \varrho_{\text{ref}} \frac{\partial \psi(\mathbf{U}^e, \mathbf{K}^e, \mathbf{q})}{\partial \mathbf{K}^e} \mathbf{U}^T, \tag{3.42}$$

$$\mathbf{y} = -\varrho_{\text{ref}} \frac{\partial \psi(\mathbf{U}^e, \mathbf{K}^e, \mathbf{q})}{\partial \mathbf{q}}, \tag{3.43}$$

as well as in the statement

$$\mathcal{D} = \boldsymbol{\Sigma} : \mathbf{L}^p + \boldsymbol{\Gamma}\, \mathbf{U}^{-1} : \dot{\mathbf{K}}^e + \mathbf{y} \cdot \dot{\mathbf{q}} > 0, \tag{3.44}$$

which specifies the dissipation function. In (3.43),(3.44), $\mathbf{y}$ has been introduced as the conjugate variable of $\mathbf{q}$. Note further that $\mathbf{L}^p$ is defined by $(3.19)_1$.

It should be mentioned that the above constitutive relations are formulated in a general form. Possible representations of these relations must allow for the fullfillment of the corresponding field equations. The discussion of such general representations is out of the scope of the paper.

Until now we have dealt with the first function of the theory, namely the free energy function ψ. The second function is the flow rule. We assume the existence of an elastic range defined by a function ϕ formulated in the stress space in terms of the real stress tensors. The material moment tensor to enter the formulation is evidently $\boldsymbol{\Gamma}$. Contrasting this, the stress tensor can be chosen either as $\boldsymbol{\Sigma}$ or as $\boldsymbol{\Xi}$. Both of them have the physical meaning of the Kirchhoff stress tensor (e.g. have the same invariants as the Kirchhoff stress tensor). Taking a look at the dissipation function it is evident that in the case of the decomposition (3.14), the tensor $\boldsymbol{\Sigma}$ is the appropriate one. Accordingly we formulate the function ϕ as

$$\phi(\boldsymbol{\Sigma}, \boldsymbol{\Gamma}, \mathbf{y}) : \mathbb{R}^9 \times \mathbb{R}^9 \times \mathbb{R}^n \to \mathbb{R}^+. \tag{3.45}$$

Elastic bahaviour is given for $\phi(\boldsymbol{\Sigma}, \boldsymbol{\Gamma}, \mathbf{y}) < 0$.

The elastic-viscoplastic theory is complete when evolution equations for the internal variables are specified. Strictly speaking this is an experimental task. In elasto-plasticity, the so-called normal flow rule has been frequently used and proved to work well especially within metal plasticity. Classically, this flow rule is equivalent and can be derived by means of Hill's postulate of maximum dissipation. It is well known that the postulate does not constitute a physical law. It should be understood as a useful instrument to derive flow rules valid for a specific class of materials. In view of the fact that sufficient experimental data

concerning the behavior of the elastic-viscoplastic Cosserat continuum is not available, we appeal to the postulate of maximum dissipation in order to derive the necessary flow rules. It is clear that these rules can and should be modified, once experimental data is available giving reason for such a modification. According to the mentioned postulate we have

$$-\mathcal{D}+\frac{1}{\eta}\phi^{+}(\boldsymbol{\Sigma},\boldsymbol{\Gamma},\mathbf{y})=\text{maximum}, \tag{3.46}$$

where $1/\eta$ can be understood as a penalty term which is physically interpreted as the viscosity. The elaboration of the postulate leads with (3.44) to the following flow rules

$$\mathbf{L}^{p}=\frac{1}{\eta}\frac{\partial\phi^{+}(\boldsymbol{\Sigma},\boldsymbol{\Gamma},\mathbf{y})}{\partial\boldsymbol{\Sigma}}, \tag{3.47}$$

$$\dot{\mathbf{K}}^{p}=\frac{1}{\eta}\frac{\partial\phi^{+}(\boldsymbol{\Sigma},\boldsymbol{\Gamma},\mathbf{y})}{\partial\boldsymbol{\Gamma}}\mathbf{U}^{T}, \tag{3.48}$$

$$\dot{\mathbf{q}}=\frac{1}{\eta}\frac{\partial\phi^{+}(\boldsymbol{\Sigma},\boldsymbol{\Gamma},\mathbf{y})}{\partial\mathbf{y}}. \tag{3.49}$$

In the case we are adopting the second decomposition (3.15), the dissipation function reads

$$\mathcal{D}=\boldsymbol{\Xi}:\overline{\mathbf{L}}^{p}+\boldsymbol{\Gamma}\,\mathbf{U}^{-1}:\dot{\mathbf{K}}^{e}+\mathbf{y}\cdot\dot{\mathbf{q}}>0, \tag{3.50}$$

where $\overline{\mathbf{L}}^{p}$ is defined by $(3.22)_1$. Accordingly, in the case of decomposition (3.15), the formulation of ϕ is appropriately carried out in terms of $\boldsymbol{\Xi}$. That is, we define the flow rule by the function

$$\phi^{+}(\boldsymbol{\Xi},\boldsymbol{\Gamma},\mathbf{y}):\mathbb{R}^{9}\times\mathbb{R}^{9}\times\mathbb{R}^{n}\to\mathbb{R}^{+}. \tag{3.51}$$

The transformation of (3.46) leads now to the alternative flow rules

$$\overline{\mathbf{L}}^{p}=\frac{1}{\eta}\frac{\partial\phi^{+}(\boldsymbol{\Xi},\boldsymbol{\Gamma},\mathbf{y})}{\partial\boldsymbol{\Xi}}, \tag{3.52}$$

$$\dot{\mathbf{K}}^{p}=\frac{1}{\eta}\frac{\partial\phi^{+}(\boldsymbol{\Xi},\boldsymbol{\Gamma},\mathbf{y})}{\partial\boldsymbol{\Gamma}}\mathbf{U}^{T}, \tag{3.53}$$

$$\dot{\mathbf{q}}=\frac{1}{\eta}\frac{\partial\phi^{+}(\boldsymbol{\Xi},\boldsymbol{\Gamma},\mathbf{y})}{\partial\mathbf{y}}. \tag{3.54}$$

Note that in (3.47) $\mathbf{L}^{p}$ is a left rate. The updating of $\mathbf{U}^{p}$ must be carried out according to the product $\exp(t\mathbf{L}^{p})\mathbf{U}^{p}$. In (3.52) the rate is a right one which means that the updating of $\mathbf{U}^{p}$ is carried out according to the product $\mathbf{U}^{p}\exp(t\overline{\mathbf{L}}^{p})$.

With the specific formulation of the functions ψ and ϕ the theory is completed. The following simple generalization of the von Mises theory can be adopted which we include for completeness:

$$\phi=h^{\epsilon},\qquad h=J+\beta I-y, \tag{3.55}$$

where we have

$$J = \operatorname{dev}\boldsymbol{\Sigma} : \operatorname{dev}\boldsymbol{\Sigma}, \qquad I = \boldsymbol{\Gamma} : \boldsymbol{\Gamma}, \qquad y = y_0 + Hq. \tag{3.56}$$

In the above equations, ϵ is a material parameter and only isotropic hardening is considered where H is the hardening parameter. β is a material parameter related directly to the influence of the moments in the flow rule. In the following two boxes the complete set of equations in either case of decomposition is summarized.

$$\mathbf{U} = \mathbf{U}^p\mathbf{U}^e, \qquad \mathbf{K} = \mathbf{K}^e + \mathbf{K}^p, \quad \dot{\mathbf{U}}^p = \mathbf{L}^p\mathbf{U}^p. \tag{3.57}$$

Internal dissipation

$$\mathcal{D} = \boldsymbol{\Sigma} : \mathbf{L}^p + \boldsymbol{\Gamma}\,\mathbf{U}^{-T} : \dot{\mathbf{K}}^p + \mathbf{y}\cdot\dot{\mathbf{q}}. \tag{3.58}$$

Constitutive relations

$$\boldsymbol{\Sigma} = \varrho_{\mathrm{ref}}\frac{\partial\psi(\mathbf{U}^e,\mathbf{K}^e,\mathbf{q})}{\partial\mathbf{U}}\mathbf{U}^T = \varrho_{\mathrm{ref}}\mathbf{U}^{p^{-T}}\frac{\partial\psi(\mathbf{U}^e,\mathbf{K}^e,\mathbf{q})}{\partial\mathbf{U}^e}\mathbf{U}^T, \tag{3.59}$$

$$\boldsymbol{\Gamma} = \varrho_{\mathrm{ref}}\frac{\partial\psi(\mathbf{U}^e,\mathbf{K}^e,\mathbf{q})}{\partial\mathbf{K}^e}\mathbf{U}^T, \qquad \mathbf{y} = -\varrho_{\mathrm{ref}}\frac{\partial\psi(\mathbf{U}^e,\mathbf{K}^e,\mathbf{q})}{\partial\mathbf{q}}. \tag{3.60}$$

Evolution equations

$$\mathbf{L}^p = \frac{1}{\eta}\frac{\partial\phi^+(\boldsymbol{\Sigma},\boldsymbol{\Gamma},\mathbf{y})}{\partial\boldsymbol{\Sigma}}, \quad \dot{\mathbf{K}}^p = \frac{1}{\eta}\frac{\partial\phi^+(\boldsymbol{\Sigma},\boldsymbol{\Gamma},\mathbf{y})}{\partial\boldsymbol{\Gamma}}\mathbf{U}, \quad \dot{\mathbf{q}} = \frac{1}{\eta}\frac{\partial\phi^+(\boldsymbol{\Sigma},\boldsymbol{\Gamma},\mathbf{y})}{\partial\mathbf{y}}. \tag{3.61}$$

$$\mathbf{U} = \overline{\mathbf{U}}^e\,\overline{\mathbf{U}}^p, \qquad \mathbf{K} = \mathbf{K}^e + \mathbf{K}^p, \qquad \dot{\overline{\mathbf{U}}}^p = \overline{\mathbf{U}}^p\overline{\mathbf{L}}^p, \tag{3.62}$$

Internal dissipation

$$\mathcal{D} = \boldsymbol{\Xi} : \overline{\mathbf{L}}^p + \boldsymbol{\Gamma}\,\mathbf{U}^{-T} : \dot{\mathbf{K}}^p + \mathbf{y}\cdot\dot{\mathbf{q}}. \tag{3.63}$$

Constitutive relations

$$\boldsymbol{\Xi} = \varrho_{\mathrm{ref}}\mathbf{U}^T\frac{\partial\psi(\overline{\mathbf{U}}^e,\mathbf{K}^e,\mathbf{q})}{\partial\mathbf{U}} = \varrho_{\mathrm{ref}}\mathbf{U}^T\frac{\partial\psi(\mathbf{U}^e,\mathbf{K}^e,\mathbf{q})}{\partial\overline{\mathbf{U}}^e}\overline{\mathbf{U}}^{p^{-T}}, \tag{3.64}$$

$$\boldsymbol{\Gamma} = \varrho_{\mathrm{ref}}\frac{\partial\psi(\overline{\mathbf{U}}^e,\mathbf{K}^e,\mathbf{q})}{\partial\mathbf{K}^e}\mathbf{U}^T, \qquad \mathbf{y} = -\varrho_{\mathrm{ref}}\frac{\partial\psi(\mathbf{U}^e,\mathbf{K}^e,\mathbf{q})}{\partial\mathbf{q}}. \tag{3.65}$$

Evolution equations

$$\overline{\mathbf{L}}^p = \frac{1}{\eta}\frac{\partial\phi^+(\boldsymbol{\Xi},\boldsymbol{\Gamma},\mathbf{y})}{\partial\boldsymbol{\Xi}}, \quad \dot{\mathbf{K}}^p = \frac{1}{\eta}\frac{\partial\phi^+(\boldsymbol{\Xi},\boldsymbol{\Gamma},\mathbf{y})}{\partial\boldsymbol{\Gamma}}\mathbf{U}, \quad \dot{\mathbf{q}} = \frac{1}{\eta}\frac{\partial\phi^+(\boldsymbol{\Xi},\boldsymbol{\Gamma},\mathbf{y})}{\partial\mathbf{y}}. \tag{3.66}$$

The question of linearization of formulations as given by (3.33) and (3.34) is of special theoretical and practical interest. This issue is discussed briefly in the Appendix.

4. Concluding remarks

A theory of the elastic-viscoplastic Cosserat continuum has been presented. Basic features of the formulation are: i) It is based on the multiplicative decomposition of the stretch tensor and an additive one for the second Cosserat deformation tensor. ii) The rotation field is treated as a kinematical variable and it was emphasized that no decomposition could be adopted for such a field. iii) Two functions determine the structure of the theory completely, the free energy function and the flow rule. As a first step, the evolution equations has been derived by means of Hill's postulate of maximum dissipation.

It was shown that two possible multiplicative decompositions can be adopted. Depending on the decomposition underlined, the flow rule has to be formulated in terms of two different stress tensors corresponding to a dissipation function. Special emphasis has been given for the definition of rates and variations. Relying on the basic concepts of Lie groups, the formulation of such rates has been systematically derived, a method which clarifies many concepts seem otherwise to be arbitrary.

5. Appendix. Second derivatives and the geometric structure of the configuration space

The question of linearization of formulations as given by (3.33) and (3.34) is of special theoretical and practical interest. At least, when computations have to be carried out. It turns out that the geometry of the configuration space as a Lie group is of crucial importance. In the context of shell computations at finite deformations, these aspects have been presented in SANSOUR and BEDNARCZYK [7] and MAKOWSKI and STUMPF [21] to which the reader is referred. In brief we sketch in the following basic aspects of the linearization process to be carried out with respect to the geometrical nonlinearities. These aspects are not restricted to the Cosserat continuum but are carried over to any configuration space defined as a Lie group; e.g. within a micromorphic continuum.

The importance of the linearization concepts becomes obvious from the following observation. The second variation of a relation as (2.36) reads

$$\delta^2 \mathbf{R} = (\delta \mathbf{R})\mathbf{W} = \mathbf{R}\,\mathbf{Y}\,\mathbf{W}. \tag{5.1}$$

Evidently the expression is not symmetric with respect to the variations $\mathbf{W}$ and $\mathbf{Y}$. Based on these formulas, the linearization of (3.33) and (3.34) with respect to the geometric nonlinearities results necessarily in a non-symmetric tangent

operator. Here we touch a crucial difference between linear vector spaces and Lie groups which are naturally defined as a nonlinear manifold. A fundamental observation is that the linearization can be carried out differently if the configuration space is equipped with the structure of a Killing metric. In that case and since the first variation $\delta\mathbf{R}$ is to be understood as a tangent vector, the second variation can be carried out as a covariant derivation of that tangent vector. A related formulation which treats the first variation of the energy function as a co-vector which then is derived covariantly, is due to SIMO [22]. Our formulation has the basic feature of operating at the level of the configuration space itself.

Let us first rewrite the tangent vectors by making use of the following notation (DUBROVIN *et al.* [17]) $L_{\mathbf{W}}(\mathbf{R}) = \mathbf{R}\,\mathbf{W}$. At an arbitrary point on $SO(3)$, say at $\mathbf{R}$, the Killing metric is defined by the scalar product of the tangent vectors defined by

$$\langle L_{\mathbf{W}}(\mathbf{R}), L_{\mathbf{Y}}(\mathbf{R})\rangle = \mathrm{tr}|\,(\mathbf{R}\,\mathbf{W}(\mathbf{R}\,\mathbf{Y})^T) = \mathrm{tr}\,(\mathbf{W}\,\mathbf{Y}^T). \tag{5.2}$$

The Lie bracket $[\mathbf{W}, \mathbf{Y}]$ is given by

$$[\mathbf{W}, \mathbf{Y}] = \mathbf{W}\,\mathbf{Y} - \mathbf{Y}\,\mathbf{W}, \qquad \mathbf{W}, \mathbf{Y} \in so(3). \tag{5.3}$$

On the space of tangent vectors there exists a connection given by the relation (BRICKELL and CLARK [23], CHOQUET *et al.* [16], DUBROVIN *et al.* [17]).

$$\begin{aligned} 2\,\langle \nabla_{\mathbf{U}}\mathbf{V}, \mathbf{W}\rangle = {} & \mathbf{U}(\langle \mathbf{V}, \mathbf{W}\rangle) + \mathbf{V}(\langle \mathbf{W}, \mathbf{U}\rangle) - \mathbf{W}(\langle \mathbf{U}, \mathbf{V}\rangle) \\ & - \langle \mathbf{U}, [\mathbf{V}, \mathbf{W}]\rangle + \langle \mathbf{V}, [\mathbf{W}, \mathbf{U}]\rangle + \langle \mathbf{W}, [\mathbf{U}, \mathbf{V}]\rangle \\ & - \langle \mathbf{U}, \mathbf{T}(\mathbf{V}, \mathbf{W})\rangle + \langle \mathbf{V}, \mathbf{T}(\mathbf{W}, \mathbf{U})\rangle + \langle \mathbf{W}, \mathbf{T}(\mathbf{U}, \mathbf{V})\rangle \end{aligned} \tag{5.4}$$

where the torsion tensor $\mathbf{T}$ is defined as

$$\mathbf{T}(\mathbf{U}, \mathbf{V}) = \nabla_{\mathbf{U}}\mathbf{V} - \nabla_{\mathbf{V}}\mathbf{U} - [\mathbf{U}, \mathbf{V}].$$

For a symmetric connection the torsion $\mathbf{T}$ vanishes and we can obtain from (5.4) the expression

$$\nabla_{L_{\mathbf{Y}}} L_{\mathbf{W}} = \frac{1}{2} L_{[\mathbf{Y},\mathbf{W}]}. \tag{5.5}$$

Hereby one has to make use of the metric as defined in (5.2) as well as of the idea that tangent vectors can be understood as derivatives operating on function spaces. By the latter fact, the first line in (5.4) vanishes identically since the metric is independent of the particular point on the curve in $\mathcal{C}$.

Dealing with vector fields, it makes sense to define with the help of this connection a covariant derivative (or covariant variation). In fact such a derivative is given on the right invariant vector fields as

$$\begin{aligned} \nabla_{\mathbf{Y}} L_{\mathbf{W}}(\mathbf{R}) = L_{\mathbf{W}\,\mathbf{Y}}(\mathbf{R}) + \nabla_{L_{\mathbf{Y}}} L_{\mathbf{W}}(\mathbf{R}) &= \mathbf{R}\,\mathbf{W}\,\mathbf{Y} + \frac{1}{2}\mathbf{R}[\mathbf{Y}, \mathbf{W}] \\ &= \frac{1}{2}\mathbf{R}(\mathbf{Y}\,\mathbf{W} + \mathbf{W}\,\mathbf{Y}). \end{aligned} \tag{5.6}$$

Evidently the relation is symmetric with respect to the variations **W**, **Y**. Accordingly, the last result and not (5.1) should be used to accomplish possible linearizations. For more details and applications to practical computations within the shell theory, the reader is referred to SANSOUR and BEDNARCZYK [7].

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TECHNISCHE HOCHSCHULE DARMSTADT,
FACHGEBIET MASCHINENELEMENTE UND AKUSTIK
Magdalenenstr. 4, 64289 Darmstadt, Germany.

Received October 7, 1997.

Arch. Mech., 50, 3, pp. 599–611, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

System symmetries and inverse variational problems in continuum theory

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

M. SCHOLLE (PADERBORN)

THE AIM of the conventional Inverse Problem in Lagrange formalism is to find a Lagrangian, the associated Euler–Lagrange equations of which are equivalent to a given set of partial differential equations of a physical system. In contrast, I am dealing with a different type of an inverse problem. I look for a Lagrangian which is associated with a given set of balance equations. My approach is based on general relations between symmetry groups (geometrical and gauge symmetries) and its associated balance equations. I follow two different mathematical lines: The first one is *Noether's theorem*: Universal Lie symmetry groups like translations (spatial and temporal), rotations and Galilei transformation are connected with the fundamental conservation laws for energy, linear momentum, angular momentum and center of mass motion. All of these balances are of the "volume-type". The second line takes account of a relationship between non-Lie symmetry groups (e.g. regauging of potentials) and balances of the "area-type". These are physically associated with *line-shaped objects* like vortex lines and dislocations. Following both lines in an inverse manner I derive the relevant symmetry properties of a yet unknown Lagrangian for a given set of balance equations of volume- and area-types. Consequently, a rough scheme for the analytical structure of the Lagrangian can be given. As an example, a Lagrangian for the elastic deformation of a body with eigenstresses due to fixed dislocations is constructed.

Notations

Subsequently I use the following notations for temporal and spatial coordinates and their corresponding first order derivatives:

$$x = (x^\alpha) = (t, \mathbf{x}) = \left(x^0 = t, x^1, \cdots, x^3\right),$$

$$\partial = (\partial_\alpha) = (\partial_t, \nabla) = \left(\partial_0 = \partial_t = \frac{\partial}{\partial t}, \partial_1 = \frac{\partial}{\partial x^1}, \cdots, \partial_3 = \frac{\partial}{\partial x^3}\right).$$

The *substantial time derivative* is the operator

$$\mathrm{D}_t := \partial_t + \mathbf{v}\cdot\nabla,$$

where $\mathbf{v}$ denotes the velocity field of the medium. Furthermore, the three canonical Euclidean base vectors $\mathbf{e}_\kappa$ of the laboratory frame are defined as

$$\mathbf{e}_1 = (1,0,0), \qquad \mathbf{e}_2 = (0,1,0), \qquad \mathbf{e}_3 = (0,0,1).$$

Let $\ell = \ell(\psi, \partial\psi, x)$ be a first order Lagrangian of a system based on N independent fields

$$\psi = \left(\psi^i(x)\right) = \left(\psi^1(x), \cdots, \psi^N(x)\right).$$

Then, the conjugated canonical field momenta $\pi^\alpha = (\pi_i^\alpha) = (\pi_1^\alpha(\psi, \partial\psi, x), \cdots, \pi_N^\alpha(\psi, \partial\psi, x))$ are given by

$$\pi_i^\alpha(\psi, \partial\psi, x) := \frac{\partial \ell}{\partial(\partial_\alpha \psi^i)}. \tag{0.1}$$

We additionally define $\boldsymbol{\pi} = \left(\pi^1, \pi^2, \pi^3\right)$.

Einstein's summation convention is implied, whenever two indices occur twice in a product, exept for special cases, where for clarity the summation is indicated explicitly.

1. The inverse problem of the second kind

IN TRADITIONAL continuum theories a system is regarded to be physically defined, if a set of relevant balance equations is established together with an associated set of constitutive equations for the densities, flux densities and production rates involved in the balance equations.

Apart from this method, Lagrange formalism (LF) gives rise to an alternative formulation of the dynamics of the system: as the main feature, all information on the processes of a particular system is contained in one function only, namely its Lagrangian. All balance equations can be derived from the Lagrangian.

However, in many cases the Lagrangian is unknown. Then, to establish an adequate Lagrangian formulation of the system, one has to start from the established set of phenomenological balance equations in order to construct the suitable Lagrangian. This is a rough description of the "inverse problem in LF". An exact mathematical definition of the inverse problem in LF is much more difficult; it depends on the viewpoint, how the phenomenological equations should be derived from the Lagrangian:

1. From the traditional viewpoint, either the phenomenological equations themselves or an equivalent self-adjoint set of equations are expected to be the *Euler–Lagrange equations* of the Lagrangian. We call this traditional concept the *inverse problem of the first kind* (IP1).

2. Noether's theorem shows us, how to derive the balance equations from a given Lagrangian. Taking universal symmetries like time- and space translation, rigid rotation and Galilei-transformation into account, the phenomenological balances for energy, linear momentum, angular momentum and center of mass motion can be derived by means of the wellknown "Noether machinery". Thus, if one interprets the relevant phenomenological balances of the system as Noether balances, a different kind of inverse problem is defined which I call the *inverse problem of the second kind* (IP2).

Taking the second viewpoint, it is practicable to treat different physical systems in the same universal way, i.e. apart from their individual constitutive laws. Lagrange formalism is a *unifying concept* for quite different physical problems.

However, not all relevant phenomenological equations can be interpreted as Noether balances, e.g. the fundamental dynamical equations for *vortices* and *dislocations* which are "area-type" balances. In order to define IP2 completely we first have to find an adequate way to treat such balances in a way which is quite analogous to Noether's theorem.

2. Symmetries and balances beyond Noether's theorem

2.1. Two types of balance equations

We refer to the wellknown homogenous balance equation of an observable A,

$$\partial_t a(\mathbf{x}, t) + \nabla \cdot \mathbf{j}_a(\mathbf{x}, t) = 0\,, \tag{2.1}$$

which we call a *volume-type balance equation*. a is the local density and $\mathbf{j}_a$ the flux density of the observable A. This local form of the balance equation is associated with a global form by integrating Eq. (2.1) over a fixed test volume V:

$$\frac{dA}{dt} = \Phi_A\,, \tag{2.2}$$

where

$$A(t) := \int_V a(\mathbf{x}, t)\, d^3x \tag{2.3}$$

is the total amount of the observable A in the volume V, and

$$\Phi_A(t) := -\int_V \nabla \cdot \mathbf{j}_a(\mathbf{x}, t)\, d^3x = -\int_{\partial V} \mathbf{j}_a(\mathbf{x}, t) \cdot d\mathbf{S} \tag{2.4}$$

is the total flux of A across the boundary ∂V of the test volume.

In the case of *point-like objects*, the quantities A and Φ_A are obviously associated with the number of objects within the test volume V and with the number of objects passing the boundary ∂V, respectively. In Eq. (2.4) we took account of Gauss' theorem. Thus the term "volume-type balance" is sufficiently motivated.

We further refer to the homogenous balance equation of the type

$$\partial_t \mathbf{w}(\mathbf{x}, t) + \nabla \times \mathbf{J}_w(\mathbf{x}, t) = 0 \tag{2.5}$$

which, with regard to the subsequent theory and applications, is supplemented by the equation

$$\nabla \cdot \mathbf{w} = 0. \tag{2.6}$$

Obviously Eq. (2.5) is formally different from (2.1); we call it an *area-type balance equation*. It is associated with an observable Γ. Let us call $\mathbf{w}$ a *generalized vortex density* and $\mathbf{J}_w$ the associated *generalized vortex flux density*. The local form

(2.5) of the balance equation is related to a global form by integrating over a fixed test area F:

$$\frac{d\Gamma}{dt} = \Phi_\Gamma , \tag{2.7}$$

where

$$\Gamma(t) := \int_F \mathbf{w}(\mathbf{x},t)\cdot d\mathbf{F} \tag{2.8}$$

is called the total *generalized circulation* of the observable Γ *referred to the test area* F.

$$\Phi_\Gamma(t) := -\int_F \nabla\times\mathbf{J}_w(\mathbf{x},t)\cdot d\mathbf{F} = -\int_{\partial F}\mathbf{J}_w(\mathbf{x},t)\cdot d\mathbf{s} \tag{2.9}$$

is called the total *generalized circulation flux* across the boundary line ∂F of the test area.

It is a wellknown fact that Eqs. (2.5), (2.6) are frequently physically realized by means of *line-shaped objects* which may be counted in a test cross-section. In this case the vortex density $\mathbf{w}$ and the vortex flux density $\mathbf{J}_w$ are associated with the number of objects piercing the test area F and with the number of objects passing the boundary line ∂F. In Eq. (2.9) we took account of Stokes' theorem. Thus the term "area-type balance" is sufficiently motivated.

Examples for two simultanous equations of the types (2.5), (2.6) are:

• *Helmholtz' equations* for the vorticity $\boldsymbol{\omega} = \frac{1}{2}\nabla\times\mathbf{v}$ of an ideal fluid ($\mathbf{v}$: velocity field):

$$\partial_t\boldsymbol{\omega} + \nabla\times[-\mathbf{v}\times\boldsymbol{\omega}] = 0, \tag{2.10}$$

$$\nabla\cdot\boldsymbol{\omega} = 0. \tag{2.11}$$

• Fundamental kinematical equations of the *dislocation theory*:

$$\partial_t\underline{\underline{\alpha}} + \nabla\times\underline{\underline{J}}_\alpha = 0, \tag{2.12}$$

$$\nabla\cdot\underline{\underline{\alpha}} = 0. \tag{2.13}$$

$\underline{\underline{\alpha}}$ is the second rank dislocation tensor and $\underline{\underline{J}}_\alpha$ the associated dislocation flux density. Equation (2.13) is related to the fact that dislocation lines cannot end within the crystal, whereas Eq. (2.12) is related to the number of dislocation lines and its balance.

These area-type balances cannot be interpreted as Noether balances! Nevertheless the question arises if the area-type balances (2.5), (2.6) can be obtained within the Lagrange formalism by means of a straightforward and unified formalism similar to the Noether theorem.

2.2. An alternative symmetry-balance-theorem

Let $\psi = (\psi^1, \cdots, \psi^N)$ be a set of fundamental field variables of a physical system, e.g. a set of potentials. Let further $\ell(\psi, \partial\psi, x)$ be the Lagrangian of the system. Then let us look at a set $\mathbb{F} = \left\{(F^1(\psi), \cdots, F^N(\psi))\right\}$ of functions $F^i \in C^2(\mathbb{R}^N)$ which induce a *regauging* of the fields ψ (potentials):

$$\begin{aligned} x^\alpha &\longrightarrow x^\alpha, \\ \psi^i &\longrightarrow F^i(\psi), \qquad F \in \mathbb{F}. \end{aligned} \tag{2.14}$$

Let us assume that these transformations (2.14) fulfil the *strict symmetry criterion*:

$$\ell(F(\psi), \partial F(\psi), x) = \ell(\psi, \partial\psi, x). \tag{2.15}$$

Then they are called *symmetry transformations of the Lagrangian*. We further assume that the set $\mathbb{F}$ is a *non-Lie group*, i.e. there are no group parameters available with the consequence that Noether's theorem is not applicable to (2.14). Nevertheless, I shall establish an alternative method to get a set of balance equations associated with the symmetry group $\mathbb{F}$: Deriving (2.15) with respect to $\partial_\alpha \psi^i$, I obtain a system of $4N$ equations

$$\left(\pi_j^\alpha\right)_{\psi \to F} \frac{\partial F^j}{\partial \psi^i} = \pi_i^\alpha, \qquad \alpha = 0, \cdots, 3, \quad i = 1, \cdots, N, \tag{2.16}$$

with the field momenta π_i^α defined in Eq. (0.1). This *differential symmetry criterion* is a system of necessary conditions for the set $\mathbb{F}$ of symmetry transformations. These $4N$ equations are not *linearly independent* in general. However, there always exists a *basic representation* of the field momenta

$$\pi^\alpha = \sum_{p=1}^{M} \mu_p^\alpha B^p \tag{2.17}$$

with *coefficients* $\mu_p^\alpha(\psi, \partial\psi, x)$ which are invariant under to the gauge transformation (2.14), and with a set of $M \leq 4$ *linearly independent basis elements* $\mathbb{B} := \left\{B^1 = (B_1^1, \cdots, B_N^1), \cdots, \ B^M = \left(B_1^M, \cdots, B_N^M\right)\right\}$. Their linear independence means that

$$\sum_{p=1}^{M} \lambda_p B^p = 0 \quad \Longleftrightarrow \quad \lambda_p = 0 \quad \forall p \tag{2.18}$$

with coefficients $\lambda_p(\psi, \partial\psi, x)$ *invariant* with respect to (2.14). The basis elements B^p are functions of $\psi, \partial\psi$ and x, in general. By means of this basis representation, the set of Eqs. (2.16) can be simplified; it can be substituted by the *reduced symmetry criterion*

$$\left(B_j^p\right)_{\psi \to F} \frac{\partial F^j}{\partial \psi^i} = B_i^p, \tag{2.19}$$

a system of $M \cdot N$ linearly independent equations which contains the same information about the non-Lie regauging group $\mathbb{F}$ as (2.16) does.

The basis elements B^p represent characteristic features of the non-Lie group $\mathbb{F}$; they are of the same importance as the infinitesimal generators for Lie-groups are.

THEOREM. *Let* $\mathbb{B} = \{B^p \,|\, p = 1, \cdots, M \leq 4\}$ *be a proper set of linearly independent basis elements due to Eq.* (2.17). *From this basis* $\mathbb{B}$ *we define the vortex densities* $\mathbf{w}^p$ *and the associated flux densities* $\mathbf{J}^p$ *as*

$$\mathbf{w}^p := \nabla B_i^p \times \nabla \psi^i, \tag{2.20}$$

$$\mathbf{J}^p := \partial_t \psi^i \nabla B_i^p - \partial_t B_i^p \nabla \psi^i. \tag{2.21}$$

Then, these quantities are invariant under regauging (2.14) *and fulfil the* M *homogenous area-type balances* $(p = 1, \cdots, M)$

$$\partial_t \mathbf{w}^p + \nabla \times \mathbf{J}^p = 0, \tag{2.22}$$

$$\nabla \cdot \mathbf{w}^p = 0. \tag{2.23}$$

P r o o f: 1. The gauge-invariance of the balance quantities $\mathbf{w}^p$ and $\mathbf{J}^p$ is a consequence of the reduced symmetry criterion (2.19). Looking at

$$\begin{aligned} \mathbf{w}^p &= \nabla B_i^p \times \nabla \psi^i = \nabla \left[\left(B_j^p \right)_{\psi \to F} \frac{\partial F^j}{\partial \psi^i} \right] \times \nabla \psi^i \\ &= \nabla \left(B_j^p \right)_{\psi \to F} \times \left(\frac{\partial F^j}{\partial \psi^i} \nabla \psi^i \right) + \left(B_j^p \right)_{\psi \to F} \frac{\partial^2 F^j}{\partial \psi^i \partial \psi^k} \nabla \psi^k \times \nabla \psi^i \end{aligned}$$

and keeping in mind that the last term vanishes [1], the gauge-invariance of the vortex densities can be easily shown:

$$\mathbf{w}^p = \nabla \left(B_j^p \right)_{\psi \to F} \times \left(\frac{\partial F^j}{\partial \psi^i} \nabla \psi^i \right) = \nabla \left(B_j^p \right)_{\psi \to F} \times \nabla F^j(\psi) = \left(\mathbf{w}^p \right)_{\psi \to F} .$$

The gauge-invariance of the vortex flux densities $\mathbf{J}^p$ can be proven in the same way.

2. Obviously, by definition (2.20), (2.21) the two identities

$$\begin{aligned} \partial_t \mathbf{w}^p &= \left(\partial_t \nabla B_i^p \right) \times \nabla \psi^i + \nabla B_i^p \times \left(\partial_t \nabla \psi^i \right) \\ &= \nabla \times \left[\partial_t B_i^p \nabla \psi^i - \partial_t \psi^i \nabla B_i^p \right] - \partial_t B_i^p \nabla \times \nabla \psi^i + \partial_t \psi^i \nabla \times \nabla B_i^p = -\nabla \times \mathbf{J}^p \\ \nabla \cdot \mathbf{w}^p &= \nabla \cdot \left[\nabla \times \left(B_i^p \nabla \psi^i \right) - B_i^p \nabla \times \nabla \psi^i \right] = 0 \end{aligned}$$

are fulfilled.

[1] This term contains a contraction of an expression symmetric with respect to the index change $i \leftrightarrow k$ and an expression antisymmetric with respect to the same operation.

The above theorem supplements Noether's theorem – it operates with another kind of symmetries and another kind of balances. For further details I refer to the forthcomming paper [8].

2.3. Helmholtz' equation of the ideal fluid as an example

It is well-known that the Lagrangian for an ideal fluid takes the form [2]

$$\ell = -\varrho\left[\partial_t \Phi + \gamma\partial_t\vartheta + \frac{1}{2}(\nabla\Phi + \gamma\nabla\vartheta)^2 + u(\varrho)\right] \tag{2.24}$$

depending on the 4 independent fields $\psi = (\psi^1, \cdots, \psi^4) = (\varrho, \Phi, \gamma, \vartheta)$, namely the mass density ϱ and the so-called Clebsch potentials which give rise to the potential representation [3, 4]

$$\mathbf{v} = \nabla\Phi + \gamma\nabla\vartheta \tag{2.25}$$

of the velocity field $\mathbf{v}$. As a consequence, the vortex field $\boldsymbol{\omega}$ takes the form

$$\boldsymbol{\omega} = \frac{1}{2}\nabla\times\mathbf{v} = \frac{1}{2}\nabla\gamma\times\nabla\vartheta\,. \tag{2.26}$$

The function $u(\varrho)$ denotes the elastic energy of the fluid. Now we apply the alternative symmetry-balance-theorem for area-type balances to this example: the conjugate canonical field momenta take the form

$$\begin{aligned}\pi^0 &= \left(\pi^0_1, \cdots, \pi^0_4\right) = (0, -\varrho, 0, -\varrho\gamma)\,,\\ \boldsymbol{\pi} &= (\boldsymbol{\pi}_1, \cdots, \boldsymbol{\pi}_4) = (0, -\varrho\mathbf{v}, 0, -\varrho\gamma\mathbf{v})\,.\end{aligned}$$

Obviously, the field momenta can be represented by means of one basis element B^0 only:

$$\begin{aligned}\pi^0_i &= -\varrho B^0_i\,,\\ \boldsymbol{\pi}_i &= -\varrho\mathbf{v}B^0_i\,,\end{aligned} \tag{2.27}$$

with

$$B^0 = \left(B^0_1, \cdots, B^0_4\right) = (0, 1, 0, \gamma). \tag{2.28}$$

According to (2.20), (2.21), this basis element gives rise to a line density $\mathbf{w}$ and its flux density $\mathbf{J}$ via

$$\mathbf{w}^0 = \nabla B^0_i \times \nabla\psi^i = \nabla\gamma\times\nabla\vartheta = 2\boldsymbol{\omega}, \tag{2.29}$$

$$\mathbf{J}^0 = \partial_t\psi^i\nabla B^0_i - \partial_t B^0_i\nabla\psi^i = -\mathbf{v}\times\mathbf{w}^0, \tag{2.30}$$

which are gauge invariant and fulfil the homogenous balance equation of the area type (2.22), (2.23). In (2.30) we took account of the two Euler–Lagrange equations [2]

$$\mathrm{D}_t\vartheta = 0, \qquad \mathrm{D}_t\gamma = 0,$$

of (2.24). Obviously, the associated balance equations (2.22), (2.23) turn out to be *Helmholtz' equations* (2.10), (2.11). Thus, the regauging group of the Clebsch potentials Φ, γ, ϑ determined by the basis element B^0 is associated with the vortex dynamics of the fluid.

3. A Lagrangian description for the dynamical theory of elasticity with eigenstresses

3.1. The general analytical form of the Lagrangian

For the ideal fluid we found that the conjugate field momenta can be represented by means of one basis element B^0 only (see Eq. (2.27), and that it is associated with the dynamics of *vortices*. Passing from the fluid to the solid we take account of *dislocations* in an analogous way. Dislocations are line-shaped objects like vortices. Let us extend Eq. (2.27) towards a generalized basis representation

$$\begin{aligned} \pi_i^0 &= -\varrho B_i^0 + \sum_{\kappa=1}^{3} \sigma_\kappa^0 B_i^\kappa , \\ \boldsymbol{\pi}_i &= -\varrho \mathbf{v} B_i^0 + \sum_{\kappa=1}^{3} \boldsymbol{\sigma}_\kappa B_i^\kappa , \end{aligned} \tag{3.1}$$

with *four basis elements* B^0, B^1, B^2, B^3, the dimension N of which is still open. B^0 corresponds to the *vortex dynamics*, whereas B^1, B^2, B^3 correspond to the *dislocation dynamics*.

The associated area-type balances (2.22), (2.23) are based on the quantities

$$2\boldsymbol{\omega} = \nabla B_i^0 \times \nabla \psi^i = \nabla \times \left(B_i^0 \nabla \psi^i \right), \tag{3.2}$$

$$2\mathbf{J}_\omega = \partial_t \psi^i \nabla B_i^0 - \partial_t B_i^0 \nabla \psi^i, \tag{3.3}$$

and

$$\underline{\underline{\alpha}} = \sum_{\kappa=1}^{3} \left(\nabla B_i^\kappa \times \nabla \psi^i \right) \otimes \mathbf{e}_\kappa = \sum_{\kappa=1}^{3} \nabla \times \left(B_i^\kappa \nabla \psi^i \right) \otimes \mathbf{e}_\kappa , \tag{3.4}$$

$$\underline{\underline{J}}_\alpha = \sum_{\kappa=1}^{3} \left[\partial_t \psi^i \nabla B_i^\kappa - \partial_t B_i^\kappa \nabla \psi^i \right] \otimes \mathbf{e}_\kappa , \tag{3.5}$$

with an open set $\psi = \left(\psi^1, \cdots, \psi^N \right)$ of fundamental field variables. $\boldsymbol{\omega}$, $\mathbf{J}_\omega$ are the *vortex field* and the *vortex flux density*, and $\underline{\underline{\alpha}}$, $\underline{\underline{J}}_\alpha$ are the *dislocation density* and the associated flux density. In the theory of *generalized Cosserat-continua* [6, 7],

the dislocation density in a crystal lattice is defined from the three (reciprocal) *Cosserat-directors* $\mathbf{a}^1$, $\mathbf{a}^2$, $\mathbf{a}^3$ via

$$\underline{\underline{\alpha}} = \sum_{\kappa=1}^{3} (\nabla \times \mathbf{a}^\kappa) \otimes \mathbf{e}_\kappa \,. \tag{3.6}$$

The Cosserat-directors are associated with the crystal lattice vectors. Comparing (3.2) with (2.26) and (3.4) with (3.6), I obtain the identifications

$$\mathbf{v} = B_i^0 \nabla \psi^i, \tag{3.7}$$

$$\mathbf{a}^\kappa = B_i^\kappa \nabla \psi^i. \tag{3.8}$$

Aditionally, we have to take account of the *Noether balances*. E.g. the momentum balance [1]

$$\partial_t \mathbf{p} + \nabla \cdot \underline{\underline{\Sigma}} = 0 \tag{3.9}$$

which is due to space translations, is defined via Noether's theorem by the constitutive equations

$$\mathbf{p} = -\pi_i^0 \nabla \psi^i = \varrho B_i^0 \nabla \psi^i + \sum_{\kappa=1}^{3} \sigma_\kappa^0 B_i^\kappa \nabla \psi^i = \varrho \mathbf{v} + \mathbf{p}^*, \tag{3.10}$$

$$\underline{\underline{\Sigma}} = \ell \underline{\underline{1}} - \pi_i \otimes \nabla \psi^i = \ell \underline{\underline{1}} + \varrho \mathbf{v} \otimes B_i^0 \nabla \psi^i - \sum_{\kappa=1}^{3} \boldsymbol{\sigma}_\kappa \otimes B_i^\kappa \nabla \psi^i$$
$$= \varrho \mathbf{v} \otimes \mathbf{v} - \underline{\underline{\sigma}}, \tag{3.11}$$

where I have made use of the basis representation (3.1) and of the following abbreviations:

$$\mathbf{p}^* := \sum_{\kappa=1}^{3} \sigma_\kappa^0 \mathbf{a}^\kappa, \tag{3.12}$$

$$\underline{\underline{\sigma}} := \sum_{\kappa=1}^{3} \boldsymbol{\sigma}_\kappa \otimes \mathbf{a}^\kappa - \ell \underline{\underline{1}}. \tag{3.13}$$

$\mathbf{p}^*$ is the *quasi-momentum density* and $\underline{\underline{\sigma}}$ the *stress tensor*. Furthermore the mass density ϱ is coupled with the Cosserat directors by means of

$$\varrho = \varrho(\mathbf{a}^\kappa) = \varrho_0 \, \mathbf{a}^1 \cdot (\mathbf{a}^2 \times \mathbf{a}^3). \tag{3.14}$$

In order to simplify the subsequent procedure, I assume that the basis elements B^0, B^κ depend on the field variables ψ only and that $\sigma_\kappa^0 = 0$, i.e. the

quasi-momentum density $\mathbf{p}^*$ is assumed to vanish. Consequently, the system of equations (3.1) takes the form

$$
\begin{aligned}
&\frac{\partial \ell}{\partial(\partial_t \psi^i)} = \pi_i^0 = -\varrho B_i^0(\psi), \\
&\frac{\partial \ell}{\partial(\nabla \psi^i)} = \pi_i = -\varrho B_i^0(\psi) + \sum_{\kappa=1}^{3} \boldsymbol{\sigma}_\kappa(\psi, \partial_t \psi, \nabla \psi) B_i^\kappa(\psi),
\end{aligned} \tag{3.15}
$$

with the quantities $\varrho, \mathbf{v}, \mathbf{a}^\kappa$ determined by (3.14), (3.7), (3.8). Substituting $\ell = \varrho \tilde{\ell}$ and taking

$$
\begin{aligned}
\frac{\partial \ell}{\partial(\partial_t \psi^i)} &= \varrho \frac{\partial \tilde{\ell}}{\partial(\partial_t \psi^i)}, \\
\frac{\partial \ell}{\partial(\nabla \psi^i)} &= \varrho \frac{\partial \tilde{\ell}}{\partial(\nabla \psi^i)} + \tilde{\ell} \sum_{\kappa=1}^{3} \frac{\partial \varrho(\mathbf{a}^\lambda)}{\partial \mathbf{a}^\kappa} \frac{\partial \mathbf{a}^\kappa}{\partial(\nabla \psi^i)}
\end{aligned}
$$

into consideration, the system (3.15) simplifies after division by the factor ϱ to

$$
\begin{aligned}
&\frac{\partial \tilde{\ell}}{\partial(\partial_t \psi^i)} = -B_i^0(\psi), \\
&\frac{\partial \tilde{\ell}}{\partial(\nabla \psi^i)} = -\frac{\partial}{\partial(\nabla \psi^i)} \left[\frac{1}{2}\mathbf{v}^2\right] + \sum_{\kappa=1}^{3} \left[\frac{\boldsymbol{\sigma}_\kappa}{\varrho} - \frac{\tilde{\ell}}{\varrho} \frac{\partial \varrho(\mathbf{a}^\lambda)}{\partial \mathbf{a}^\kappa}\right] \frac{\partial \mathbf{a}^\kappa}{\partial(\nabla \psi^i)}.
\end{aligned} \tag{3.16}
$$

This system of partial differential equations for $\tilde{\ell}$ can be integrated if and only if the condition

$$
\frac{\boldsymbol{\sigma}_\kappa}{\varrho} - \frac{\tilde{\ell}}{\varrho} \frac{\partial \varrho(\mathbf{a}^\lambda)}{\partial \mathbf{a}^\kappa} = -\frac{\partial u(\mathbf{a}^\lambda, \psi)}{\partial \mathbf{a}^\kappa} \tag{3.17}
$$

is fulfilled with an adequate scalar function $u = u(\mathbf{a}^\lambda, \psi)$. Then, we result in the *general analytical form* of the Lagrangian:

$$
\ell = \varrho \tilde{\ell} = -\varrho(\mathbf{a}^\kappa) \left[B_i^0(\psi) \partial_t \psi^i + \frac{1}{2}\mathbf{v}^2 + u(\mathbf{a}^\kappa, \psi)\right]. \tag{3.18}
$$

Making use of Noether's theorem with respect to time translation, the term $\varrho u(\mathbf{a}^\kappa, \psi)$ is identified as the *internal energy density*. It should be mentioned that the rough scheme (3.18) of the Lagrangian can be applied to many different physical systems in continuum mechanics!

3.2. The concrete Lagrangian for elasticity with eigenstresses

Having established the general scheme (3.18) for the Lagrangian, we have to go into more details: How many independent field variables ψ^i are necessary to

determine the state of the system and which analytical form of the yet unknown structures $B^0, B^\kappa, u(\mathbf{a}^\kappa, \psi)$ in the Lagrangian (3.18) should be used? In this paper I prefer a more heuristic treatment:

At first, we may choose the internal energy density u according to *Hooke's law* of an isotropic material

$$u = u(\mathbf{a}^\kappa) = K \ln \varrho + \frac{\mu}{2} \varrho^{-2/3} \sum_{\kappa=1}^{3} (\mathbf{a}^\kappa)^2 \tag{3.19}$$

with the *bulk modulus* K and the *shear modulus* μ. By means of Eq. (3.13), this implies the well-known form of the stress tensor:

$$\underline{\underline{\sigma}}(\mathbf{a}_\kappa) = K \varrho \underline{\underline{1}} + \mu \varrho^{1/3} \sum_{\kappa=1}^{3} \left[\mathbf{a}^\kappa \otimes \mathbf{a}^\kappa - \frac{1}{3} (\mathbf{a}^\kappa)^2 \underline{\underline{1}} \right]. \tag{3.20}$$

This formula is Hooke's law rewritten in terms of Cosserat-directors.

Secondly, in analogy with (2.25) I make a *Clebsch-ansatz*

$$\mathbf{a}^\kappa = \nabla \varphi^\kappa + \zeta^\kappa \nabla \vartheta^\kappa \tag{3.21}$$

for each of the three Cosserat directors $\mathbf{a}^\kappa$ with 9 independent potentials φ^κ, ζ^κ, ϑ^κ; $\kappa = 1, 2, 3$. Comparing (3.8) with (3.21), the three basis elements B^1, B^2, B^3 are determined. Consequently, by means of (3.4), the *dislocation density tensor* reads

$$\underline{\underline{\alpha}} = \sum_{\kappa=1}^{3} (\nabla \zeta^\kappa \times \nabla \vartheta^\kappa) \otimes \mathbf{e}_\kappa , \tag{3.22}$$

whereas according to (3.5) the *dislocation flux density tensor* takes the form

$$\underline{\underline{J}} = -\mathbf{v} \times \underline{\underline{\alpha}} + \sum_{\kappa=1}^{3} [\mathrm{D}_t \vartheta^\kappa \nabla \zeta^\kappa - \mathrm{D}_t \zeta^\kappa \nabla \vartheta^\kappa] \otimes \mathbf{e}_\kappa . \tag{3.23}$$

Until this point the considerations took only account of the symmetry properties. Equation (3.23) will be used for fitting the ansatz for the Lagrangian to real dislocation dynamics.

The model is now restricted to purely convective dislocation dynamics. Then, the first term in (3.23) is sufficient and the second term has to vanish according to a particular ansatz for the Lagrangian. Supplementing the already introduced field variables φ^κ, ζ^κ, ϑ^κ by an additional set Φ, χ_κ, γ_κ, ξ_κ of field variables, I make the ansatz

$$\ell = -\varrho \left[\partial_t \Phi + \sum_{\kappa=1}^{3} (\chi_\kappa \partial_t \varphi^\kappa + \gamma_\kappa \partial_t \vartheta^\kappa + \xi_\kappa \partial_t \zeta^\kappa) + \frac{1}{2} \mathbf{v}^2 + u(\mathbf{a}^\kappa) \right] \tag{3.24}$$

for the Lagrangian of the elastically deformed crystal with fixed dislocations. In (3.24) the mass density has to be replaced by (3.14), the quantities $\mathbf{a}^i$ and $u(\mathbf{a}^\kappa)$ by (3.21), (3.19). Finally, the quantity $\mathbf{v}$ has to be understood as

$$\mathbf{v} = \nabla\Phi + \sum_{\kappa=1}^{3} [\chi_\kappa \nabla\varphi^\kappa + \gamma_\kappa \nabla\vartheta^\kappa + \xi_\kappa \nabla\zeta^\kappa]. \tag{3.25}$$

This expression is in accordance with Eqs. (3.7) and (3.15). Thus, it turns out that $\mathbf{v}$ is the velocity field. As compared with the original Clebsch-ansatz (2.25) in (3.25), there are involved 10 potentials Φ, χ_κ, γ_κ, ξ_κ. We should not worry about this unusual potential representation: (3.25) is a straightforvard result of the theory. The essence of it is its *regauging group* which is associated with the *vortex dynamics* by means of the symmetry-balance theorem developed in Sec 2.2..

Variation with respect to $\Phi, \chi_\kappa, \gamma_\kappa, \xi_\kappa, \varphi^\kappa, \vartheta^\kappa, \zeta^\kappa$ – the free and independent fields – results in the Euler – Lagrange equations

$$\delta\Phi : \partial_t\varrho + \nabla\cdot(\varrho\mathbf{v}) = 0, \tag{3.26}$$

$$\delta\varphi^\kappa : \partial_t(\varrho\chi_\kappa) + \nabla\cdot[\varrho\chi_\kappa\mathbf{v} - \boldsymbol{\sigma}_\kappa] = 0, \tag{3.27}$$

$$\delta\vartheta^\kappa : \partial_t(\varrho\gamma_\kappa) + \nabla\cdot[\varrho\gamma_\kappa\mathbf{v} - \zeta^\kappa\boldsymbol{\sigma}_\kappa] = 0 \tag{3.28}$$

$$\delta\zeta^\kappa : \partial_t(\varrho\xi_\kappa) + \nabla\cdot[\varrho\xi_\kappa\mathbf{v}] + \boldsymbol{\sigma}_\kappa\cdot\nabla\vartheta^\kappa = 0, \tag{3.29}$$

$$\delta\chi_\kappa : -\varrho \mathrm{D}_t\varphi^\kappa = 0, \tag{3.30}$$

$$\delta\gamma_\kappa : -\varrho \mathrm{D}_t\vartheta^\kappa = 0, \tag{3.31}$$

$$\delta\xi_\kappa : -\varrho \mathrm{D}_t\zeta^\kappa = 0. \tag{3.32}$$

$\boldsymbol{\sigma}_\kappa$ is determined by Eq. 3.17). Equation (3.26) is the *mass balance* which can also be obtained via Noether's theorem with respect to the gauge transformation $\Phi \longrightarrow \Phi+\epsilon$, whereas Eqs. (3.27)–(3.32) are the essential dynamical field equations for the potentials. Making use of (3.31), (3.32) the dislocation flux density tensor (3.23) simplifies to

$$\underline{\underline{J}} = -\mathbf{v} \times \underline{\underline{\alpha}}. \tag{3.33}$$

Thus, the dynamical equations (2.12), (2.13) for the dislocations can be obtained by means of the *theorem for area-type balances* stated in Sec. 2.2.:

$$\begin{aligned} \partial_t\underline{\underline{\alpha}} + \nabla\times\left[-\mathbf{v}\times\underline{\underline{\alpha}}\right] &= 0 \\ \nabla\cdot\underline{\underline{\alpha}} &= 0. \end{aligned} \tag{3.34}$$

Obviously I am dealing with a purely convective dislocation dynamics: in terms of a microscopic picture, the dislocations are fixed at their initial lattice position. Thus, the deformations of the crystal are purely elastic ones and the Lagrangian (3.24) describes a *dynamical generalization of Kröner's static theory of eigenstresses* [5] *due to dislocations.*

4. Conclusion

By means of this paper I have shown the method of determination of a Lagrangian along the line of the inverse problem of the second kind. Noether's theorem associated with volume-type balances has been used as well as a new theorem associated with area-type balances. A Lagrangian for the convective generalization of the eigenstress theory of (fixed) dislocations opens perspectives towards a theory of moving dislocations, i.e. of plastic deformations. Investigations are in progress.

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FB 6, THEORETISCHE PHYSIK,
UNIVERSITÄT PADERBORN
Warburger Straße 100, D-33095 Paderborn, Germany.

Received October 27, 1997.

Arch. Mech., 50, 3, pp. 613–621, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

A note on kinematics of surfaces

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

M.L. SZWABOWICZ (GDAŃSK)

THE QUESTION how to describe effectively the motion of a deformable surface in ordinary Euclidean space is discussed. Two alternative formulations are supplied, both based on the assumption that the Riemannian metric of the moving surface must appear explicitly in the system describing the motion. The motivation for this assumption is to divide the variables responsible for the evolution of the intrinsic geometry (strains) of the surface from those responsible for the evolution of its extrinsic geometry (bending). Exemplary application of these results to the large deflection/small strain class of deformations of thin shells is considered.

1. Introduction

IN MECHANICS surfaces appear generally in two contexts:

(i) as boundaries of three-dimensional domains;

(ii) as an idealization of thin structures, that is objects with one dimension negligible in comparison with the other two.

The first of the above categories includes all phenomena that can be modeled by three-dimensional topological manifolds with boundary, such like interface dynamics, crystal growth and contact problems, whereas the second – all those that can be directly modeled by two-dimensional manifolds like soap films, membranes, thin plates and shells. Consequently, one faces surfaces of any topological type: most often – with boundary, frequently - closed compact, and occasionally – complete.

For problems belonging to category (i) it frequently happens that it is only the evolution of the boundary itself, and not the ambient domain, that is of main interest (capillarity, crystal growth, solidification, friction and wear). Yet, to find how the boundary evolves in time requires solving a three-dimensional differential or even integro-differential problem for the entire domain, with input data sometimes difficult to come by due to the limitations and/or obstacles in applying the measurement techniques. A remedy is to introduce a coarser, yet simpler, model founded on a geometrical approach, wherein the velocity field of the particles on the boundary or the surface energy are expressed as functionals of the physical quantities driving the evolution process:

see the monograph by KOSIŃSKI [1] on propagation of singularities in media, the article by BLINOWSKI and TRZĘSOWSKI [2] on generalized theory of capillary phenomena, the article by BROWER, KESSLER, KOPLIK and LEVINE [3] for discussion in the context of interface dynamics and papers by ZMITROWICZ [4], STRÖMBERG [5] and STARMANS, BREKELMANS and JANSSEN [6] for friction and wear problems. This step converts the original three-dimensional problem into a two-dimensional one for a surface, which allows to move it to the second category.

Problems from (ii) are posed ab initio as two-dimensional by suitable approximations of different forms of energy appearing in the phenomenon and subsequent construction of some two-dimensional constitutive equations. If the surface is deformable (and usually it is), these constitutive equations must contain the kinematical variables accounting for the influence of the actual configuration of the surface on the physical state of the body the surface models.

Once all the physical factors are enclosed in mathematical formulae, one has to cast the problem into its final form, which will then become an evolution problem on a two-dimensional topological manifold. The evolution parameter may be the time (interface dynamics), forces (statics of shells) or some other variables depending on the nature of the problem. In the course of this evolution not only the geometry but also the topology of the surface may vary (cracks, ruptures, bifurcations, branching of soap films). However, the common background is the kinematics, which in this case is the theory of immersions of two-dimensional manifolds into R^3. Thus, the optimal, from the analytical point of view, final formulation of the problem arises as a compromise between the group of equations responsible for the physics and those accounting for kinematics. At this stage the key element is the choice of primary variables, which subsequently will become the unknown functions in the systems of PDE's to be solved for some initial and/or boundary conditions. The right choice may not only facilitate the analysis by setting the problem in a form as compact as possible (say, for the fewest number of unknowns) or exposing the group of parameters dominating in the problem; it may also reveal interdisciplinary connections and analogies, which help in understanding the underlying phenomenon.

Due to the above, kinematics of a moving surface has been treated from different aspects in various places in the literature: the most recent references are [1, 3, 8, 7, 10, 9, 14, 15]. Specifically, the theory of shells contributed to the subject so abundantly that it is impossible to cite here even the most important references (take, for instance, [11] as the starting point). All the same, as the recent advances in mathematical theory of surfaces indicate [13], the subject is far from being exhausted. Below I discuss possible novel formulations of the evolution problem under the assumption that the surface metric must appear as an explicit primary variable and show how they can be applied to the large deflection/small strain theory of thin shells. This material has been treated in more detail in [9, 15].

2. Intrinsic and reduced formulations; evolution

Let our surface, moving in $\mathbf{R}^3$, be given at time t by the position vector

$$\mathbf{r} = x\mathbf{i} + y\mathbf{j} + z\mathbf{k}, \tag{2.1}$$

where $x = x(\vartheta^\alpha, t)$, $y = y(\vartheta^\alpha, t)$, $z = z(\vartheta^\alpha, t)$ are the Cartesian coordinates in some fixed in time Cartesian frame $\mathbf{i}$, $\mathbf{j}$, $\mathbf{k}$, and ϑ^α, $\alpha = 1, 2$, are convective curvilinear coordinates (i.e. $\dot{\vartheta}^\alpha \equiv 0$). Then, the local basis consists of the two tangent vectors $\mathbf{r}_{,\alpha}$ (commas denote partial derivatives with respect to the coordinates ϑ^α) and the normal to the surface $\mathbf{n}$. Let the velocity field on the surface be $\dot{\mathbf{r}} = V^\alpha \mathbf{r}_{,\alpha} + U\mathbf{n}$. For V^α and U as known functionals on the surface, the latter equation yields a quasi-linear evolution system of three PDE's for the three unknown Cartesian coordinates of the immersion $\mathbf{r}$ (see [9]). This type of formulation corresponds to the displacement formulations. Although being simple, it gives, however, no insight into what is happening with physically measurable quantities characterizing the surface (like internal distances between adjacent points or curvatures), as the motion progresses.

The intrinsic formulations lie at the other extremity. They abstract the problem of the evolution from the ambient Euclidean space. The fundamental theorem of the theory of surfaces establishes a local one-to-one correspondence between the space of non-congruent surfaces and sets of six functions $a_{\alpha\beta}$ and $b_{\alpha\beta}$ (coefficients of the metric and the second fundamental form) satisfying the compatibility conditions: the Gauss - Mainardi - Codazzi equations

$$\frac{1}{2}\varepsilon^{\alpha\lambda}\varepsilon^{\beta\mu}b_{\alpha\beta}b_{\lambda\mu} = K, \tag{2.2}$$

$$b_{\alpha\beta}|_\lambda \varepsilon^{\beta\lambda} = 0, \tag{2.3}$$

where $(.)|_\alpha$ denotes the covariant derivative, $\varepsilon^{\alpha\lambda}$ are the contravariant components of the permutation tensor and K is the Gaussian curvature. Formally, Eqs. (2.2) and (2.3), written down in maps from some atlas, form a nonlinear underdetermined system of three partial differential equations for six unknown functions of points on some two-dimensional differentiable manifold representing the topology of the surface. For a given topological type of the manifold, solutions of these equations correspond to all possible mutually homeomorphic and non-congruent configurations of the surface. By choosing any one-parameter family of such solutions (with some parameter t) and interpreting this parameter as time, we obtain a full description of a topology-preserving evolution corresponding to some motion of a surface in $\mathbf{R}^3$.

The fact that the system is underdetermined leaves a gap to be filled with additional three equations whose connotation lends a definite meaning to the whole system. In geometry these additional equations are predominantly of finite type, like in the problem of isometric bending: $\dot{a}_{\alpha\beta} \equiv 0$. In physics they are

usually systems of PDE that additionally relate the coefficients of both forms, thus closing the system. For instance, in theory of shells these are the equations of motion and in interfacial dynamics – the velocity functionals (see [3]).

The connected evolution system (see [1, 3, 7, 8] for discussion and derivation) consists of the following six PDE's:

$$\dot{a}_{\alpha\beta} = -2b_{\alpha\beta}U + V_\alpha|_\beta + V_\beta|_\alpha\,, \tag{2.4}$$

$$\dot{b}_{\alpha\beta} = U|_{\alpha\beta} - U(2Hb_{\alpha\beta} - Ka_{\alpha\beta}) + b_{\alpha\lambda}V^\lambda|_\beta + b_{\beta\lambda}V^\lambda|_\alpha + V^\lambda b_{\alpha\beta}|_\lambda \tag{2.5}$$

for six unknown functions $a_{\alpha\beta} = a_{\alpha\beta}(\vartheta^\lambda, t)$ and $b_{\alpha\beta} = b_{\alpha\beta}(\vartheta^\lambda, t)$ of points on the manifold and time. H in Eq. (2.5) denotes the mean curvature of the surface.

Although mathematically satisfactory, this system suffers from excessive, for physical applications, number (six) of equations and unknowns. A question arises: does the information about the kinematics of a moving surface have to be scattered on so many functions? Besides, the evolution of the metric informs us about the variation of the local distances between the adjacent points of the surface, but no such clear interpretation may be ascribed to the evolution of the second fundamental form.

As a remedy, we may replace the coefficients of the second fundamental form with its invariants: the mean and Gaussian curvatures, and its principal directions. The curvatures certainly bear more physical meaning than abstract functions $b_{\alpha\beta}$ (in support of this statement see [2], where the authors used this idea in connection with their considerations about the changes of surface energy under transitions of the Euler–Poincaré characteristic of the interfacial surface). Then, the Gaussian curvature may be eliminated from the system with the use of the Gauss equation (2.2). This step leads to replacement of the compatibility equations (2.2), (2.3) with a system of two nonlinear PDE's for five unknown functions: the coefficients of the metric, the mean curvature and the angle φ between a fixed convective field of directions on the surface and one of the principal directions. In [9] I have shown that if one picks the directions tangent to ϑ^1 coordinate lines to be the reference field of directions, then the corresponding evolution system consists of the following five equations:

$$\begin{aligned}\dot{a}_{\alpha\beta} = {} & -2HU\,a_{\alpha\beta} \\ & - 2\sqrt{H^2 - K}\,U(\cos 2\varphi\,\delta^\mu_\alpha - \sin 2\varphi\,\varepsilon_{\alpha\lambda}\,g^{\lambda\mu})\left(\frac{1}{a^{11}}\,\delta^1_\mu\,\delta^1_\beta - \frac{1}{a_{22}}\,a_{2\mu}a_{2\beta}\right) \\ & + V_\alpha|_\beta + V_\beta|_\alpha\,,\end{aligned} \tag{2.6}$$

$$\dot{H} = H_{,\alpha}\,V^\alpha + (2H^2 - K)U + \frac{1}{2}\,\Delta U\,, \tag{2.7}$$

$$\begin{aligned}\dot{\varphi} = {} & (\varphi_{,\alpha} + k^{\vartheta^1}_\alpha)V^\alpha + \frac{\sqrt{a}}{a_{22}}V^1|_2 + \frac{1}{2a_{22}}\sqrt{\frac{a}{H^2 - K}}\,a^{1\alpha}U|_{\alpha 2}\cos 2\varphi \\ & + \frac{1}{2\sqrt{H^2 - K}}\left[\frac{1}{a_{22}}\,U|_{22} - \frac{1}{2}\Delta U + 2(H^2 - K)U\right]\sin 2\varphi\,.\end{aligned} \tag{2.8}$$

In the above formulae Δ denotes the Laplace – Beltrami operator, $\dot{\varphi}$ is the angular velocity of the principal directions of the second fundamental form, $a = \det(a_{\alpha\beta})$ and $k_\alpha^{\vartheta^1}$ are the components of the connection vector (the co-form of the connection form in the Maurer – Cartan equations) given by the formulae:

$$\mathbf{k}^{\vartheta^1} = \frac{1}{2\sqrt{a}}\left[\left(\frac{a_{12}}{a_{22}}a_{22,1} - a_{11,2}\right)\mathbf{a}^1 + \left(\frac{a_{12}}{a_{22}}a_{22,2} + a_{22,1} - 2a_{12,2}\right)\mathbf{a}^2\right]. \tag{2.9}$$

Locally, away from an umbilical point, the evolution system (2.6)–(2.8) is completely equivalent to the original system (2.4)-(2.5). Above all, it preserves the bijective nature of the relation between the space of its solutions and the space of non-rigid motions. It still contains, however, five unknown functions.

To obtain any further reduction of the evolution system and, thus, a more compact description of motion of a surface, one may choose to decompose the motion into the part responsible for the evolution of its intrinsic geometry and the other, describing the evolution of the extrinsic geometry. This approach is particularly useful in mechanics of deformable material surfaces. Then, evolution of the intrinsic geometry is described by the strain rate, and that of extrinsic geometry corresponds to the isometric bending (the other terms in common use for this kind of motion are: pure bending, geometric bending, inextensional deformation). There are exactly two alternative ways to make description of this kind as compact as possible. Both are based on the so-called Darboux equations – two nonlinear second-order PDE derived independently by Darboux and Bianchi in connection with the problem of finding all isometric immersions of a given two-dimensional Riemannian manifold into the ordinary Euclidean space. For a fixed metric they become equations of the Monge – Ampère type, i.e. equations whose leading term is the determinant of the second covariant derivative of the unknown function.

The unknown function in the case of the first of the two equations has the interpretation of a distance function from some fixed, but otherwise arbitrary, plane in R^3. Suppose this plane coincides with the $z = 0$ plane. Then, the unknown function is exactly the z Cartesian coordinate of the immersion sought and the corresponding equation is:

$$d_z - K(1 - z_{,\alpha}\, z_{,\beta}\, a^{\alpha\beta}) = 0\,, \tag{2.10}$$

where $d_z = 1/2\varepsilon^{\alpha\lambda}\varepsilon^{\beta\mu} z|_{\alpha\beta} z|_{\lambda\mu}$ is the Monge – Ampère operator of the function z and K should be replaced with the Gauss formula expressing the Gaussian curvature of a given metric via its coefficients. Upon solving this equation, the second fundamental form of the related immersion is furnished by the formula:

$$b_{\alpha\beta} = (1 - z_{,\lambda}\, z_{,\mu}\, a^{\lambda\mu})^{-1/2}\, z|_{\alpha\beta}\,, \tag{2.11}$$

and the remaining two Cartesian coordinates x, y follow from the coefficients of the metric and the solution z via quadratures (see [9, 12]). Note that the above

set of relations provides complete information about the surface at a fixed time t in terms of just four quantities. By letting z and the metric vary with time we obtain systematic account of its evolution. Then, evolution of the metric describes the evolution of its intrinsic geometry, whereas evolution of z supplies information about the evolution of the second fundamental form and, thus, the isometric bending, as desired.

As follows from [9], the corresponding evolution system is:

$$\dot{a}_{\alpha\beta} = -\frac{2U}{\sqrt{1 - z_{,\lambda}\, z_{,\mu}\, a^{\lambda\mu}}}\, z|_{\alpha\beta} + V_\alpha|_\beta + V_\beta|_\alpha\,, \tag{2.12}$$

$$\dot{z} = V^\alpha z_{,\alpha} + U\sqrt{1 - z_{,\lambda}\, z_{,\mu}\, a^{\lambda\mu}}\,. \tag{2.13}$$

An alternative description of the evolution problem may be based on the second of the two Darboux equations after minor modifications. The unknown function in this case is the function $r = r(\vartheta^\alpha, t)$ describing the distance of the points of the surface at some moment t from some fixed, but otherwise arbitrary, point O in $\mathbf{R}^3$. Take O to be the origin of the Cartesian system. Then r is the length of the position vector and the equation is:

$$d_{r^2} - 2\Delta r^2 + K(r^2_{,\alpha}\, r^2_{,\beta}\, a^{\alpha\beta} - 4r^2) + 4 = 0\,. \tag{2.14}$$

Again, upon solving this equation the second fundamental form follows from the formula

$$b_{\alpha\beta} = \frac{1}{\sqrt{r^2 - \frac{1}{4}(r^2)_{,\alpha}\,(r^2)_{,\beta}\, a^{\alpha\beta}}}\left(\frac{1}{2}r^2|_{\alpha\beta} - a_{\alpha\beta}\right). \tag{2.15}$$

The related evolution system is:

$$\dot{a}_{\alpha\beta} = \frac{1}{r\sqrt{1 - r_{,\alpha}\, r_{,\beta}\, a^{\alpha\beta}}}(2a_{\alpha\beta} - r^2|_{\alpha\beta})U + V_\alpha|_\beta + V_\beta|_\alpha\,, \tag{2.16}$$

$$\dot{r} = V^\alpha r_{,\alpha} + U\sqrt{1 - r_{,\lambda}\, r_{,\mu}\, a^{\lambda\mu}}\,. \tag{2.17}$$

3. Application to large deflection/small strain type of thin shell theories

For purposes of demonstration let us consider how the selection of a proper description of surface kinematics may be helpful in modification of the nonlinear theory of thin shells within the class of large deflection/small strain deformations. The practical significance of this class follows from the fact that for metals, most frequently used materials in construction of thin-walled structures, the admissible strain is approximately a quantity of the order 10^{-3}. This limitation on the admissible deformations the middle surface of the shell may assume, considerably

reduces the practically accessible states of its equilibrium (see [14, 15]). Yet, this fact is nowhere visible in the framework of the classical shell theory, due to the fact that it is based on description of motion via displacements.

As I have argued in [15], to pose the problem in a form convenient for qualitative as well as quantitative analysis, it is necessary to employ one of the two descriptions of motion based on the Darboux equations. With this choice the strains appear as the primary variables in the theory. Besides, the whole extrinsic geometry of the shell's middle surface is described by a single function z or r. Thus, the shell problem is governed by a determined system of four nonlinear PDE for four unknown functions, one of them being the Darboux equation and the remaining three – the equations of motion. In view of "smallness" of strains, this system may be subsequently linearized in these three variables. This step simplifies the whole problem, because we then have to deal with a system linear in three functions and nonlinear in only one, although the whole class of nonlinear large deflection/small strain deformations is covered effectively. Besides, upon solving this system, the displacements may be computed *via* quadratures.

For demonstrative purposes, let us see how this procedure works in the simplest case of statics of thin linearly elastic shells (see [15] for a more detailed discussion). To distinguish the deformed configuration of the shell middle surface from the undeformed one, the objects pertaining to the deformed configuration are marked by overbars, e.g. $\overline{a}_{\alpha\beta}$, $\overline{b}_{\alpha\beta}$, etc. That is, for this whole section and in contradistinction to the notation from the previous one, $a_{\alpha\beta}$ are now coefficients of the metric *only* at some initial time t_0, and $\overline{a}_{\alpha\beta}$ at some later time t. Then, $\gamma_{\alpha\beta} = (1/2)(\overline{a}_{\alpha\beta} - a_{\alpha\beta})$ is the surface strain tensor, $\kappa_{\alpha\beta} = -\overline{b}_{\alpha\beta} + b_{\alpha\beta}$ is the curvature change measure and $J = \dfrac{d\overline{A}}{dA} = \sqrt{\dfrac{\overline{a}}{a}}$. It may be shown (see [15]) that with the above notation we have:

$$\overline{a}^{\alpha\beta} = \frac{1}{J}\left[(1-2\gamma)a^{\alpha\beta} + 2\gamma^{\alpha\beta}\right], \tag{3.1}$$

where $\gamma = \operatorname{tr}(\boldsymbol{\gamma})$,

$$\overline{\varepsilon}_{\alpha\beta} = J\,\varepsilon_{\alpha\beta}\,, \qquad \overline{\varepsilon}^{\alpha\beta} = J^{-1}\varepsilon^{\alpha\beta}, \qquad J^2 = 4\det(\boldsymbol{\gamma}) + 2\gamma + 1\,. \tag{3.2}$$

Besides, the Christoffel symbols in both configurations are related by the formula

$$\overline{\Gamma}^{\lambda}_{\alpha\beta} - \Gamma^{\lambda}_{\alpha\beta} = \overline{a}^{\,\lambda\mu}\gamma_{\mu\alpha\beta}\,, \qquad \text{where} \quad \gamma_{\mu\alpha\beta} = \gamma_{\mu\alpha}|_{\beta} + \gamma_{\mu\beta}|_{\alpha} - \gamma_{\alpha\beta}|_{\mu}\,. \tag{3.3}$$

Now use the above to pull the Darboux equation (2.10) from the deformed configuration to the undeformed one and subsequently, to linearize the result in $\gamma_{\alpha\beta}$. This leads to the equation

$$d_{\overline{z}} - [\overline{z}|_{\alpha\beta} - (\Delta\overline{z})a_{\alpha\beta}]\,\overline{z}_{,\lambda}\,\gamma^{\lambda\alpha\beta} - \left(\gamma^{\lambda\mu}|_{\lambda\mu} - \Delta\gamma\right)\left(1 - \overline{z}_{,\alpha}\,\overline{z}_{,\beta}\,a^{\alpha\beta}\right) - K\left\{1 - \overline{z}_{,\alpha}\,\overline{z}_{,\beta}\left[a^{\alpha\beta}(1+\gamma) - 2\gamma^{\alpha\beta}\right]\right\} = 0, \tag{3.4}$$

which is a second-order PDE, linear in strains and nonlinear in the function $\overline{z}$ – a Cartesian coordinate of the deformed shell middle surface. By assumption, this equation approximates the kinematics of the shell middle surface in the neighborhood of its undeformed state for sufficiently small strains and their derivatives, but arbitrary bendings. To obtain a determined system of equations, we need three further equations relating our four unknown functions. These are granted by the balance conditions.

Suppose we have derived the balance conditions from the virtual work principle by routine variational methods, starting from the strain energy density of the form $\mathcal{W} = \mathcal{W}(\gamma_{\alpha\beta}, \kappa_{\alpha\beta})$ (if $\mathcal{W}$ is a quadratic function of its arguments, we get the Koiter–Sanders first approximation theory). Then, the resulting Lagrangian equilibrium equations take the form

$$
\begin{aligned}
(3.5)\qquad & \left(-\frac{\partial \mathcal{W}}{\partial \gamma_{\alpha\beta}} + \overline{b}^{\alpha}_{\lambda}\frac{\partial \mathcal{W}}{\partial \kappa_{\lambda\beta}}\right)\Big|_{\beta} + \overline{b}^{\alpha}_{\lambda}\frac{\partial \mathcal{W}}{\partial \kappa_{\lambda\beta}}\Big|_{\beta} + \left[\left(-\frac{\partial \mathcal{W}}{\partial \gamma_{\alpha\mu}} + 2\overline{b}^{\alpha}_{\lambda}\frac{\partial \mathcal{W}}{\partial \kappa_{\lambda\mu}}\right)\overline{a}^{\beta\nu}\right. \\
& \left. + \left(-\frac{\partial \mathcal{W}}{\partial \gamma_{\mu\beta}} + \overline{b}^{\mu}_{\lambda}\frac{\partial \mathcal{W}}{\partial \kappa_{\lambda\beta}}\right)\overline{a}^{\alpha\nu} + \overline{b}^{\alpha}_{\lambda}\frac{\partial \mathcal{W}}{\partial \kappa_{\lambda\beta}}\overline{a}^{\lambda\nu}\right]\gamma_{\nu\beta\mu} + p^{\alpha} = 0, \\
(3.6)\qquad & -\frac{\partial \mathcal{W}}{\partial \kappa_{\alpha\beta}}\Big|_{\alpha\beta} - \left[\left(\frac{\partial \mathcal{W}}{\partial \kappa_{\alpha\mu}}\overline{a}^{\beta\lambda} + \frac{\partial \mathcal{W}}{\partial \kappa_{\mu\beta}}\overline{a}^{\alpha\lambda}\right)\gamma_{\lambda\alpha\mu}\right]\Big|_{\beta} \\
& + \left(-\frac{\partial \mathcal{W}}{\partial \gamma_{\alpha\beta}} + \overline{b}^{\alpha}_{\lambda}\frac{\partial \mathcal{W}}{\partial \kappa_{\lambda\beta}}\right)\overline{b}_{\alpha\beta} \\
& - \left[\frac{\partial \mathcal{W}}{\partial \kappa_{\lambda\beta}}\overline{a}^{\alpha\mu} + \left(\frac{\partial \mathcal{W}}{\partial \kappa_{\lambda\psi}}\overline{a}^{\beta\varphi} + \frac{\partial \mathcal{W}}{\partial \kappa_{\psi\beta}}\overline{a}^{\lambda\varphi}\right)\gamma_{\varphi\lambda\psi}\overline{a}^{\alpha\mu}\right]\gamma_{\mu\alpha\beta} + p = 0,
\end{aligned}
$$

where p^{α} and p account for the contributions from the external loads. Now, replace in the above $\overline{a}^{\alpha\beta}$ and $\overline{b}^{\alpha\beta}$ with the right-hand sides of (3.1) and (2.11), respectively. The two equations (3.5) are of the order three in $\overline{z}$ and two in $\gamma_{\alpha\beta}$, and the equation (3.6) – of the order four in $\overline{z}$ and three in $\gamma_{\alpha\beta}$. Therefore, linearization in $\gamma_{\alpha\beta}$ transforms them into the following three PDE:

$$
\mathcal{H}^{\alpha} + \mathcal{H}^{\alpha\kappa\lambda}\gamma_{\kappa\lambda} + \mathcal{H}^{\alpha\kappa\lambda\mu}\gamma_{\kappa\lambda}|_{\mu} = 0, \tag{3.7}
$$

$$
\mathcal{V} + \mathcal{V}^{\alpha\beta}\gamma_{\alpha\beta} + \mathcal{V}^{\alpha\beta\lambda}\gamma_{\alpha\beta}|_{\lambda} + \mathcal{V}^{\alpha\beta\lambda\mu}\gamma_{\alpha\beta}|_{\lambda\mu} = 0. \tag{3.8}
$$

The tensor coefficients $\mathcal{H}$ and $\mathcal{V}$ in the above are nonlinear functions of: the derivatives of $\overline{z}$ (up to the third order in the case of $\mathcal{H}$ and fourth of $\mathcal{V}$), the parameters of the undeformed configuration $a_{\alpha\beta}$ and $b_{\alpha\beta}$, material constants, and the external loads (for large deformations they may depend on the configuration and, therefore, they may enter all of the coefficients). Their precise form will depend on the physical model of the shell material and the external loads applied to the shell.

Acknowledgments

This work was supported by the State Committee for Scientific Research, KBN grant No. 7 T07A 025 09.

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INSTITUTE OF FLUID-FLOW MACHINERY
POLISH ACADEMY OF SCIENCES, GDAŃSK, POLAND
e-mail: mls@imppan.imp.pg.gda.pl

Received October 6, 1997.

Arch. Mech., 50, 3, pp. 623–627, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

The Maxwell rule in phase-transitions

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

C. TRIMARCO (PISA)

THE MAXWELL RULE, also known as the rule of equal areas, represents a basic notion in the phase transition processes. Although the rule might need amending for solids, it is treated as unquestionable for fluids. This belief relies on a thermodynamical argument. Namely, that the Gibbs thermodynamical potential should remain stationary during the transition process. Surprisingly, from the same thermodynamical argument, the Maxwell rule can be invalidated, even for fluids. Nonetheless, a revised form of the rule can be proposed.

1. Introduction

THE MAXWELL RULE applies to the pressure-volume or, in solids, to the stress-strain isothermal diagrams of materials undergoing a phase transition process. With specific reference to the Van der Waals equation [1–5], the liquid-vapour transition possibly occurs in the oscillating branch of the (P, V) state diagram. The rule states that: the state points of the (P, V) isothermal diagram have to be aligned along a horizontal isobaric segment during the transition. This segment divides the oscillating branch of the Van der Waals isothermal curve into two lobes of equal areas.

The rule can be easily extended to any phase transition.

A complementary method for phase transitions in solids and fluids deals with the isothermal families of the free energy diagrams [2]. The phase transition is believed to occur whenever the free energy loses the convexity property in one of its arguments. In this case, the linear convexity of the free energy is assumed to account for the phase transition process. Such a procedure is also known as the *method of the tangent* and is widely employed by metallurgists [2–6]. The method of the tangent and the Maxwell rule turn out to be equivalent one to the other as they represent two aspects of the same idea [6, 9]. Both rely on the stationarity of the Gibbs thermodynamical potential. However, the equivalence may fail whenever two different forms of the free energy, one for each phase respectively, exist. More epecifically, the temperature dependence of the free energy may differ in the two phases whereas the volume dependence may not. From the mathematical standpoint, in this case the free energy is a continuous but not necessarily differentiable function of the temperature. From the physical

standpoint, one notices that the isothermal pressure-volume diagrams alone may show a deficiency in describing the process. Information about the specific heat in the two phases may also be of primary importance.

2. The Gibbs identity

The Maxwell rule is based on the Gibbs identity [2]. For homogeneous processes in simple fluids [10], the identity reads:

$$d\mathcal{E} = -P\,dV + T\,dS. \tag{2.1}$$

$\mathcal{E}$ represents the internal energy, P the pressure, V the specific volume, T the temperature, S the entropy. The identity (2.1) suggests that $\mathcal{E}$ should be understood as a differentiable function of V and S, P, by contrast, is usually given as a function of V and T in order to be consistent with the experimental diagrams. Thus, one is inclined to choose V and T rather than V and S as independent variables. Accordingly, the integrability conditions read:

$$\begin{aligned} \left.\frac{\partial \mathcal{E}}{\partial V}\right|_T &= T \left.\frac{\partial P}{\partial T}\right|_V - P\,, \\ \left.\frac{\partial P}{\partial T}\right|_V &= T \left.\frac{\partial S}{\partial V}\right|_T . \end{aligned} \tag{2.2}$$

One can introduce the free energy $\mathcal{F}(V,T) \equiv \mathcal{E} - TS$ by a Legendre transformation so that the following meaningful expressions

$$-P = \frac{\partial \mathcal{F}}{\partial V} \qquad \text{and} \qquad -S = \frac{\partial \mathcal{F}}{\partial T} \tag{2.3}$$

are attained.

By performing again a Legendre transform, one can introduce the Gibbs thermodynamical potential $G(P,T) = \mathcal{F} + PV$. Such a quantity is very useful for phase transition processes which occur at the thermomechanical equilibrium. In fact, as pressure and temperature do not vary during the process, G must also remain constant accordingly.

3. The Maxwell rule

During a process of phase transition there are regions in which two (or more) phases coexist [1–6]. In such regions the validity of an *a priori* settled constitutive law generally fails. By examining the experimental (P,V,T) diagrams of the related processes one may note that a bounded domain corresponds to such regions [1]. In such a domain any branch of the constitutive curves has to be

replaced by isobaric curves. Unfortunately, the boundary of this domain is *unknown*. The related thermomechanical problem is mostly concerned with finding this boundary. In the isothermal (P, V) diagrams the required boundary reduces to two points which have to be horizontally aligned along an isobaric segment. These two points are uniquely found by appealing to the stationarity condition for the Gibbs potential [1–6].

Having denoted by A and B the two boundary-points of interest in the isothermal (P, V) diagrams, one can write the following equation:

$$G_B - G_A \equiv \mathcal{F}_B - \mathcal{F}_A + \overline{P}(V_B - V_A) = 0. \tag{3.1}$$

Notice that $P_A = P_B \equiv \overline{P}$, according to the previous assumptions.

$\mathcal{F}_B - \mathcal{F}_A$ can be evaluated along the isothermal path $P(V, T_0)$, $V \in (V_A, V_B)$, $T_0 \equiv$ constant. More specifically:

$$\mathcal{F}_B - \mathcal{F}_A = \int\limits_{(V_A, T_0)}^{(V_B, T_0)} \left.\frac{\partial \mathcal{F}}{\partial V}\right|_{T_0} dV = -\int\limits_{V_A}^{V_B} P(V, T_0)\, dV. \tag{3.2}$$

Note that

$$-\left.\frac{\partial \mathcal{F}}{\partial V}\right|_{T_0} \equiv P(V, T_0).$$

The unknowns $\overline{P}$, V_A and V_B are uniquely found by Eq. (3.1) with reference to the (P, V) diagrams.

A geometrical interpretation of Eq. (3.1) in the (P, V) isothermal diagram leads to the Maxwell rule of equal areas.

The weak point of these arguments resides in the choice of the path for the integral on the r.h.s. of the expression (3.2). In fact, the free energy is there evaluated along the isothermal branch of a curve which includes the so-called *spinodal region* (pressure increasing with increasing volume). Such a branch does not represent *physically reversible processes*. A possible different choice may be that of performing the path integral along any other path out of the transition region. Such a path needs not be an isothermal curve; it is only required to represent a reversible process whose initial and final states are at the same temperature and pressure.

Assume now that the proposed path of integration crosses the border between the pure phase domains in the (T, V) diagram. The free energy may change its form in the temperature dependence passing across such a border. As the border is *a priori known*, one is able to evaluate the path-integral of interest.

In the specific case of the V.d.W. curves one achieves the following final result:

$$\mathcal{F}_B^* - \mathcal{F}_A = -\int\limits_{(V_A, T_0)}^{(V_B, T_0)} P(V, T(V))\, dV + \lambda(T_0). \tag{3.3}$$

The superscribed star in $\mathcal{F}_B^*$ stresses the different form of $\mathcal{F}_B^*$ with respect to $\mathcal{F}_A$.

The reader interested in further details is referred to the paper by KAHL [7].

The expressions (3.2) and (3.3) differ from each other by the amount $\lambda(T_0)$. Should the two forms of the free energy coincide, $\lambda(T_0)$ would vanish. In this circumstance the equivalence between the aforementioned expressions is completely recovered. The quantity $\lambda(T_0)$ is related to the different forms of the specific heat in the two pure phases.

One can summarize the result by remarking the following. The free energy $\mathcal{F}$ is continuous across the border between the pure phases, but possibly not differentiable with respect to temperature; at least, not twice differentiable.

The expounded argument can be extended to any two-phase diagram, provided that no hysteresis occurs and no progress of transition fronts [4, 6, 8, 9] takes place. The Gibbs thermodynamical potential still remains stationary, though the Maxwell geometrical rule of equal areas may not hold any longer. Nevertheless, an amendment to the Maxwell rule can be proposed in the presence of *spinodal regions*. The amended rule could be restated as follows: the areas of the cut lobes are possibly unequal but may differ from one another by a quantity which depends only on the temperature.

4. Final comments

The Maxwell rule can be questioned even for the classical Van der Waals diagrams for fluids. The failure of such a basic rule can be attributed to the two different forms the free energy may exhibit in the two phases.

In solids and in crystals the phase transition processes can be much more involved. For thermoelastic materials, the free energy depends on the strain (a second order tensor) whereas in fluids the only geometrical quantity considered is the specific volume (a scalar quantity). The strain addresses the geometrical compatibility conditions and, in turn, the notion of *coherence* [2–4, 6, 8, 9]. Additional remarkable differences can be envisaged with respect to fluids. In fact, the notions of *natural state*, of *self-strain* and of *strain energy* may be relevant in solids. By contrast, they are meaningless in fluids. Such notions lead to different forms of the free energy, each for one of the pure phases, even in the simplest one-dimensional problems of phase transition [6, 9].

Hence, the validity of the Maxwell rule is once more undermined.

Acknowledgments

This work was supported by GNFM of CNR.

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DIPARTIMENTO DI MATEMATICA APPLICATA "U.DINI",
UNIVERSITA DI PISA, PISA, ITALY.

Received October 10, 1997.

Arch. Mech., 50, 3, pp. 629–644, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

Diffusion

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

Ł.A. TURSKI (WARSZAWA)

THE CLASSICAL FIELD of statistical mechanics – the theory of diffusion processes – is still offering considerable challenge when the physical problems to be described by it are more "realistic" than those easily envisioned as simple random walk. In this lecture I shall present our recent results on diffusion processes in two wide classes of physical problems: i) Diffusion in dense quasi-two-dimensional adsorbates on surfaces of the crystals, where the interparticle interactions and the interaction with the host solid cannot be neglected and play a mutually complementary role. These phenomena can be conveniently called the dynamics in $d = 2 + 1$ dimensions. ii) Diffusion in the crystals containing topological (line) defects, such as dislocations and disclinations. I shall present our results on use of the combined continuum theory of defects and the path integral approach to description of such diffusion processes. Possibility of generalization of these models for quantum particles will also be outlined.

1. Introduction

THE PHYSICAL PROCESS which keeps the fragrance producers and sellers in their lucrative business is the diffusion. Indeed, it is slow motion of the concentration profile, as compared to the thermal speed of a gas particle, which keeps the fragrance particle component close to our body. It also prevents the smell of burned bacon, or bouquet of just opened bottle of *Frankenwein*, from filling the interior of the house instantaneously. The slowness and the persistence of the diffusion is one of the reasons why this dynamical process is of such an importance in various branches of biology [1].

The theory of diffusion appears to be a mature field. Close scrutiny, however, reveals that it is still in the developing stage particularly when one attempts to describe phenomena, which albeit on the first glance are not that much different from the other "diffusion" processes, nevertheless, show dramatic differences from the textbook definition of diffusion as the long–time large–distances limit of the random walk. In this lecture I shall discuss two classes of such problems related to two fields of solid state physics: surface physics and theory of imperfect solids. Both of them can play an important role in analysis of the crystal growth phenomena, no attempts, however, will be made to discuss these potential applications in greater detail.

The plan of my lecture is then as follows. In the following Sec. 2, I shall present a brief account of our recent extensive work on the use of a novel statistical mechanics technique – the local mean field theory – to the description of the diffusion on the surface of a solid. In particular I shall discuss recent attempt to formulate a theory of diffusion in dense adsorbates, in which, due to adparticle interactions, one observes mutual competition between the flow and hopping characteristics of particle dynamics. In Sec. 3, I shall review our extensive work on the simple diffusion in the medium containing random arrangement of topological defects, i.e. dislocations and disclinations. I shall show that in this case, the long time and long distance limit of the mean square displacement of a particle is no longer proportional to time and that diffusion might show nonmarkovian character. In some special and highly idealized situations it may even exhibit Sinay-like behavior in more than one dimension. In Sec. 4, I shall very briefly discuss the problem of a single quantum particle moving on a lattice with topological defects. This section serves as an introduction to our recent and ongoing work in that field.

2. Surface diffusion

When a freshly cleaved surface of a crystal is exposed to an ambient gas, some of the gas particles get stuck to the surface in a process which we call adsorption. The adatoms do not get just to any point on the surface but to its specific points, called adsorption sites, which form a $d = 2$ lattice with structure not necessarily the same as the crystallographic structure of crystal surface. Formation of an adsorbate is a complex phenomenon, particularly since in most of the circumstances, electronic degrees of freedom of the adatoms are mixed with these of the host solid providing chemical-like binding between adatoms and the crystal. I shall restrict myself to seemingly simpler situation of a *physisorption*, that is when the chemical structure of adatom remains intact throughout the formation, equilibration and future dynamical history of the adsorbate. As we shall see, this is a sufficiently rich model to analyze fundamental problems of the diffusion theory [2–4]. It is a very important model, for it permits us to asses how the intricacies of interactions between the adsorbed particles and the host solid, mediated by solid phonons (both bulk and surface) can be handled in description of the dynamical properties of the adsorbates. Understanding of particle migration over the solid surface is also of considerable applied interest, for example the particle diffusion, along the surface of growing crystal, might change the morphological mode of the crystal growth [5]. In this lecture I shall be mostly concerned with fundamental aspects of the surface diffusion, particularly for dense adsorbates, when mutual interactions among the adsorbate particles cannot be neglected. The wealth of phenomena in dense adsorbates becomes enormous, offering possibility of studying transitions from localized (registered and nonregistered) phases

to orientationally ordered (hexatic) fluids to two-dimensional fluid layers. Their extensive discussion can be found in the recent collection of articles [2]. In some sense these are $2+1$ dimensional systems, that is they permit us to see how the truly three-dimensional properties of the system are turned off and replaced by two-dimensional ones.

How do we describe diffusion in the adsorbates? Conventionally the starting point would be the kinetic lattice gas approach in which one postulates certain equation of motion for the multiparticle probability distribution function of finding $n_{\mathbf{R}}, n_{\mathbf{R}'}, \ldots$ particles at lattice sites $\mathbf{R}, \mathbf{R}', \ldots$ at a given instant of time – $P(\{n_{\mathbf{R}}\}, t)$. This equation, called the *Master* equation, is difficult to derive from the first principles for the lattice gas model does not have its own, endogeneous, dynamics. In contrast, the static properties of the lattice gas, and *eo ipso* these of modeled adsorbate, are fully determined by:

1) the lattice gas Hamiltonian, conveniently and conventionally written as:

$$\mathcal{H}(\{n_{\mathbf{R}}\}) = -\sum_{\mathbf{R},\mathbf{R}'} J_{\mathbf{R},\mathbf{R}'} n_{\mathbf{R}} n_{\mathbf{R}'} + \sum_{\mathbf{R}} V(\mathbf{R}) n_{\mathbf{R}} \,, \tag{1}$$

where the "exchange integral" $J_{\mathbf{R},\mathbf{R}'}$ describes the interparticle interactions and $V(\mathbf{R})$ is the on-site potential, describing, for example, binding of the particle to the host solid;

2) the choice of the ensemble used in the evaluation of the statistical sum; that is deep physical insight into what are the proper constraints imposed on the system.

To describe the lattice gas dynamics we must supply it with a model dynamics given by the master equation of the form:

$$\begin{aligned} &\partial_t P(\{n_{\mathbf{R}}\}, t) \\ &\quad = \sum_{\{n'_{\mathbf{R}}\}} W(\{n_{\mathbf{R}}\}, \{n'_{\mathbf{R}}\}) P(\{n'_{\mathbf{R}}\}, t) - \sum_{\{n'_{\mathbf{R}}\}} W(\{n'_{\mathbf{R}}\}, \{n_{\mathbf{R}}\}) P(\{n_{\mathbf{R}}\}, t) \,, \end{aligned} \tag{2}$$

with the properly chosen transition amplitudes W, which are functionally dependent on the occupations $\{n_{\mathbf{R}}\}$. The only guiding principles we have in constructing these transition amplitudes are: our knowledge of underlying physics (which might be far from complete) and the detailed balance condition. The later assures that all the solutions of Eq. (2) tend asymptotically to the equilibrium solution $P^{\mathrm{eq}}(\{n_{\mathbf{R}}\}) \propto \exp(-\beta \mathcal{H}(\{n_{\mathbf{R}}\}))$.

As it stands, Eq. (2) presents formidable, and with exception of simple cases, unsolvable, mathematical problem. Variety of approximate schemes have been advocated in the literature. In a series of publications [6–8] we have proposed a new method to analyze such an equation which uses so-called local mean field approximation. We found our method to be quite useful for moderately dense adsorbates with attractive interactions, for which a good agreement can be obtained

between predictions of our model [7] and Monte Carlo simulation results [9]. For systems with repulsive interactions [8] we have obtained sensible agreement between our prediction for the behavior of the diffusion coefficient in the 2×2 ordered region of the phase diagram, shown in Fig. 1, and the reported experimental data. In Fig. 2 we have shown the behavior of the diffusion coefficient as a function of the lattice gas density plotted for various values of the temperature, corresponding to ordered and disordered region of the phase diagram in Fig. 1.

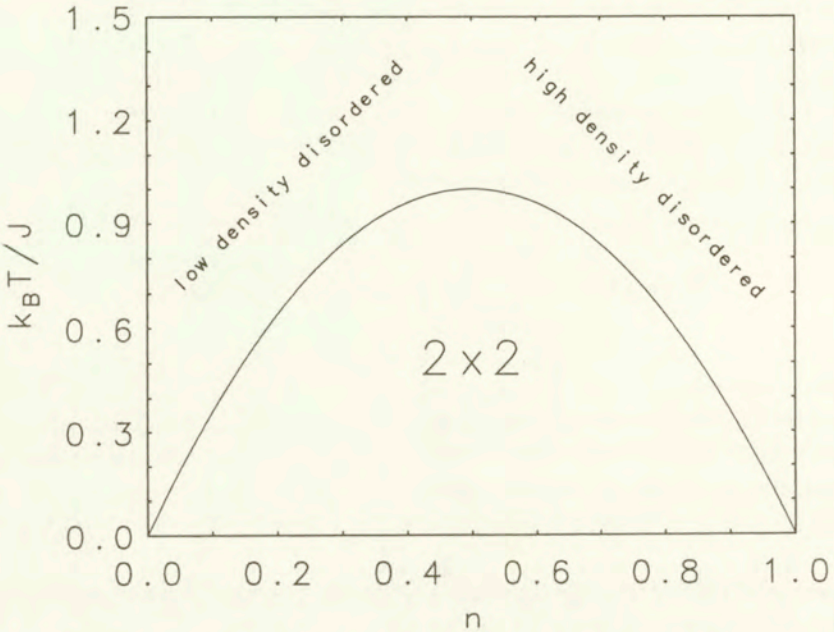

FIG. 1. The mean field phase diagram for lattice gas with repulsive interactions.

In spite of this progress one easily recognizes that the lattice gas models suffer from a serious drawback, namely they cannot account for any *flow* properties of the dense adsorbate. When the density of adsorbate increases, particularly above that of a monolayer, fluid-like properties of the adsorbate gain importance, diffusion ceases to be hopping-like, and the kinetic lattice gas approach becomes deficient. To analyze such situations we have proposed in Ref. [10] a fluid-like mesoscopic model which takes into account details of dynamic (phonon mediated) interactions between the adsorbate and the host solid. This model results in a hydrodynamic-like equations for the adsorbate fluid. These equations describe the fluid flow for which the momentum is not conserved on account of a single particle friction term violating the Gallilean invariance of the model containing new "transport" coefficient $\check{\zeta}$. This breakdown of conservation law for momentum emerges from the fully Gallilean invariant original model after phonons are projected out and transient in time terms are averaged out. This procedure effectively assumes that the host solid is "infinitely" heavy, and that

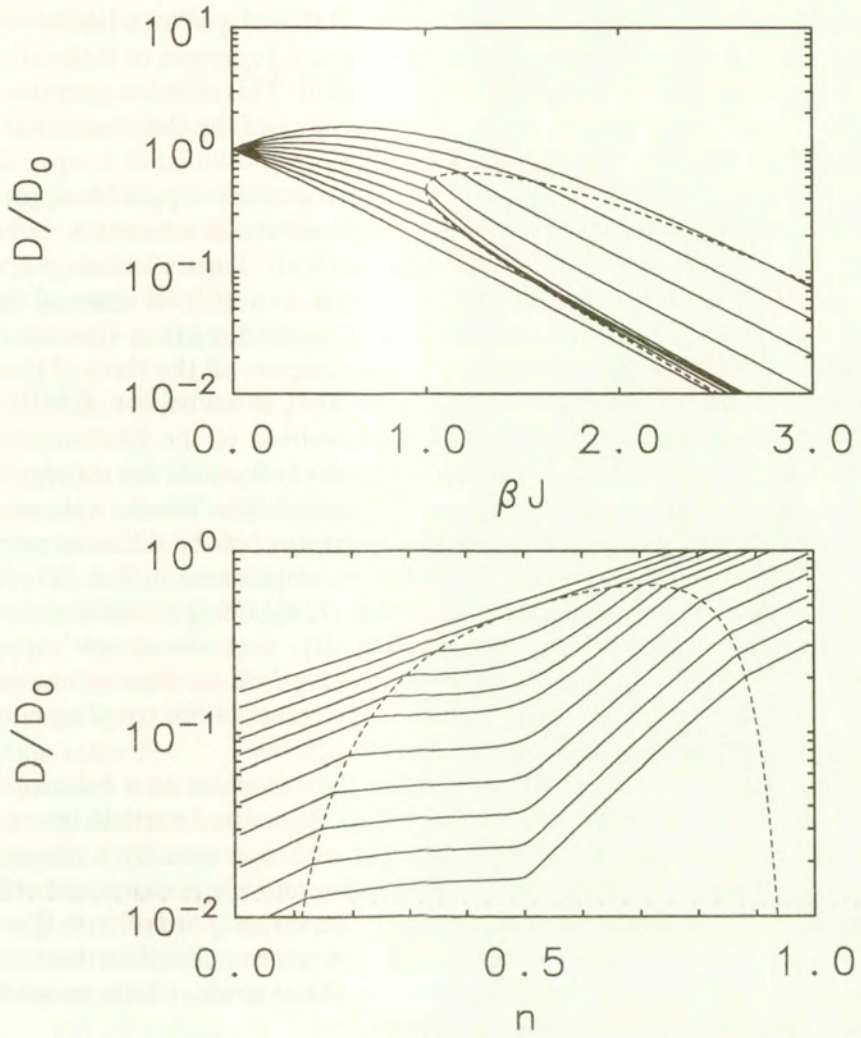

FIG. 2. a. Diffusion coefficient of the interacting lattice gas D/D_0 versus βJ. Adsorbate concentrations n decrease by 0.1, from $n = 0.9$ for the topmost line down to $n = 0.1$ for the lowest one. b. Adsorbate concentration dependence of D/D_0. Parameter βJ increases by 0.1 from $\beta J = 0.9$ for the topmost line up to $\beta J = 1.4$ and then by 0.2 up to 3.0 for the lowest one. $V = 1.5J$ and $D_0 = \nu_0 z/2d$ in both panels.

its center of mass can "absorb" arbitrary amount of momentum restoring the overall Gallilean invariance.

This new hydrodynamic picture of the dense adsorbate dynamics is difficult to use. In order to see how it can be utilized in practice we have created its toy version [11] based on the cellular automata paradigm [12–14]. The cellular automata models explore the complementary to lattice gas feature of the lattice models concentrating entirely on the velocity degrees of freedom of the migra-

ting particles. The important role in the model [11] is played by a lattice collision operator constructed such as to mimic the physical processes of interaction between the adatom and the phonons of the host solid. This collision operator turns out to be closely related to cellular automata version of the Boltzmann – Lorentz model, well known from the classical kinetic theory.

As we have discussed it above, we do have three different possible approaches to the analysis of the seemingly simplest problem of the adsorbate dynamics, namely the diffusion processes. Each of the methods, kinetic lattice gas, mesoscopic density functional, and cellular automaton, can address some of the features of the adsorbed dynamics and fails to account for the other. Can one devise a model which will, within some limitations, encompass all the three of them? In a recent paper [15] we have proposed a model which, as we believe, does actually this. The basic ingredient of our model is generalized to the $2d$-dimensional μ space master equation which in well defined limits reduces to the standard form of master equation [7] or to the Boltzmann – Lorentz-like kinetic equation [11]. We have shown that our model provides a description of the diffusion processes in which fluid – like characters of the processes, emphasized in Ref. [10, 11] are combined with the hopping mechanism of Ref. [7, 8]. Using suitable generalization of the local mean field analysis from Ref. [7], we derive a new expression for the diffusion coefficient which permits us to analyze its dependence on several parameters, like temperature, density and a value of the coupling constant measuring the strength of mutual particle interactions.

Within the model of Ref. [15] we envisage the adsorbate as a d-dimensional, classical, many-particle system dense enough so the mutual particle interactions cannot be neglected. We describe the state of such a system by a μ-space distribution function $F(\mathbf{r}, \mathbf{v}, t)$ where $\mathbf{r}$ and $\mathbf{v}$ denote particle position and velocity, respectively. The customary normalization of $F(\mathbf{r}, \mathbf{v}, t)$ is $\int d\mathbf{r}d\mathbf{v}F(\mathbf{r}, \mathbf{v}, t) = N_{\text{tot}}$, where N_{tot} is the total number of particles in the system. This distribution function obeys the generalized master equation in the μ-space, which we postulate in accord with two fundamental requirements.

The first one is that this equation reduces to the well known master equation for a lattice gas (in the continuum limit) when the velocity degrees of freedom of particles are "averaged out". This means that in some limit, discussed below, the diffusion process described by our new model has to reduce to that discussed in Ref. [7]. The second requirement is that in the opposite limit, when fluid properties of the system are of greater importance than the hopping ones embodied in master equation of Ref. [7], we recover the description provided either by mesoscopic model of Ref. [10] or by the cellular automaton model [11]. This in turn implies that the master equation in the μ-space must bear a similarity to the Boltzmann–Lorentz kinetic equation, an essential ingredient of the model in Ref. [11]. The third condition imposed on our model is that it must take into account mutual interactions between particles in such a way as to make the applications of the local mean field model discussed in Ref. [7] possible.

The master equation, which fulfills the above conditions reads:

$$\partial_t F(\mathbf{r},\mathbf{v},t) = -\mathbf{v}\cdot\nabla F(\mathbf{r},\mathbf{v},t) + \widehat{W}\{F\}\,. \tag{3}$$

To construct the operator $\widehat{W}$ we follow the lattice gas parlance and consider the full μ space distribution as a cell variable. The μ-space cells are constructed by splitting the configuration space into (quasi) lattice with a spacing a, and letting a particle in each configuration space cell to explore the entire momentum (or velocity) space.

The operator $\widehat{W}$ acting on the phase space function $F(\mathbf{r},\mathbf{v},t)$ can be written down explicitly in the following form:

$$\widehat{W}F(\mathbf{r},\mathbf{v},t) = \phi_B(\mathbf{v})\int d\mathbf{v}' \sum_{\mathbf{a}} \Gamma(\mathbf{r}+\mathbf{a},t)F(\mathbf{r}+\mathbf{a},\mathbf{v}',t) - z\Gamma(\mathbf{r})F(\mathbf{r},v,t)\,, \tag{4}$$

where $\phi_B(\mathbf{v})$ is the Maxwell–Boltzmann distribution function. The sum in Eq. (4) runs over all z nearest neighbors of the particle located at a site $\mathbf{r}$. The coefficients Γ are the transition rates for particle short range "jumps" between the sites $\mathbf{r}$ and $\mathbf{r}+\mathbf{a}$. Equation (4) resembles closely the generalization of the Boltzmann–Lorentz collision operator [15]. Indeed, replacing Γ's by averaged values and replacing $\phi_B(\mathbf{v})\int d\mathbf{v}'$ by the integral operator averaging velocities over the surface of a unit sphere in the velocity space, we obtain the Boltzmann–Lorentz operator. In a general case, the operator $\widehat{W}$ is nonlinear due to the F dependence of the transition rates Γ.

To proceed with analysis of Eq. (4) we follow our version of the local mean field theory discussed in length in Refs. [6, 7]. In this procedure one is replacing the many-body master equation by an effective single particle one in which the transition rates are functionally dependent on a single-site effective field which is randomly distributed. The effective master equation has to obey the H-theorem, thus for each realization of the local field distribution the density differs from its global mean value ρ_0 by a factor $\propto \Gamma^{-1}$:

$$\rho(h) = \Gamma^{-1}(h)\frac{\rho_0}{\int dh f(h)\Gamma^{-1}(h)}\,, \tag{5}$$

where $\Gamma(h)$ is the effective transition rate which depends on the value of the local field h, and $f(h)$ is the field distribution. The main point is now how one gets the field distribution $f(h)$. The explicit mean field procedure for the construction of $f(h)$ was provided in our earlier work Ref. [6, 7], we quote here only the final result. Denoting by $\subset A \supset = \int dh f(h)A(h)$ the average over the random local field, we obtain the following expression for the diffusion coefficient [15]:

$$D = \frac{a^2}{\subset \Gamma^{-1} \supset} + \frac{c^2 \subset \Gamma^{-2} \supset}{\subset \Gamma^{-1} \supset} = D_{\text{hopping}}\left(1 + \frac{c^2}{a^2} \subset \Gamma^{-2} \supset\right), \tag{6}$$

where D_{hopping} is the value of the diffusion coefficient following the kinetic lattice gas model discussed in Ref. [7] and at the beginning of this section.

The above equation combines two contributions to the diffusion process: the one which is due to fluid – like properties of the system and that which is due to its lattice gas properties. It is the inverse averaged transition rate dependence of this coefficient which makes a comparison with the Monte Carlo data in our recent work [7] so effective.

Following the analysis from [7], one can obtain from Eq. (6) the following „engineering"-like expression for the diffusion coefficient

$$D = D_0 \left[\exp[-\rho_0 z(e^{\beta J} - 1)] + AT \exp[\rho_0 z e^{\beta J}(e^{\beta J} - 1)] \exp[2\beta V]\right], \tag{7}$$

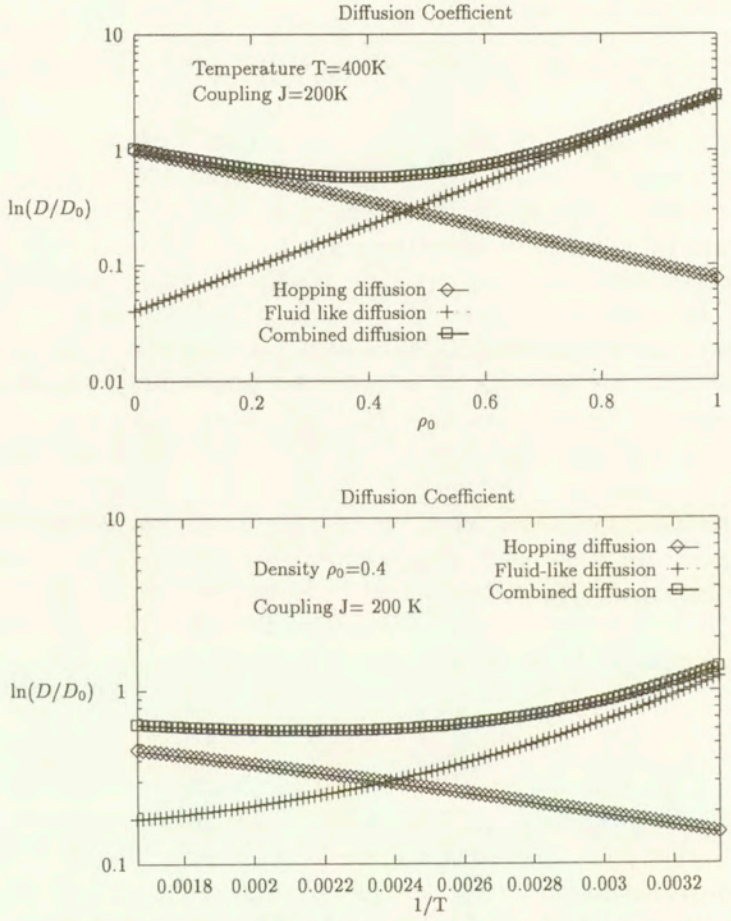

FIG. 3. a. Diffusion coefficient for $T = 400$ K plotted as a function of density ρ_0. The dotted line is for pure lattice gas model, the dashed one is the "fluid" contribution to the diffusion coefficient, and the solid one is the total diffusion coefficient. b. Diffusion coefficient for density $\rho_0 = 0.4$ plotted as a function of inverse temperature $1/T$. The dotted line is for pure lattice gas model, the dashed one is the "fluid" contribution to the diffusion coefficient, and the solid one is the total diffusion coefficient. $A = 10^{-4}\,\mathrm{K}^{-1}$ and $J = 200$ K in both panels.

where $A = k_B/(mz\nu_0 a^2)$ and ν_0 is the overall rate factor setting a universal inverse time unit of our model. $D_0 = \nu_0 a^2 \exp(-\beta V)$ is the diffusion coefficient for the noninteracting lattice gas. For heavy adsorbates on metal surfaces the prefactor ν_0 is typically of the order of 10^{12}sec^{-1}. Assuming the mass of an adatom to be that of an oxygen atom and using the square lattice model with $a = 10^{-8}$ cm we obtain $A = 0.00143\,\text{K}^{-1}$. Varying the mass and using different values of the prefactor we find that A may change between $10^{-1} < A < 10^{-5}\text{K}^{-1}$. Values of the on-site potential and of the exchange coupling are chosen as in the Monte Carlo simulations of GOMER *et al.* [9] and in Ref. [7]. At low densities the hopping term dominates, while for larger ones the contribution due to the fluid – like behavior starts to grow and eventually it dominates. For reasons discussed in Ref. [15] our model should be treated with caution for large densities. In Fig. 3 we have shown the density and temperature dependence of the diffusion coefficient, respectively. The general behavior of it agrees with the physical picture one has concerning in what regime which contribution, hopping one or fluid one should dominate.

3. Diffusion in the presence of topological defects

So far we have discussed diffusion in systems where interparticle interactions modify the usual picture of diffusion viewed as a limit of the random walk. The resulting description still gives Einstein-like relation between the root mean square displacement of a "typical" particle and time $\langle r^2 \rangle \propto t$. The difficulty was how to calculate the proportionality coefficient i.e the diffusion coefficient. In this section I would like to discuss a different problem. I shall consider as simple random walk problem as possible – a single particle making unbiased jumps on a *locally* perfect lattice. The point here is in the word "locally". The lattice of adsorption sites in Sec. 2 was perfect. What happens when this lattice, and as a matter of fact any lattice, is imperfect?

The analysis of influence of various types of defects on simple diffusion is clearly beyond the scope of the lecture. I shall concentrate here on a particular type of extended line defects in solids, namely the *topological defects*. To be specific I shall consider edge and screw dislocations and disclinations of a sort (Kleinert disclinations). The latter are of a rather academic interest but they lead to a dramatic change in the diffusion behavior, they lead to so-called Sinay diffusion in more than $d = 1$ case. The material in this section is based on recent series of publications [16–19] and covers only salient features of our theory. No dislocation theory primer is included in this paper. The reader is referred to the wealth of available literature for necessary details of continuum dislocation theory [20–22].

Imagine a two-dimensional plane on which a Brownian particle has left its chalk–trace. Take now a black marble and roll it down that plane over the particle trajectory,without the slip. The chalk leaves the image on the marble surface.

The question might arise, and actually it did to BOCHNER [23], what are the statistical properties of this image trace. The mathematical problem is that at each instance of the marble motion the plane is tangent to it, and in that tangent plane we have quite ordinary random walk; that is an "easy" part of the story. The difficult one is that we have to paste together pieces of locally normal random walks all over the *curved* surface. This kind of "academic" problem is precisely the one one encounters when studying diffusion in crystal which contains continuous distribution of dislocations and/or disclinations [21, 22]. Following main assumptions of this theory, a diffusing particle sees a locally perfect crystal. It recognizes that it moves in topologically distorted medium only after completing its path. Since the diffusion process involves all paths between two remote points, thus the presence of topological defects might affect the diffusion. Moreover, in a real crystal one controls neither the position nor the topological charges (Burgers vectors and Frank angles) of the defects. Both of these characteristics of the defects and their distribution are therefore random quantities. The statistics of them is independent of the thermal ensemble used to discuss the diffusion. Defects are a random *quenched* distortion of the lattice and therefore we have to incorporate them carefully into description of the diffusion.

In a series of papers [16–19] we just have proposed such an approach in which the diffusion process in the crystal with a given density of dislocations is visualized as a random walk in which the particle makes a jump from one allowed lattice site to another, with the jump probabilities the same as in the simple random walk, but only in the local frame. In local coordinates (ξ^α) the Langevin equation for such a process is then very simple and reads:

$$\frac{d}{dt}\xi^\alpha = l^\alpha , \tag{8}$$

where l^α is the usual Langevin force representing white noise with zero average and variance

$$\langle l^\alpha(t) l^\beta(t')\rangle = 2D\delta^{\alpha\beta}\delta(t-t') . \tag{9}$$

In the above formula $\langle f\rangle$ denotes the ensemble average and D is the bare diffusion coefficient in the medium free of dislocations.

Transforming the Langevin equation Eq. (8) back to the laboratory frame (x^i) we have:

$$\dot{x}^i(t) = B^i_\alpha(x(t)) l^\alpha(t) , \tag{10}$$

where $B^i_\alpha(x)$ is the "distortion"tensor (which differs from Kröner's by a unit tensor) specific to, and *known*, for all interesting types of defects. In Ref. [17] we have shown that the correct interpretation of the stochastic equation (10) is the Stratonovich one, which leads to the covariant diffusion equation of the form

$$\partial_t P(x,t) = D\Delta^T P(x,t), \tag{11}$$

where

$$\Delta^T = g^{ij}\nabla_i^T\nabla_j^T\,, \qquad \nabla_i^T = \nabla_i + 2T_{ik}^k\,, \tag{12}$$

and g^{ij}, the inverse metric tensor, and the torsion vector $2T_{ik}^k$, are all given in terms of the distortion field B_α^i. In Eq. (11) $P(x,t)$ is a scalar probability distribution for a particle occupying site x at the time t.

Note, that equation (11) is the most general Fokker–Planck equation describing random walk on a manifold with non-zero torsion. Note also that the coefficients of this equation depend on the distortion field generated by dislocations. In case of random distribution of defects these coefficients become quenched random variables. I note in passing, that Eq. (11) is the fundamental equation in a not really explored field of random statistical geometry, which has many applications in general relativity, pattern recognition etc.

To discuss the diffusion process one has to average over a quenched random distribution of topological defects. This is conveniently done in a Martin–Siggia–Rose-type path-integral representation [24]. In refs. [16, 17] we have discussed in greater detail the predictions of the above outlined theory for quenched distribution of random disclinations and screw dislocations. Disclinations are the most prominent "topological" defects and their presence leads to the dramatic changes in the character of diffusion processes. Equation (11) for disclination case assumes the form of the Fokker–Planck equation with random drift velocity $V^i = -D\delta^{ij}\partial_j\Omega\Phi$, where Ω is the Frank angle and Φ is the two-dimensional Coulomb potential. For distribution of dislocation, statistical properties of the defects density $\rho(x)$ becomes important. We have studied defects distribution which is Gaussian with zero mean and has translational invariant second moments which include possibility of screening of topological charges [16, 17]. Denoting the screening length as κ we have shown that the particle exhibits nonuniversal subdiffusion with:

$$\overline{\langle x^2\rangle}(t) \sim t^{1-\gamma/8\pi\kappa}\,, \tag{13}$$

where γ is the strength of the defects distribution correlation.

The unscreened case is even more dramatic. For $\kappa = 0$ we have shown, following arguments of BOUCHARD, COMTET, GEORGE and LE DOUSSAL [25] that the particle diffusion becomes Sinay-like:

$$\overline{\langle x^2\rangle}(t) \sim (\ln t)^2. \tag{14}$$

As far as I know, it is the first example for Sinay diffusion in more than one dimension.

The quenched distribution of screw dislocations is more interesting due to the role played by these defects in crystal growth phenomena [26]. In this case our statistical model turns out to be, in a sense, exactly solvable (viz. Ref. [16, 17]). For the mean-square displacement of the particle we find an anisotropic normal diffusion behavior, enhanced in the z-direction. The latter is plausible since the

locally isotropic random steps globally lead to climbing up or down of the particle on the spiral staircases of the screw dislocations. This effect is not strong enough to generate a superdiffusive (at least logarithmic) correction in the z-direction. However, anomalies do show up in higher cumulants of the particle position. E.g., for the fourth-order cumulants we find $\langle x^4 \rangle_c = 0$, and

$$\langle x^2 z^2 \rangle_c \sim \langle z^4 \rangle_c \sim t \ln t \tag{15}$$

for $t \to \infty$. Thus, topological defects give rise to a non-Gaussian random walk process. A measure of the deviation from Gaussian behavior are the relative cumulants which exhibit long-time tails, e.g. $\langle z^4 \rangle_c / \langle z^2 \rangle^2 \sim \ln t / t$. It is an open question whether one can observe this anomaly either in computer simulations or in laboratory experiments.

4. Quantum dynamics

In previous section I have analyzed the classical diffusion of a Brownian particle on a Riemann–Cartan manifold representing a crystal with frozen-in (quenched) topological defects [16, 17] (see also [27]). In an identical setting we now want to establish a general framework for the discussion of the long-wavelength quantum states of a single particle. For special cases of single straight dislocation lines this problem has repeatedly been discussed in the literature. The main physical effects connected with screw dislocations are the Bohm–Aharonov-type interference effects [28] and the (questionable) possibility of bound states of the particle to the dislocation lines [29]. For edge dislocations the existence of bound states has been demonstrated [30] on the basis of the deformation-potential approximation, see e.g. [31]. We will specify our general form of the Schrödinger equation on a manifold to these cases and comment on the most significant physical implications. This section contains most of the results contained in a recent work by RICHARD BAUSCH, RUDI SCHMITZ and myself [19].

In order to construct a foundation for our quantum mechanical analysis, in Ref. [19], we propose a model guided by the picture of a classical random walk of a particle in a topologically distorted crystal, which is the quantum tight-binding model on a d-dimensional lattice being coherently deformed due to the presence of frozen-in topological defects. With the notations $\mathbf{n}$ for the position vectors of the lattice sites and $\mathbf{a}(\mathbf{n})$ for the vectors pointing from $\mathbf{n}$ to the nearest-neighbor sites of $\mathbf{n}$, our model Hamiltonian reads

$$H = -\frac{1}{2} \sum_{\mathbf{n}} v(\mathbf{n}) \sum_{\mathbf{a}(\mathbf{n})} t(\mathbf{a}(\mathbf{n})) \left[\varphi^\dagger(\mathbf{n} + \mathbf{a}(\mathbf{n})) \varphi(\mathbf{n}) + \varphi^\dagger(\mathbf{n}) \varphi(\mathbf{n} + \mathbf{a}(\mathbf{n})) \right]. \tag{16}$$

Here $v(\mathbf{n})$ is the volume of the lattice unit cell at $\mathbf{n}$, $t(\mathbf{a}(\mathbf{n}))$ is the transfer energy along the bond $\mathbf{a}(\mathbf{n})$, and $\varphi^\dagger$, φ are the particle creation and annihilation operators obeying the commutation (or anti-commutation) relations.

In order to reveal the long-wavelength quantum states of the particle, one has to expand the φ-operators depending on $\mathbf{a}(\mathbf{n})$ in (16) to second order in the lattice constant a of the undistorted lattice. The details of this analysis require careful but rather straightforward application of the rules of differential geometry. The resulting continuum limit of the Hamiltonian (16) for a model with a distortion-independent transfer energy $t = \hbar^2/(2ma^2)$ where m is an effective mass of the particle is:

$$H = -\frac{\hbar^2}{2m} \int d^d x \sqrt{g}\, \varphi^\dagger \left[g^{ij} \nabla_i^T \nabla_j + (g^{ij} \nabla_i^T T_{jk}{}^k) \right] \varphi , \tag{17}$$

where the operators $\varphi, \varphi^\dagger$ obey the commutation relations $\left[\varphi(x), \varphi^\dagger(y)\right] = \delta(x-y)/\sqrt{g(x)}$.

The Hamiltonian (17) is manifestly covariant as a consequence of the special form (16) chosen for the lattice model. The expression $g^{ij}\nabla_i^T \nabla_j$ in the kinetic part of (17) is identical to the Laplace–Beltrami operator $(1/\sqrt{g})\partial_i \sqrt{g} g^{ij} \partial_j$ and in general differs from the operator $g^{ij}\nabla_i^T \nabla_j^T$ entering the diffusion equation on a manifold [16]. The potential energy in (17) is proportional to the divergence of the torsion vector $T^i \equiv g^{ij} T_{jk}{}^k$ which is the only nontrivial scalar of the manifold in addition to the scalar curvature R. Whereas one finds $\nabla_i T^i = 0$ for screw dislocations and $\nabla_i T^i \neq 0$ for edge dislocations, the condition $R = 0$ is valid for both types of dislocations [32]. As an example of a defect with $R \neq 0$, we mention a kind of disclination defined by a distortion field $B_i^\alpha(x)$ which describes local rotations of the lattice [33] and implies $\nabla_i T^i = R/4$.

In Ref. [19] we have discussed application of Eq. (17) to the problems known in the literature and concerning the existence and/or nonexistence of the bound states formed for quantum particles by the topological lattice defects. We have clarified this issue by showing that the model in Eq. (17) does not allow for existence of the bound states for edge and screw dislocations. To describe the possibility of these bounds state one has to generalize the model allowing the transfer energy t to become space-dependent. Details of that discussion are outside of the scope of this lecture.

The other quantum mechanical model of the particle motion in the presence of the topological disorder was discussed by Andrzej ŁUSAKOWSKI and myself [34]. This model analyzes the tight binding Hamiltonian Eq. (16) in the presence of the random arrangement of the Bohm–Aharonov magnetic field fluxes penetrating the lattice cells. The position and value of the flux are quenched random variables. The analysis provides the analytic expression for the density of states of the particle shown in Fig. 4. The divergence of the density of states typical for a two-dimensional system is gone but the density is shrinked, the zone boundary is moved inwards. The shrinking of the zone depends on the jump anisotropy coefficient r but it is already clearly visible for isotropic case $r = 1$. This unexpected and puzzling result is well confirmed by the numerical simulations [35]. The the-

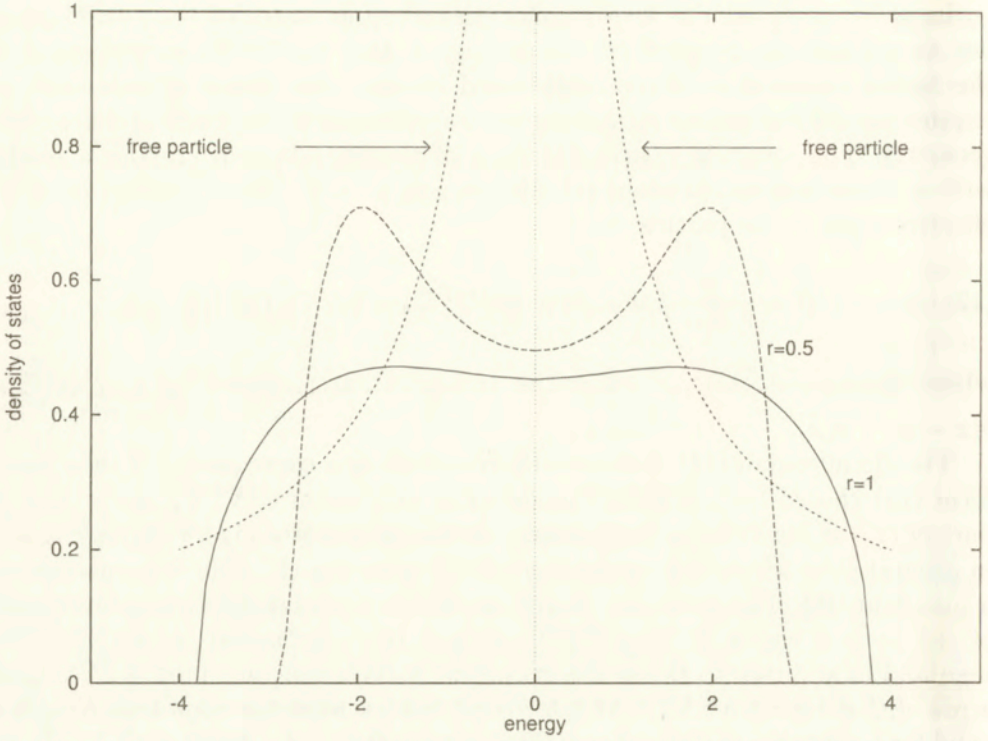

FIG. 4. Density of states plotted for various values of the ratio $r = K_x/K_y$. Upper line $r = 0.5$. Bottom line $r = 1$. Two-dimensional density of states for free particle is shown for comparison.

ory presented in Ref. [34] is a "first step" to the analysis of one of the most challenging problems in contemporary quantum statistical mechanics, namely the theory of quantum particle motion in a random magnetic field. Preliminary results obtained by us recently indicate, among others, that there is no simple diffusion there and that the system exhibits long time tails in the current–current correlation functions leading to the not yet fully explored memory effects in the dynamics of particles in random magnetic field. Work along this line has just been published [36].

Acknowledgments

Most of the material in this lecture is based on results of fruitful and ongoing collaboration with R. BAUSCH, Z. GORTEL, A. ŁUSAKOWSKI, R. SCHMITZ and M. ZAŁUSKA-KOTUR.

This work was partially supported by KBN (Poland) Grant 2 P03B 11712.

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CENTER FOR THEORETICAL PHYSICS,
POLISH ACADEMY OF SCIENCES AND COLLEGE OF SCIENCE
Al. Lotników 32/46, 02-668 Warszawa, Poland.
e-mail: laturski@cft.edu.pl

Received September 12, 1997.

Arch. Mech., 50, 3, pp. 645–655, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

On generalized Weber and Clebsch transformations

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

H.-J. WAGNER (PADERBORN)

SUITABLE generalizations of the Weber and Clebsch transformations of the hydrodynamic equations are introduced which have some bearing in the treatment of the inverse problem of Lagrangian field theory. In particular these generalizations open the way to equivalence proofs for several Lagrangians proposed in the realm of ideal (magneto-)hydrodynamics. This means that the Euler–Lagrange equations corresponding to these Lagrangians do not only imply but are also implied by the original field equations of the systems under study.

1. Introduction

GIVEN A SET of field equations for a dynamical system, the inverse problem of Lagrangian field theory deals with the question whether one can find an action principle for it. In other words, it is examined whether Lagrangians can be constructed whose Euler–Lagrange equations are equivalent to a given set of field equations.

Concerning the "Eulerian" field equations of ideal fluid flow in hydrodynamics, magnetohydrodynamics, and plasma dynamics, a large number of proposed Lagrangians can be found in the literature. To quote only a few surveys of the whole field, see [1–6]. However, in several cases it has only been shown that the respective Euler–Lagrange equations imply the validity of the original hydrodynamical flow equations. But to establish full equivalence between the Euler–Lagrange equations and the original field equations, it is also necessary to examine whether the Euler–Lagrange equations are capable of describing *all* possible solutions of the original equations.

Up to now, complete equivalence proofs for certain Lagrangians have been given for the cases of the barotropic and the non-barotropic ideal fluid [1, 7]. The main tools involved in these proofs are representations of vector fields in terms of special potential classes as well as the so-called Weber and Clebsch transformations of the hydrodynamic equations.

One aim of this paper is to show that – employing suitable generalizations of these Weber and Clebsch transformations – complete equivalence proofs can also be given for many other Lagrangians in hydrodynamics, magnetohydrodynamics, and plasma dynamics. The class of systems which can be treated on more or

less the same footing is rather large and comprises e. g. charged ideal fluids in external electromagnetic fields and ideal magnetohydrodynamic fluids with infinite conductivity. Even a certain case of fluid flow in porous media – obeying a nonstationary extension of Darcy's law – turns out to be covered. The present paper is organized as follows:

Section 2 is devoted to fixing of the notation. In Sec. 3, the original Weber and Clebsch transformations for barotropic fluids are shortly revisited and their connection to the solution of the inverse problem of Lagrangian field theory is pointed out. In Sec. 4 we then introduce suitable generalizations of the Weber and the Clebsch transformations, starting from a generalized form of the Euler equation. In the next section it is demonstrated that there is a considerable number of hydrodynamical systems whose respective Euler equations can be cast into such a generalized form. The paper is then concluded with a list of Lagrangians for these systems for which equivalence proofs are now available.

Due to limitations of space, not all the – sometimes lengthy – derivations can be given here. Only the generalized Weber and Clebsch transformations are treated in some detail, whereas we have to restrict ourselves to summary remarks in the remaining sections. The full length considerations can be found elsewhere [6].

2. Notation

The trajectories of the material points of the continuum are given as follows:

$$\mathbf{x} = \mathbf{x}(\mathbf{x}_0, t)\,. \tag{2.1}$$

Here t means time and $\mathbf{x}_0$ denotes the material (Lagrangian) coordinates:

$$\mathbf{x}_0 = \mathbf{x}(\mathbf{x}_0, 0)\,. \tag{2.2}$$

We require (2.1) to be invertible, thus leading to the "index field"

$$\mathbf{x}_0 = \mathbf{x}_0(\mathbf{x}, t). \tag{2.3}$$

The "Eulerian" velocity field $\mathbf{u}(\mathbf{x}, t)$ is given as

$$\mathbf{u}(\mathbf{x}, t) = \frac{\partial}{\partial t}\mathbf{x}(\mathbf{x}_0, t)\Big|_{\mathbf{x}_0=\mathbf{x}_0(\mathbf{x},t)}\,. \tag{2.4}$$

Generally, the fields of the form $\varepsilon(\mathbf{x}, t)$ – i.e., described as functions of $\mathbf{x}$ and t – are called "Eulerian fields". They give rise to the corresponding "Lagrangian fields" $\varepsilon^{(L)}$ depending on $\mathbf{x}_0$ and t:

$$\varepsilon^{(L)}(\mathbf{x}_0, t) = \varepsilon(\mathbf{x}(\mathbf{x}_0, t), t)\,. \tag{2.5}$$

The following abbreviation for the substantial time derivative is used in this paper:

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla\,. \tag{2.6}$$

It mainly comes into the play by means of the "local transport theorem"

$$\frac{\partial}{\partial t}\varepsilon^{(L)}(\mathbf{x}_0,t)\Big|_{\mathbf{x}_0=\mathbf{x}_0(\mathbf{x},t)} = \frac{D}{Dt}\varepsilon(\mathbf{x},t)\,. \tag{2.7}$$

3. Weber and Clebsch transformations revisited

In this section we give a rather condensed review of the Weber and Clebsch transformations for the barotropic ideal fluid, i.e., for a fluid where the pressure p is a function of the mass density ϱ only. For details the reader is referred to §§ 15, 167 of [8] and § 29 of [1].

Our starting point is the Euler equation

$$\frac{D}{Dt}\mathbf{u} = -\nabla\left(\int\frac{dp(\varrho)}{\varrho} + U\right) = -\nabla(P+U). \tag{3.1}$$

After transition to the Lagrangian picture (Lagrangian equations of motion), one can derive the so-called "Weber transformation of the hydrodynamic equations"

$$\sum_k u_k^{(L)}(\mathbf{x}_0,t)\frac{\partial}{\partial x_{0i}}x_k(\mathbf{x}_0,t) = u_i^{(L)}(\mathbf{x}_0,0) + \frac{\partial}{\partial x_{0i}}\phi^{(L)}(\mathbf{x}_0,t) \tag{3.2}$$

with

$$\phi^{(L)}(\mathbf{x}_0,t) = \int_0^t\left(\frac{1}{2}\mathbf{u}^{(L)}(\mathbf{x}_0,t')^2 - P^{(L)}(\mathbf{x}_0,t') - U^{(L)}(\mathbf{x}_0,t')\right)dt'\,. \tag{3.3}$$

Transition back to the Eulerian picture implies the "Lin representation" of the velocity field

$$\mathbf{u}(\mathbf{x},t) = \nabla\phi(\mathbf{x},t) + \sum_i \alpha_i(\mathbf{x},t)\nabla x_{0i}(\mathbf{x},t) \tag{3.4}$$

with

$$\boldsymbol{\alpha}(\mathbf{x},t) = \mathbf{u}^{(L)}(\mathbf{x}_0(\mathbf{x},t),0)\,, \qquad \phi(\mathbf{x},t) = \phi^{(L)}(\mathbf{x}_0(\mathbf{x},t),t)\,. \tag{3.5}$$

Due to (2.7), $\boldsymbol{\alpha}$, $\mathbf{x}_0$, ϕ solve the following equations:

$$\frac{D}{Dt}\boldsymbol{\alpha} = 0\,, \qquad \frac{D}{Dt}\mathbf{x}_0 = 0\,, \qquad \frac{D}{Dt}\phi = \frac{1}{2}\mathbf{u}^2 - P - U\,. \tag{3.6}$$

Note that the Euler equation (3.1) can be rederived from (3.4), (3.6).

Now, what has this to do with the inverse problem of Lagrangian field theory? The Euler–Lagrange equations of the so-called "Lin Lagrangian" [9]

$$\mathcal{L} = \frac{1}{2}\varrho \mathbf{u}^2 - \varrho P(\varrho) + p(\varrho) - \varrho U + \phi\left(\frac{\partial}{\partial t}\varrho + \nabla\cdot(\varrho\mathbf{u})\right) - \varrho\boldsymbol{\alpha}\cdot\frac{D}{Dt}\mathbf{x}_0 \tag{3.7}$$

can be shown to include (3.4), (3.6), whereas the Euler equation is missing. The above considerations now show that (3.4), (3.6) are an equivalent substitute for the original Euler equation.

The Lin representation of the velocity field is globally valid. If one only looks for a local representation, one can achieve a much simpler expression for $\mathbf{u}$. This is due to the fact that – at least locally – any vector field $\mathbf{A}$ can be represented in terms of the "Clebsch potentials":

$$\mathbf{A} = \nabla\psi_0 + \alpha_0\nabla\beta_0\,. \tag{3.8}$$

For a proof see e.g. [10] and the references quoted there.

In particular, $\mathbf{u}^{(L)}(\mathbf{x}_0, 0)$ can thus be represented as

$$u_i^{(L)}(\mathbf{x}_0, 0) = \frac{\partial}{\partial x_{0i}}\psi_0(\mathbf{x}_0) + \alpha_0(\mathbf{x}_0)\frac{\partial}{\partial x_{0i}}\beta_0(\mathbf{x}_0). \tag{3.9}$$

Insertion of this representation into the Weber transformation and subsequent transition to the Eulerian picture implies

$$\mathbf{u} = \nabla\tilde{\phi} + \alpha\nabla\beta \tag{3.10}$$

with

$$\frac{D}{Dt}\tilde{\phi} - \frac{\mathbf{u}^2}{2} + P + U = 0\,, \qquad \frac{D}{Dt}\alpha = 0\,, \qquad \frac{D}{Dt}\beta = 0\,. \tag{3.11}$$

Again, the Euler equation can be rederived from these expressions.

Equations (3.10), (3.11) are included in the set of Euler–Lagrange equations of the "Davydov Lagrangian" [11]

$$\mathcal{L} = \frac{1}{2}\varrho \mathbf{u}^2 - \varrho P(\varrho) + p(\varrho) - \varrho U + \phi\left(\frac{\partial}{\partial t}\varrho + \nabla\cdot(\varrho\mathbf{u})\right) - \varrho\alpha\frac{D}{Dt}\beta \tag{3.12}$$

which arises from (3.7) by replacing $\boldsymbol{\alpha}\cdot(D/Dt)\mathbf{x}_0$ with the simplified expression $\alpha(D/Dt)\beta$. Therefore, the Euler equation is locally equivalently substituted within the Euler–Lagrange equations of (3.12).

REMARK. In the literature instead of the Davydov Lagrangian one often finds the "Bateman Lagrangian" [12]

$$\mathcal{L} = \frac{1}{2}\varrho \mathbf{u}^2 - \varrho P(\varrho) + p(\varrho) - \varrho U - \varrho\frac{D}{Dt}\phi - \varrho\alpha\frac{D}{Dt}\beta \tag{3.13}$$

which differs from the Davydov Lagrangian only by a 4-divergence and thus gives rise to the same Euler–Lagrange equations.

4. Generalized Weber and Clebsch transformations

Our starting points in this section are field quantities $\mathbf{Y}(\mathbf{x},t)$ and $\psi(\mathbf{x},t)$ which are supposed to satisfy the "generalized Euler equation"

$$\frac{D}{Dt}\mathbf{Y} + \sum_j Y_j \nabla u_j = \nabla\psi\,. \tag{4.1}$$

Just as the usual Euler equation (3.1) for a barotropic fluid in an external potential field serves as a starting point for the derivation of the original Weber transformation, the generalized Euler equation (4.1) will be shown to imply a certain "generalized Weber transformation". The following steps rather closely resemble those for the barotropic fluid which can be recovered as a special case by putting $\mathbf{Y} = \mathbf{u}$ and $\psi = \mathbf{u}^2/2 - P - U$.

Reexpressing (4.1) in Lagrangian coordinates, with (2.7) we get

$$\frac{\partial}{\partial t}\mathbf{Y}^{(L)}(\mathbf{x}_0,t) + \sum_j Y_j^{(L)}(\mathbf{x}_0,t)\nabla u_j(\mathbf{x},t)\Big|_{\mathbf{x}=\mathbf{x}(\mathbf{x}_0,t)} = \nabla\psi(\mathbf{x},t)\Big|_{\mathbf{x}=\mathbf{x}(\mathbf{x}_0,t)}\,. \tag{4.2}$$

This implies the "generalized Lagrangian equations of motion"

$$\begin{aligned}\sum_k \frac{\partial}{\partial t}Y_k^{(L)}(\mathbf{x}_0,t)\frac{\partial}{\partial x_{0i}}x_k(\mathbf{x}_0,t) &\\ + \sum_{j,k} Y_j^{(L)}(\mathbf{x}_0,t)\frac{\partial}{\partial x_k}u_j(\mathbf{x},t)\Big|_{\mathbf{x}=\mathbf{x}(\mathbf{x}_0,t)}\frac{\partial}{\partial x_{0i}}x_k(\mathbf{x}_0,t) &\\ = \sum_k \frac{\partial}{\partial x_k}\psi(\mathbf{x},t)\Big|_{\mathbf{x}=\mathbf{x}(\mathbf{x}_0,t)}\frac{\partial}{\partial x_{0i}}x_k(\mathbf{x}_0,t)\,.&\end{aligned} \tag{4.3}$$

Making use of the chain rule, and employing the fact that $\mathbf{u}^{(L)} = \partial\mathbf{x}/\partial t$, we are led to

$$\sum_k \frac{\partial}{\partial t}\left(Y_k^{(L)}(\mathbf{x}_0,t)\frac{\partial}{\partial x_{0i}}x_k(\mathbf{x}_0,t)\right) = \frac{\partial}{\partial x_{0i}}\psi^{(L)}(\mathbf{x}_0,t). \tag{4.4}$$

Integrating with respect to t and using $(\partial x_k/\partial x_{0i})(\mathbf{x}_0,0) = \partial x_{0k}/\partial x_{0i} = \delta_{ik}$, we end up with the following "generalized Weber transformation":

$$\sum_k Y_k^{(L)}(\mathbf{x}_0,t)\frac{\partial}{\partial x_{0i}}x_k(\mathbf{x}_0,t) = Y_i^{(L)}(\mathbf{x}_0,0) + \frac{\partial}{\partial x_{0i}}\int_0^t \psi^{(L)}(\mathbf{x}_0,t')\,dt'\,. \tag{4.5}$$

Transformation to the Eulerian picture leads to

$$\begin{aligned}\sum_i \left(\sum_k Y_k^{(L)}(\mathbf{x}_0,t)\frac{\partial}{\partial x_{0i}}x_k(\mathbf{x}_0,t)\right)\Big|_{\mathbf{x}_0=\mathbf{x}_0(\mathbf{x},t)}\frac{\partial}{\partial x_j}x_{0i}(\mathbf{x},t) &\\ = \sum_i \left(Y_i^{(L)}(\mathbf{x}_0,0) + \frac{\partial}{\partial x_{0i}}\int_0^t \psi^{(L)}(\mathbf{x}_0,t')\,dt'\right)\Big|_{\mathbf{x}_0=\mathbf{x}_0(\mathbf{x},t)}\frac{\partial}{\partial x_j}x_{0i}(\mathbf{x},t)\,.&\end{aligned} \tag{4.6}$$

Employing the chain rule, we finally get:

$$Y_j(\mathbf{x},t) = \sum_i Y_i^{(L)}(\mathbf{x}_0(\mathbf{x},t),0)\frac{\partial}{\partial x_j}x_{0i}(\mathbf{x},t) + \frac{\partial}{\partial x_j}\int_0^t \psi^{(L)}(\mathbf{x}_0(\mathbf{x},t),t')\,dt'\,. \tag{4.7}$$

Defining

$$\boldsymbol{\alpha}(\mathbf{x},t) = \mathbf{Y}^{(L)}(\mathbf{x}_0(\mathbf{x},t),0)\,, \qquad \phi(\mathbf{x},t) = \int_0^t \psi^{(L)}(\mathbf{x}_0(\mathbf{x},t),t')\,dt'\,, \tag{4.8}$$

we end up with the following decomposition of $\mathbf{Y}$:

$$\mathbf{Y}(\mathbf{x},t) = \nabla\phi(\mathbf{x},t) + \sum_i \alpha_i(\mathbf{x},t)\nabla x_{0i}(\mathbf{x},t). \tag{4.9}$$

The time evolution equations of the fields α_i are simply

$$\frac{D}{Dt}\alpha_i(\mathbf{x},t) = 0, \tag{4.10}$$

due to the fact that $\alpha_i(\mathbf{x},t) = f_i(\mathbf{x}_0(\mathbf{x},t))$. Moreover, (4.8) implies

$$\frac{\partial}{\partial t}\phi^{(L)}(\mathbf{x}_0,t) = \psi^{(L)}(\mathbf{x}_0,t)\,. \tag{4.11}$$

In Eulerian coordinates, this corresponds to

$$\frac{D}{Dt}\phi(\mathbf{x},t) = \psi(\mathbf{x},t)\,. \tag{4.12}$$

Vice versa, the generalized Euler equation (4.1) can be rederived from (4.9) with (4.10) and (4.12). Using the obvious commutation relation

$$\nabla\frac{D}{Dt} - \frac{D}{Dt}\nabla = \sum_j (\nabla u_j)\frac{\partial}{\partial x_j} \tag{4.13}$$

we get

$$\begin{aligned}\frac{D}{Dt}\mathbf{Y} &= \frac{D}{Dt}\nabla\phi + \sum_i \underbrace{\left(\frac{D}{Dt}\alpha_i\right)}_{=0}\nabla x_{0i} + \sum_i \alpha_i\frac{D}{Dt}\nabla x_{0i} \\ &= \nabla\underbrace{\left(\frac{D}{Dt}\phi\right)}_{=\psi} - \sum_j(\nabla u_j)\frac{\partial}{\partial x_j}\phi + \sum_i \alpha_i\nabla\underbrace{\left(\frac{D}{Dt}x_{0i}\right)}_{=0} - \sum_{i,j}\alpha_i(\nabla u_j)\frac{\partial}{\partial x_j}x_{0i} \\ &= \nabla\psi - \sum_j(\nabla u_j)Y_j\,.\end{aligned} \tag{4.14}$$

The results obtained so far can be summed up as follows:

PROPOSITION 1. (Generalized Weber Transformation)

The validity of the generalized Euler equation $(D/Dt)\mathbf{Y} + \sum_j Y_j \nabla u_j = \nabla\psi$ gives rise to the following generalized Weber transformation:

$$\sum_k Y_k^{(L)}(\mathbf{x}_0, t)\frac{\partial}{\partial x_{0i}} x_k(\mathbf{x}_0, t) = Y_i^{(L)}(\mathbf{x}_0, 0) + \frac{\partial}{\partial x_{0i}}\int_0^t \psi^{(L)}(\mathbf{x}_0, t')\, dt' . \tag{4.15}$$

PROPOSITION 2. (Generalized Lin Representation)

The validity of the generalized Euler equation $(D/Dt)\mathbf{Y} + \sum_j Y_j \nabla u_j = \nabla\psi$ is globally equivalent to the existence of the representation

$$\mathbf{Y} = \nabla\phi + \sum_i \alpha_i \nabla x_{0i} , \tag{4.16}$$

where α_i, x_{0i} and ϕ are solutions of the following time evolution equations:

$$\frac{D}{Dt}\alpha_i = 0 , \qquad \frac{D}{Dt} x_{0i} = 0 , \qquad \frac{D}{Dt}\phi = \psi . \tag{4.17}$$

With regard to the derivation of a generalized Clebsch transformation, we now make use of the fact that $\mathbf{Y}^{(L)}(\mathbf{x}_0, 0)$ can be locally represented in terms of Clebsch potentials:

$$Y_i^{(L)}(\mathbf{x}_0, 0) = \frac{\partial}{\partial x_{0i}}\eta_0(\mathbf{x}_0) + \alpha_0(\mathbf{x}_0)\frac{\partial}{\partial x_{0i}}\beta_0(\mathbf{x}_0) . \tag{4.18}$$

Thus, (4.7) implies

$$\begin{aligned} Y_j(\mathbf{x}, t) &= \sum_i Y_i^{(L)}(\mathbf{x}_0(\mathbf{x}, t), 0)\frac{\partial}{\partial x_j} x_{0i}(\mathbf{x}, t) + \frac{\partial}{\partial x_j}\phi(\mathbf{x}, t) \\ &= \sum_i \left(\frac{\partial}{\partial x_{0i}}\eta_0(\mathbf{x}_0)\right)\Big|_{\mathbf{x}_0 = \mathbf{x}_0(\mathbf{x}, t)} \frac{\partial}{\partial x_j} x_{0i}(\mathbf{x}, t) \\ &\quad + \sum_i \left(\alpha_0(\mathbf{x}_0)\frac{\partial}{\partial x_{0i}}\beta_0(\mathbf{x}_0)\right)\Big|_{\mathbf{x}_0 = \mathbf{x}_0(\mathbf{x}, t)} \frac{\partial}{\partial x_j} x_{0i}(\mathbf{x}, t) + \frac{\partial}{\partial x_j}\phi(\mathbf{x}, t) . \end{aligned} \tag{4.19}$$

Defining

$$\alpha(\mathbf{x}, t) = \alpha_0(\mathbf{x}_0(\mathbf{x}, t)) , \quad \beta(\mathbf{x}, t) = \beta_0(\mathbf{x}_0(\mathbf{x}, t)) , \quad \eta(\mathbf{x}, t) = \eta_0(\mathbf{x}_0(\mathbf{x}, t)) , \tag{4.20}$$

and using the chain rule, we get

$$Y_j(\mathbf{x}, t) = \frac{\partial}{\partial x_j}(\eta(\mathbf{x}, t) + \phi(\mathbf{x}, t)) + \alpha(\mathbf{x}, t)\frac{\partial}{\partial x_j}\beta(\mathbf{x}, t) . \tag{4.21}$$

Putting $\tilde{\phi}(\mathbf{x},t) = \eta(\mathbf{x},t) + \phi(\mathbf{x},t)$, we end up with a Clebsch representation for $\mathbf{Y}$:

$$\mathbf{Y}(\mathbf{x},t) = \nabla\tilde{\phi}(\mathbf{x},t) + \alpha(\mathbf{x},t)\nabla\beta(\mathbf{x},t)\,, \tag{4.22}$$

where α, β, and η are solutions of

$$\frac{D}{Dt}\alpha = 0\,, \qquad \frac{D}{Dt}\beta = 0\,, \qquad \frac{D}{Dt}\eta = 0\,. \tag{4.23}$$

Moreover

$$\frac{D}{Dt}\tilde{\phi} = \frac{D}{Dt}\eta + \frac{D}{Dt}\phi = \frac{D}{Dt}\phi = \psi\,. \tag{4.24}$$

Vice versa, in analogy to (4.14) it can be shown that the generalized Euler equation is derivable from (4.22) together with the above time evolution equations for α, β, and $\tilde{\phi}$.

Again we summarize:

PROPOSITION 3. (Generalized Clebsch Transformation)

The validity of the generalized Euler equation $(D/Dt)\mathbf{Y} + \sum_j Y_j \nabla u_j = \nabla\psi$ is locally equivalent to the existence of the representation

$$\mathbf{Y} = \nabla\tilde{\phi} + \alpha\nabla\beta\,, \tag{4.25}$$

where α, β and $\tilde{\phi}$ are solutions of the following time evolution equations:

$$\frac{D}{Dt}\alpha = 0\,, \qquad \frac{D}{Dt}\beta = 0\,, \qquad \frac{D}{Dt}\tilde{\phi} = \psi\,. \tag{4.26}$$

We conclude the present section with the remark that due to

$$\begin{aligned}\frac{D}{Dt}\tilde{\phi} &= \frac{\partial}{\partial t}\tilde{\phi} + (\mathbf{u}\cdot\nabla)\tilde{\phi} = \frac{\partial}{\partial t}\tilde{\phi} + \mathbf{u}\cdot(\mathbf{Y} - \alpha\nabla\beta) \\ &= \frac{\partial}{\partial t}\tilde{\phi} + \mathbf{u}\cdot\mathbf{Y} - \alpha(\mathbf{u}\cdot\nabla)\beta = \frac{\partial}{\partial t}\tilde{\phi} + \mathbf{u}\cdot\mathbf{Y} - \alpha\left(\frac{D}{Dt}\beta - \frac{\partial}{\partial t}\beta\right) \\ &= \frac{\partial}{\partial t}\tilde{\phi} + \mathbf{u}\cdot\mathbf{Y} + \alpha\frac{\partial}{\partial t}\beta\,,\end{aligned} \tag{4.27}$$

the time evolution equation (4.24) may be replaced with the "generalized Bernoulli theorem"

$$\frac{\partial}{\partial t}\tilde{\phi} + \alpha\frac{\partial}{\partial t}\beta + \mathbf{u}\cdot\mathbf{Y} - \psi = 0\,. \tag{4.28}$$

5. Examples

It remains to show that there indeed exists a sufficiently nontrivial list of hydrodynamical systems with Euler equations that can be cast into the generalized form (4.1).

The first example on this list to be mentioned is the non-barotropic ideal fluid. Here the energy density e, the temperature $T = \partial e/\partial s$, and the pressure $p = \varrho^2 \partial e/\partial \varrho$ are depending on both the mass density ϱ and the entropy density s. In addition to the Euler and the continuity equation we require the isentropy relation $Ds/Dt = 0$ to be valid.

We define the following quantity (sometimes called "thermasy" [13]):

$$\theta = \int_0^t T^{(L)}(\mathbf{x}_0(\mathbf{x}, t), t')\, dt' . \tag{5.1}$$

It is a solution of $D\theta/Dt = T$ and one can show that the Euler equation

$$\frac{D}{Dt}\mathbf{u} = -\frac{\nabla p}{\varrho} - \nabla U \tag{5.2}$$

can be cast into the form of the generalized Euler equation (4.1) with

$$\mathbf{Y} = \mathbf{u} - \theta \nabla s , \qquad \psi = \frac{\mathbf{u}^2}{2} - e - \frac{p}{\varrho} - U . \tag{5.3}$$

If the forces exerted on the non-barotropic ideal fluid are due to an external electromagnetic field, then the respective Euler equation

$$\frac{D}{Dt}\mathbf{u} = -\frac{\nabla p}{\varrho} + \frac{q}{m}\left(\mathbf{E} + \frac{1}{c}\mathbf{u} \times \mathbf{B}\right) \tag{5.4}$$

can be cast into the form (4.1) with

$$\mathbf{Y} = \mathbf{u} + \frac{q}{mc}\mathbf{A} - \theta \nabla s , \qquad \psi = \frac{\mathbf{u}^2}{2} - e - \frac{p}{\varrho} - \frac{q}{m}\left(\varphi - \frac{1}{c}\mathbf{u}\cdot\mathbf{A}\right), \tag{5.5}$$

where φ and $\mathbf{A}$ denote the usual electromagnetic scalar and vector potentials.

Another example consists of the Euler equation for a non-barotropic ideal fluid in magnetohydrodynamics with infinite conductivity:

$$\frac{D}{Dt}\mathbf{u} = -\frac{\nabla p}{\varrho} + \frac{1}{4\pi\varrho}\left((\nabla \times \mathbf{B}) \times \mathbf{B}\right) . \tag{5.6}$$

Introducing an auxiliary vector field $\mathbf{h}(\mathbf{x}, t)$ *via*

$$h_j(\mathbf{x}, t) = \frac{1}{4\pi}\sum_k \int_0^t B_k^{(L)}(\mathbf{x}_0(\mathbf{x}, t), t')\frac{\partial}{\partial x_j}\Big(x_k(\mathbf{x}_0(\mathbf{x}, t), t')\Big)dt' , \tag{5.7}$$

Eq. (5.6) can be cast into the form (4.1) with

$$\mathbf{Y} = \mathbf{u} - \theta\nabla s - \frac{1}{\varrho}(\nabla \times \mathbf{h}) \times \mathbf{B}, \qquad \psi = \frac{\mathbf{u}^2}{2} - e - \frac{p}{\varrho}. \tag{5.8}$$

Here one has to make use of the fact that $\mathbf{h}(\mathbf{x}, t)$ is a solution of

$$\frac{\mathbf{B}}{4\pi} = \frac{\partial}{\partial t}\mathbf{h} - \mathbf{u} \times (\nabla \times \mathbf{h}) + \nabla(\mathbf{u}\cdot\mathbf{h}) \tag{5.9}$$

which implies

$$\frac{\nabla \times \mathbf{B}}{4\pi} = \frac{\partial}{\partial t}(\nabla \times \mathbf{h}) - \nabla \times [\mathbf{u} \times (\nabla \times \mathbf{h})]. \tag{5.10}$$

As a last example, we mention the following nonstationary extension of Darcy's law for the seepage of a barotropic fluid in a porous medium:

$$\frac{D}{Dt}\mathbf{u} = -\nabla P - \nabla U - \lambda\mathbf{u}. \tag{5.11}$$

Here, (4.1) can be achieved by putting

$$\mathbf{Y} = \mathbf{u}e^{\lambda t}, \qquad \psi = \left(\frac{\mathbf{u}^2}{2} - P - U\right)e^{\lambda t}. \tag{5.12}$$

For all these examples there exist Lagrangians for which – with the help of the generalized Lin representations – one can show that the Euler equation is always equivalently substituted within the respective Euler–Lagrange equations.

For the sake of completeness, we list up these Lagrangians but – due to the limited space – this has to be done without giving any further details:

(i) Non-barotropic ideal fluid [9]

$$\mathcal{L} = \frac{1}{2}\varrho\mathbf{u}^2 - \varrho e(\varrho, s) - \varrho U + \phi\left(\frac{\partial}{\partial t}\varrho + \nabla\cdot(\varrho\mathbf{u})\right) - \varrho\theta\frac{D}{Dt}s - \varrho\boldsymbol{\alpha}\cdot\frac{D}{Dt}\mathbf{x}_0. \tag{5.13}$$

(ii) Non-barotropic ideal fluid in an external electromagnetic field

$$\mathcal{L} = \frac{1}{2}\varrho\mathbf{u}^2 - \varrho e(\varrho, s) - \frac{q}{m}\varrho\left(\varphi - \frac{1}{c}\mathbf{u}\cdot\mathbf{A}\right) + \phi\left(\frac{\partial}{\partial t}\varrho + \nabla\cdot(\varrho\mathbf{u})\right) - \varrho\theta\frac{D}{Dt}s - \varrho\boldsymbol{\alpha}\cdot\frac{D}{Dt}\mathbf{x}_0. \tag{5.14}$$

(iii) Non-barotropic ideal fluid in magnetohydrodynamics with infinite conductivity [14]

$$\mathcal{L} = \frac{1}{2}\varrho\mathbf{u}^2 - \varrho e(\varrho, s) - \frac{\mathbf{B}^2}{8\pi} + \phi\left(\frac{\partial}{\partial t}\varrho + \nabla\cdot(\varrho\mathbf{u})\right) - \varrho\theta\frac{D}{Dt}s - \varrho\boldsymbol{\alpha}\cdot\frac{D}{Dt}\mathbf{x}_0 - \mathbf{h}\cdot\left(\frac{\partial}{\partial t}\mathbf{B} - \nabla \times (\mathbf{u} \times \mathbf{B})\right) - \kappa\nabla\cdot\mathbf{B}. \tag{5.15}$$

(iv) Barotropic fluid in a porous medium

$$\mathcal{L} = e^{\lambda t}\left\{\frac{1}{2}\varrho\mathbf{u}^2 - \varrho P(\varrho) + p(\varrho) - \varrho U\right\} + \phi\left(\frac{\partial}{\partial t}\varrho + \nabla\cdot(\varrho\mathbf{u})\right) - \varrho\boldsymbol{\alpha}\cdot\frac{D}{Dt}\mathbf{x}_0. \tag{5.16}$$

Making the replacement $\boldsymbol{\alpha}\cdot(D/Dt)\mathbf{x}_0 \to \alpha(D/Dt)\beta$ in the above expressions, one is left with Lagrangians that are no longer global but still local solutions of the inverse problem of Lagrangian field theory. This can be proved with the aid of the generalized Clebsch transformations discussed above.

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FB 6, THEORETISCHE PHYSIK,
UNIVERSITÄT PADERBORN
Pohlweg 55, D-33098 Paderborn, Germany.

Received October 27, 1997.

Arch. Mech., 50, 3, pp. 657–669, Warszawa 1998
FIFTY YEARS OF THE ARCHIVES OF MECHANICS

On the time of existence of weak discontinuity waves in poroelastic materials

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

K. WILMAŃSKI (BERLIN)

IN THE PAPER, we consider the possibility of the growth of strong discontinuity waves in the two-component poroelastic materials. We use the model with the hyperbolic set of field equations described in the paper by K. WILMAŃSKI [8]. It is shown that indeed, the critical time (i.e. the maximum time of existence of classical solutions) is finite and it assumes realistic values for real physical systems, such as biological tissues.

1. Introduction

THE PROBLEM of propagation of waves in porous and granular materials bears special features which do not appear in other media with microstructure. The most characteristic one is the presence of additional modes of propagation. For porous materials, such a mode has been described for the first time by M.A. BIOT [1, 2], and it is called the P2-wave in contrast to P1-waves (longitudinal) and S-waves (transversal) appearing in one-component elastic solids. These additional modes are usually connected with a very high attenuation and this yields, in turn, certain difficulties in their experimental observation.

The second characteristic feature is the wave scattering on microscopic heterogeneities. Certainly, this phenomenon appears as well, for instance, in polycrystals. However, in contrast to relatively small grains of polycrystals, the size of the microstructure of typical granular and porous materials is much larger. It means that the strong scattering of sound waves appears in granular and porous materials for much longer waves (waves of much lower frequency) than it is the case for polycrystals. For instance, in the extreme case of a very coarse gravel (the typical size of particles $\sim$ 4.5 mm), the waves of frequencies higher than app. 300 kHz cannot propagate at all, primarily due to their scattering.

The third feature is connected with the diffusion (relative motion) of components. The influence of the diffusion is particularly dramatic for the value of the attenuation coefficient and it has a smaller effect on the speeds of propagation (e.g. see K. WILMAŃSKI [7, 8, 9]).

Finally, in contrast to linear elastic models of polycrystals or composites, the models of porous materials with the linear elastic skeleton admit the growth of

shock waves, i.e. strong discontinuity waves. This is due to the non-linearity of the contribution of fluid components, which is characteristic for the bulk of such systems appearing in nature.

The literature of the subject contains a rather extensive batch of work on propagation conditions, speeds of propagation and attenuation of acoustic waves in granular and porous materials based on various models (e.g. T. BOURBIE, O. COUSSY, B. ZINSZNER [4], R.I. NIGMATULIN [5], V.N. NIKOLAEVSKIJ [6]). On the other hand, scattering of acoustic waves in such materials has been investigated to a very small extent and solely for one-component models. Even less has been done in the field of growth and propagation of shock waves.

In this paper, we investigate the possibility of the growth of the strong discontinuity wave in a porous material, described by the hyperbolic set of field equations and proposed in my papers [8, 11]. In the next section, we present the model. In the third section, we derive the evolution equation for the amplitude of weak discontinuities. As usual, it appears to be the Bernoulli equation along each characteristic. The solution of this equation may become infinite after a finite time. This critical time defines the range of existence of classical solutions of field equations. For times larger than critical, there exist solely weak solutions which define the shock waves. The fourth section is devoted to the dynamical compatibility conditions which describe the propagation of such waves. We show that the present model yields these conditions in the form similar, to a certain extent, to the classical Rankine–Hugoniot conditions for gases. The problem which still remains unsolved is connected with the admissibility (selection) criterion for the shock waves. We shall return to this problem in a separate forthcoming paper.

2. The model

We consider temperature-independent processes in a two-component porous medium described by the following six fields:

$$(\mathbf{x}, t) \mapsto \left\{ \varrho_t^S, \varrho_t^F, \mathbf{v}^S, \mathbf{v}^F, n, \mathbf{e}^S \right\}, \qquad \mathbf{x} \in \mathcal{B}_t, \quad t \in \mathcal{T}, \tag{2.1}$$

where ϱ_t^S denotes the current mass density of the skeleton, ϱ_t^F – the current mass density of the fluid, $\mathbf{v}^S$ – the velocity field of the skeleton, $\mathbf{v}^F$ – the velocity field of the fluid, n – porosity, and $\mathbf{e}^S$ – the symmetric deformation tensor of the skeleton.

The field equations for these fields follow from the balance equations of partial mass and momentum for both components and from the balance equation for porosity. In addition, the velocity field $\mathbf{v}^S$ and the deformation tensor $\mathbf{e}^S$ must satisfy the integrability condition. Under the following assumption of small deformation of the skeleton:

$$\sup_{|\mathbf{n}|=1} \left| \mathbf{e}^S \cdot \mathbf{n} \otimes \mathbf{n} \right| \ll 1, \tag{2.2}$$

these balance equations have the form presented in the table below. On the left-hand side, we quote the equations in points $\mathbf{x} \in \mathcal{B}_t$ in which the fields are of the class C^1 with respect to time and space variables. On the left-hand side, we quote the dynamical compatibility relations in points of a singular surface, on which the fields may have finite discontinuities.

In addition to the small deformation of the skeleton (2.2), it has been assumed that the speed of the relative motion $|\mathbf{v}^F - \mathbf{v}^S|$ is much smaller than the partial speeds of components. This yields the linearity of the diffusive forces in the momentum balance equations. We assume as well that the deviation of porosity from the equilibrium value $\Delta = n - n_E$ is much smaller than unity.

Table 1.

regular point $\mathbf{x} \in \mathcal{B}_t$		singular point $\mathbf{x} \in \mathcal{S}_t$	
(2.3)	$\dfrac{\partial \varrho_t^S}{\partial t} + \operatorname{div}(\varrho_t^S \mathbf{v}^S) = 0,$	(2.9)	$[[\varrho_t^S(\mathbf{v}^S \cdot \mathbf{n} - c)]] = 0,$
(2.4)	$\dfrac{\partial \varrho_t^F}{\partial t} + \operatorname{div}(\varrho_t^F \mathbf{v}^F) = 0,$	(2.10)	$[[\varrho_t^F(\mathbf{v}^F \cdot \mathbf{n} - c)]] = 0,$
(2.5)	$\varrho_t^F \left(\dfrac{\partial \mathbf{v}^F}{\partial t} + \operatorname{grad} \mathbf{v}^F \mathbf{v}^F \right) = -\operatorname{grad} p^F - \pi(\mathbf{v}^F - \mathbf{v}^S),$	(2.11)	$[[\varrho_t^F(\mathbf{v}^F \cdot \mathbf{n} - c)\mathbf{v}^F]] = -[[p^F]]\,\mathbf{n},$
(2.6)	$\dfrac{\partial \Delta}{\partial t} + \mathbf{v}^S \cdot \operatorname{grad} \Delta + \varphi \operatorname{div}(\mathbf{v}^F - \mathbf{v}^S) = -\dfrac{\Delta}{\tau}, \quad \Delta := n - n_E.$	(2.12)	$[[\varrho_t^S(\mathbf{v}^S \cdot \mathbf{n} - c)\Delta]] + \varphi \varrho^S [[\mathbf{v}^F - \mathbf{v}^S]] \cdot \mathbf{n} = 0,$
(2.7)	$\varrho^S \dfrac{\partial \mathbf{v}^S}{\partial t} = \operatorname{div} \mathbf{T}^S + \pi(\mathbf{v}^F - \mathbf{v}^S),$	(2.13)	$[[\varrho_t^S(\mathbf{v}^S \cdot \mathbf{n} - c)\mathbf{v}^S]] - [[\mathbf{T}^S]]\,\mathbf{n} = 0,$
(2.8)	$\dfrac{\partial \mathbf{e}^S}{\partial t} = \dfrac{1}{2}\left(\operatorname{grad} \mathbf{v}^S + \operatorname{grad}^T \mathbf{v}^S \right),$	(2.14)	$[[\mathbf{e}^S]] + \dfrac{1}{2c}[[\mathbf{v}^S \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{v}^S]] = 0,$

The constitutive relations for poroelastic materials are assumed to have the form

$$(2.15)\ (^1) \qquad p^F = \wp^F(\varrho_t^F; n_E) + \beta\Delta, \qquad \mathbf{T}^S = \lambda^S(\mathbf{e}^S \cdot \mathbf{1})\mathbf{1} + 2\mu^S \mathbf{e}^S + \beta\Delta\mathbf{1},$$

where all constitutive parameters λ^S, μ^S, φ, β, π and τ depend solely on the equilibrium constant value of the porosity n_E. This is the value of porosity, which

(0) In my previous works the material constant describing the coupling of stresses has been denoted by $\mathcal{M}$. It is related to β in the following way: $\beta = \varphi(\mathcal{M}\tau)^{-1}$.

the material reaches after the full relaxation under the constant load. In addition, the propagation of shock waves, considered further in this work, is considered for the following form of the intrinsic pressure $\wp^F$:

$$\frac{d\wp^F}{\wp^F} = \gamma \frac{d\varrho_t^F}{\varrho_t^F}, \quad \Rightarrow \quad U^{F2} := \frac{\partial \wp^F}{\partial \varrho_t^F} = \gamma \frac{\wp^F}{\varrho_t^F}, \tag{2.16}$$

where γ is a constant.

Let us notice that the solution of equation (2.3) for small deformations of the skeleton

$$\varrho_t^S \approx (1 - \mathbf{e}^S \cdot \mathbf{1})\varrho^S \approx \varrho^S, \tag{2.17}$$

allows us to eliminate ϱ_t^S from the list of fields in regular points. It is not any more the case of the singular surfaces as we will see further in this work.

3. Propagation condition for plane waves, evolution of the amplitude

3.1. Speeds and amplitudes of weak discontinuity waves

In this section we consider a simple case of propagation of plane waves. The purpose of these considerations is primarily the derivation of the so-called evolution equation of the amplitude of the weak discontinuity waves. The solution of this equation leads to the time of existence of classical solutions of the field equations. For a given set of initial conditions, it enables the analysis of the growth of shock waves.

We consider the motion of both components to be described by the single component of velocities v^F and v^S in the direction of x-axis. The deformation $\mathbf{e}^S$ reduces to the extension in the x-direction e^S. Simultaneously, in order to estimate the magnitude of contribution of various effects, we introduce the dimensionless description. In the definition of dimensionless quantities, we use the material parameters U^S, τ and ϱ^S. Namely,

$$\begin{aligned}
&\widehat{t} = \frac{t}{\tau}, \qquad \widehat{x} = \frac{x}{U^S \tau}, \qquad U^S := \sqrt{\frac{\lambda^S + 2\mu^S}{\varrho^S}}, \\
&\widehat{\varrho}^F = \frac{\varrho_t^F}{\varrho^S}, \qquad \widehat{v}^F = \frac{v^F}{U^S}, \qquad \widehat{v}^S = \frac{v^S}{U^S}, \qquad \widehat{\Delta} = \Delta, \qquad \widehat{e}^S = e^S, \\
&\widehat{\wp}^F = \frac{\wp^F}{\varrho^S U^{S2}} \Rightarrow \frac{\partial \widehat{\wp}^F}{\partial \widehat{\varrho}^F} = (U^S)^{-2} \frac{\partial \wp^F}{\partial \varrho_t^F} \equiv \left(\frac{U^F}{U^S}\right)^2, \qquad U^F = \sqrt{\frac{\partial \wp^F}{\partial \varrho_t^F}}, \\
&\widehat{\varphi} = \varphi, \qquad \widehat{\beta} = \frac{\beta}{\varrho^S U^{S2}}, \qquad \widehat{\pi} = \frac{\pi \tau}{\varrho^S}.
\end{aligned} \tag{3.1}$$

Consequently, the set of unknown fields is as follows:

$$\mathbf{w} := \left(\widehat{\varrho}_t^F, \widehat{v}^F, \widehat{\Delta}, \widehat{v}^S, \widehat{e}^S\right)^T \in \mathcal{V}^5, \qquad (\widehat{x}, \widehat{t}) \mapsto \mathbf{w} \in \Re^5, \quad \widehat{x} \in \Re^1, \quad \widehat{t} \in \Re^1. \tag{3.2}$$

These fields satisfy the field equations following from (2.4)–(2.8), i.e.

$$\begin{aligned}
&\frac{\partial \widehat{\varrho}^F}{\partial \widehat{t}} + \widehat{v}^F \frac{\partial \widehat{\varrho}^F}{\partial \widehat{x}} + \widehat{\varrho}^F \frac{\partial \widehat{v}^F}{\partial \widehat{x}} = 0,\\
&\frac{\partial \widehat{v}^F}{\partial \widehat{t}} + \widehat{v}^F \frac{\partial \widehat{v}^F}{\partial \widehat{x}} + \left(\frac{1}{\widehat{\varrho}^F} \frac{\partial \widehat{\wp}^F}{\partial \widehat{\varrho}^F}\right) \frac{\partial \widehat{\varrho}^F}{\partial \widehat{x}} + \frac{\widehat{\beta}}{\widehat{\varrho}^F} \frac{\partial \widehat{\Delta}}{\partial \widehat{x}} = -\frac{\widehat{\pi}}{\widehat{\varrho}^F}\left(\widehat{v}^F - \widehat{v}^S\right),\\
&\frac{\partial \widehat{\Delta}}{\partial \widehat{t}} + \widehat{v}^F \frac{\partial \widehat{\Delta}}{\partial \widehat{x}} + \widehat{\varphi} \frac{\partial}{\partial \widehat{x}}\left(\widehat{v}^F - \widehat{v}^S\right) = -\widehat{\Delta},\\
&\frac{\partial \widehat{v}^S}{\partial \widehat{t}} - \frac{\partial \widehat{e}^S}{\partial \widehat{x}} - \beta \frac{\partial \widehat{\Delta}}{\partial \widehat{x}} = \widehat{\pi}\left(\widehat{v}^F - \widehat{v}^S\right),\\
&\frac{\partial \widehat{e}^S}{\partial \widehat{t}} - \frac{\partial \widehat{v}^S}{\partial \widehat{x}} = 0.
\end{aligned} \tag{3.3}$$

We write this set of equations in the form

$$\frac{\partial w_\alpha}{\partial \widehat{t}} + A_{\alpha\beta} \frac{\partial w_\beta}{\partial \widehat{x}} = B_\alpha, \qquad \alpha = 1, ..., 5, \tag{3.4}$$

with the following definitions of the matrices **A** and **B**

$$(A_{\alpha\beta}) = \begin{pmatrix}
\widehat{v}^F & \widehat{\varrho}^F & 0 & 0 & 0\\
\dfrac{1}{\widehat{\varrho}^F} \dfrac{\partial \widehat{\wp}^F}{\partial \widehat{\varrho}^F} & \widehat{v}^F & \dfrac{\widehat{\beta}}{\widehat{\varrho}^F} & 0 & 0\\
0 & \widehat{\varphi} & \widehat{v}^F & -\widehat{\varphi} & 0\\
0 & 0 & -\widehat{\beta} & 0 & -1\\
0 & 0 & 0 & -1 & 0
\end{pmatrix}, \tag{3.5}$$

$$(B_\alpha) = \left(0 \quad -\frac{\widehat{\pi}}{\widehat{\varrho}^F}\left(\widehat{v}^F - \widehat{v}^S\right) \quad -\Delta \;\; \widehat{\pi}\left(\widehat{v}^F - \widehat{v}^S\right) \quad 0\right).$$

Hyperbolicity of the set of field equations (3.4) means that the eigenvalues of the matrix **A** are real and the eigenvectors of this matrix span the space of solutions. We proceed to find these eigenvalues and eigenvectors.

We solve the equation for the eigenvalues

$$\det\left(A_{\alpha\beta} - \lambda \delta_{\alpha\beta}\right) = 0, \tag{3.6}$$

under the assumption

$$\left|\widehat{v}^F\right| \ll 1 \;\Rightarrow\; \lambda \approx \lambda_0 + \widehat{v}^F \lambda_1. \tag{3.7}$$

For λ_0 we easily obtain the following values:

$$\lambda_0^{(1)} = 0,$$

$$\left(\lambda_0^{(2-5)}\right)^2 = \frac{1}{2}\left\{1 + \frac{\partial\widehat{\wp}^F}{\partial\widehat{\varrho}^F} + \left(1 + \frac{1}{\widehat{\varrho}^F}\right)\widehat{\varphi}\widehat{\beta} \pm \sqrt{\left[1 - \frac{\partial\widehat{\wp}^F}{\partial\widehat{\varrho}^F} + \left(1 - \frac{1}{\widehat{\varrho}^F}\right)\widehat{\varphi}\widehat{\beta}\right]^2 + 4\frac{\widehat{\varphi}^2\widehat{\beta}^2}{\widehat{\varrho}^{F2}}}\right\}. \tag{3.8}$$

For the second term λ_1 in the perturbation series (3.7), we have

$$\lambda_1 = \frac{a}{b}, \qquad a := -2\lambda_0^2\left(\lambda_0^2 - 1 - \widehat{\varphi}\widehat{\beta}\right) - \left(\lambda_0^2 - \frac{\partial\widehat{\wp}^F}{\partial\widehat{\varrho}^F} - \frac{\widehat{\varphi}\widehat{\beta}}{\widehat{\varrho}^F}\right)(\lambda_0^2 - 1),$$

$$b := -2\lambda_0^2\left(\lambda_0^2 - 1 - \widehat{\varphi}\widehat{\beta}\right) - \left(\lambda_0^2 - \frac{\partial\widehat{\wp}^F}{\partial\widehat{\varrho}^F}\right)\left[(\lambda_0^2 - 1) + 2\lambda_0^2 - \widehat{\varphi}\widehat{\beta}\right] + \left[(\lambda_0^2 - 1) + 2\lambda_0^2\right]\frac{\widehat{\varphi}\widehat{\beta}}{\widehat{\varrho}^F}. \tag{3.9}$$

It can be easily checked that this contribution is of the order of magnitude of the unity. This means that we can limit the attention to the zeroth approximation (3.8) of the eigenvalues. Due to the assumption of a small deviation from the thermodynamical equilibrium, we can hardly distinguish between the contributions of $\widehat{v}^F$ and $\widehat{v}^S$ anyway. Consequently, we use the approximation $\lambda \approx \lambda_0$.

Let us notice that relations (3.8) reduce to the classical relations for speeds of propagation of longitudinal waves in the elastic solid and the ideal fluid, respectively, if the coupling coefficient $\varphi\beta$ vanishes. The normalized right and left eigenvectors follow in the form

$$\mathbf{r} = \frac{\overline{\mathbf{r}}}{\overline{r}}, \qquad \overline{\mathbf{r}} := \left(\frac{\lambda^2 - 1}{\lambda^2 - \frac{\partial\widehat{\wp}^F}{\partial\widehat{\varrho}^F}}, \frac{\lambda}{\widehat{\varrho}^F}\frac{\lambda^2 - 1}{\lambda^2 - \frac{\partial\widehat{\wp}^F}{\partial\widehat{\varrho}^F}}, \frac{1}{\widehat{\beta}}(\lambda^2 - 1), -\lambda, 1\right)^T,$$

$$\overline{r} := \sqrt{\overline{\mathbf{r}}\cdot\overline{\mathbf{r}}}, \tag{3.10}$$

$$\mathbf{l} = \frac{\overline{\mathbf{l}}}{\overline{l}}, \qquad \overline{\mathbf{l}} := \left(\frac{1}{\widehat{\varrho}^F}\frac{\partial\widehat{\wp}^F}{\partial\widehat{\varrho}^F}\frac{\lambda^2 - 1}{\lambda^2 - \frac{\partial\widehat{\wp}^F}{\partial\widehat{\varrho}^F}}, \lambda\frac{\lambda^2 - 1}{\lambda^2 - \frac{\partial\widehat{\wp}^F}{\partial\widehat{\varrho}^F}}, \frac{1}{\widehat{\varphi}}(\lambda^2 - 1), -\lambda, 1\right),$$

$$\overline{l} := \sqrt{\overline{\mathbf{l}}\cdot\overline{\mathbf{l}}},$$

Evaluation of the jump of field equations (3.4) yields easily the following property of the amplitude of the weak discontinuity, i.e. the jump of the gradient of the field $\mathbf{w}$. We have

$$(3.11)\qquad [[\mathbf{w}]] = 0 \;\Rightarrow\; \left[\left[\frac{\partial \mathbf{w}}{\partial \widehat{t}}\right]\right] + \mathbf{A}\left[\left[\frac{\partial \mathbf{w}}{\partial \widehat{x}}\right]\right] = (\mathbf{A} - c\mathbf{1})\left[\left[\frac{\partial \mathbf{w}}{\partial \widehat{x}}\right]\right] = 0$$

$$\Rightarrow\; \widehat{c} = \lambda \,\&\, \left[\left[\frac{\partial \mathbf{w}}{\partial \widehat{x}}\right]\right] = \mathsf{a}\,\mathbf{r}, \qquad \mathsf{a} := \sqrt{\left[\left[\frac{\partial \mathbf{w}}{\partial \widehat{x}}\right]\right] \cdot \left[\left[\frac{\partial \mathbf{w}}{\partial \widehat{x}}\right]\right]}, \qquad \widehat{c} := \frac{c}{U^S},$$

i.e. the speeds of propagation are identical with the eigenvalues of the matrix $\mathbf{A}$, and the amplitude of discontinuity is parallel to the right eigenvector of the matrix $\mathbf{A}$.

3.2. Evolution of the amplitude

We proceed to investigate the time changes of the magnitude a of the amplitude. In order to simplify the calculations we assume that the medium ahead of the wave (i.e. on the positive side of the surface which is defined, in general, by the direction of the normal vector $\mathbf{n}$) is in the static undeformed state. Then the differentiation of the field equations with respect to x, multiplication by the right eigenvector and evaluation of the jump on the singular surface yields the following equation:

$$(3.12)\qquad \frac{\delta \mathsf{a}}{\delta \widehat{t}} - \Gamma_1 \mathsf{a}^2 + \Gamma_2 \mathsf{a} = 0, \qquad \frac{\delta}{\delta \widehat{t}} := \frac{\partial}{\partial \widehat{t}} + \lambda \frac{\partial}{\partial \widehat{x}},$$

where

$$(3.13)\qquad \Gamma_1 := \frac{1}{\mathbf{l}\cdot\mathbf{r}} l_\alpha \frac{\partial A_{\alpha\beta}}{\partial w_\gamma} r_\gamma r_\beta, \qquad \Gamma_2 := \frac{1}{\mathbf{l}\cdot\mathbf{r}} l_\alpha \frac{\partial B_\alpha}{\partial w_\gamma} r_\gamma,$$

and the standard kinematical compatibility conditions have been used. The eigenvectors and the coefficients Γ_1 and Γ_2 are known because they are evaluated for the fields in the static undeformed state ahead of the wave, i.e.

$$(3.14)\qquad \mathbf{w}^+ = \left(\widehat{\varrho}^{F+} = \frac{\varrho_0^F}{\varrho^S},\ \widehat{v} = 0,\ \widehat{\Delta} = 0,\ \widehat{v}^S = 0,\ e^S = 0\right)^T.$$

The evolution equation of the amplitude (3.12) is of the Bernuolli type and it is typical for the quasi-linear hyperbolic systems of equations (e.g. see: M.F. MCCARTHY [3]). Certainly, it can be immediately solved. In the most general case, we have

$$(3.15)\qquad \frac{1}{\mathsf{a}} = \frac{1}{\mathsf{a}_0}\exp\left(\Gamma_2(\widehat{t} - \widehat{t}_0)\right) - \int_{\widehat{t}_0}^{\widehat{t}} \Gamma_1 \exp\left(\Gamma_2(\widehat{t} - \eta)\right) d\eta, \qquad \mathsf{a}_0 := \mathsf{a}(\widehat{t} = \widehat{t}_0).$$

Let us mention a few most important properties of the above evolution equation. First of all, it is obvious that the nonlinearity of the field equations is necessary for the existence of the non-zero coefficient Γ_1. If this is not the case, the evolution of the amplitude has an exponential character. Such an amplitude is constant if the sources **B** are absent and it grows or decays exponentially otherwise.

The situation changes in the case of presence of Γ_1. Then it may happen that the amplitude a grows to infinity in a finite time – say t_c. According to the relation (3.15), it can happen iff

$$\exp\left(\Gamma_2(\hat{t}_c - \hat{t}_0)\right) = \mathsf{a}_0 \int_{\hat{t}_0}^{\hat{t}_c} \Gamma_1 \exp\left(\Gamma_2(\hat{t}_c - \eta)\right) d\eta \,. \tag{3.16}$$

Consequently, the existence of the critical time t_c depends on the initial data, on the signs of coefficients Γ_1, Γ_2, as well as on the choice of the characteristic, i.e. on the choice of the eigenvalue of **A** and of the corresponding eigenvector. We shall investigate this problem for the system (3.4).

Bearing in mind the form (3.5) of the matrix **A**, we obtain after easy manipulations the following form of the coefficients Γ_1, Γ_2:

$$\Gamma_1 = \frac{\lambda^+}{\varrho_0^{F2}\mathbf{l}\cdot\mathbf{r}} \left(\frac{\lambda^{+2} - 1}{\lambda^{+2} - \left(\dfrac{U^{F+}}{U^{S+}}\right)^2} \right)^3 \cdot \left[\varrho_0^F \frac{\partial^2 \wp^F}{\partial \varrho^{F2}}\bigg|^+ + 2\left(\frac{U^{F+}}{U^{S+}}\right)^2 + \frac{\varrho_0^F}{\varphi\beta}\left(\lambda^{+2} - \left(\frac{U^{F+}}{U^{S+}}\right)^2\right)\right],$$

$$\Gamma_2 = \frac{1}{\mathbf{l}\cdot\mathbf{r}} \left\{ \lambda^{+2} \left(\frac{\lambda^{+2} - 1}{\lambda^{+2} - \left(\dfrac{U^{F+}}{U^{S+}}\right)^2} \right)^2 \frac{\pi}{\varrho_0^{F2}} \right.$$

$$\left. + 2\lambda^{+2} \frac{\lambda^{+2} - 1}{\lambda^{+2} - \left(\dfrac{U^{F+}}{U^{S+}}\right)^2} \frac{\pi}{\varrho_0^F} + \frac{(\lambda^{+2} - 1)^2}{\varphi\beta} + \lambda^{+2}\pi \right\}, \tag{3.17}$$

$$\lambda^{+2} \equiv \frac{1}{2}\left\{ 1 + \left(\frac{U^{F+}}{U^{S+}}\right)^2 + \left(1 + \frac{1}{\varrho_0^F}\right)\varphi\beta \right.$$

$$\left. \pm \sqrt{\left[1 - \left(\frac{U^{F+}}{U^{S+}}\right)^2 - \left(1 + \frac{1}{\varrho_0^F}\right)\varphi\beta\right]^2 + 4\varphi\beta\left(1 - \left(\frac{U^{F+}}{U^{S+}}\right)^2\right)} \right\},$$

where we have skipped the hat for the typographical reasons. The plus sign means that the quantity should be evaluated in the state $\mathbf{w}^+$ given by (3.14).

For the zero value of λ both coefficients vanish. Consequently, the amplitude of discontinuity a does not change in time along this characteristic.

It remains to establish the initial conditions. We have in general

$$\left[\left[\frac{\partial \mathbf{w}}{\partial \widehat{x}}\right]\right] = -\left(\frac{\partial \mathbf{w}}{\partial \widehat{x}}\right)^- = \mathsf{a}\,\mathbf{r}, \tag{3.18}$$

i.e.

$$\left.\frac{\partial \widehat{\varrho}^F}{\partial \widehat{x}}\right|^- = -\mathsf{a}\,r_1, \qquad \left.\frac{\partial \widehat{v}^F}{\partial \widehat{x}}\right|^- = -\mathsf{a}\,r_2, \qquad \left.\frac{\partial \widehat{\Delta}}{\partial \widehat{x}}\right|^- = -\mathsf{a}\,r_3,$$

$$\left.\frac{\partial \widehat{v}^S}{\partial \widehat{x}}\right|^- = -\mathsf{a}\,r_4, \qquad \left.\frac{\partial \widehat{e}^S}{\partial \widehat{x}}\right|^- = -\mathsf{a}\,r_5.$$

Let us consider the case of a given initial acceleration of the fluid component. For a given a_0^F, we have

$$\left.\frac{\partial \widehat{v}^F}{\partial \widehat{t}}\right|^-_{t=t_0} = \frac{\tau}{U^S} a_0^F, \qquad \text{i.e.} \qquad \left.\frac{\partial \widehat{v}^F}{\partial \widehat{t}}\right|^-_{t=t_0} = -\frac{1}{\lambda^+}\frac{\tau}{U^S} a_0^F = -\mathsf{a}|_{t=t_0} r_2\,. \tag{3.19}$$

Bearing in mind the relation (3.10) for the eigenvector, we get finally

$$\mathsf{a}_0 := \mathsf{a}|_{t=t_0} = \frac{\widehat{\varrho}^{F+}}{\lambda^{+2}} \frac{\lambda^{+2} - \left(\dfrac{U^{F+}}{U^{S+}}\right)^2}{\lambda^{+2} - 1} \frac{\tau}{U^S} a_0^F\,. \tag{3.20}$$

This choice of the initial conditions has no essential influence on the qualitative properties of the amplitude a. This is due to the fact that the initial disturbance of any quantity appearing in (3.18) yields the disturbances of all the remaining gradients. Consequently, it is solely the problem of proper normalization of initial conditions.

It is seen that the coefficients Γ_1, Γ_2 and the eigenvectors $\mathbf{r}^+$, $\mathbf{l}^+$ are constant in this example. Hence we can easily integrate in (3.16). It follows that

$$\widehat{t}_c = \widehat{t}_0 - \frac{1}{\Gamma_2} \ln\left(1 - \frac{\Gamma_2}{\mathsf{a}_0 \Gamma_1}\right). \tag{3.21}$$

Then the existence of positive critical times requires that the initial amplitude must be greater than the critical value given by the relation

$$\mathsf{a}_c := \frac{\Gamma_2}{\Gamma_1} > 0. \tag{3.22}$$

If this is the case, the classical solution of field equations ceases to exist and the shock wave is created. It shall happen on the characteristic with the shortest critical time. Consequently, in order to find it, we have to check four characteristic critical times for the present example.

We illustrate these conditions by a numerical example. We choose the following data of material parameters:

$$
\begin{aligned}
&U^S = 1.5 \times 10^3 \mathrm{m/s}, \quad U_0^F = 0.9 \times 10^3 \mathrm{m/s}, \quad n_E = 0.4, \quad \varphi = 0.4,\\
&\varrho^S = 1.2 \times 10^3 \mathrm{kg/m^3}, \quad \varrho_0^F = 0.4 \times 10^3 \mathrm{kg/m^3},\\
&\pi = 10^7 \mathrm{kg/m^3 s}, \quad \tau = 10^{-5} \mathrm{s}, \quad \beta = 0.3 \times 10^9 \mathrm{m^2/s^2}.
\end{aligned} \tag{3.23}
$$

They describe a rather soft skeleton (the relatively small value of the speed U^S) with the coefficient of permeability π smaller than the typical values for, say, rocks. These data have the order of magnitude typical for, for instance, biological tissues.

For these data, the critical initial acceleration, defined by the relation (3.22), has the value $a_0^F = 11.43\,\mathrm{m/s^2}$. Consequently, one can expect the growth of the shock wave in this two-component system provided the initial acceleration is large enough.

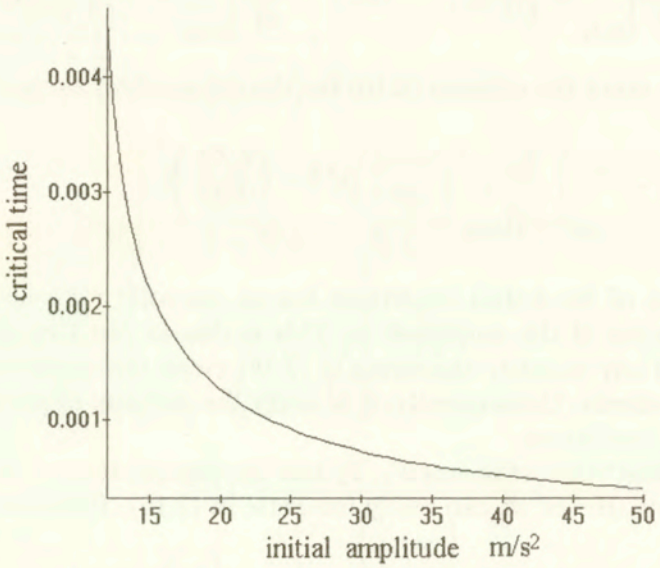

FIG. 1. Critical time in [s] vs. initial amplitude in [m/s^2] for the data (3.23).

In Fig. 1, we present the critical time as the function of the initial amplitude. As expected, this time becomes shorter for larger amplitudes. Also its order of magnitude seems to be realistic even though we are not aware of the experimental data, from which this time could be estimated.

4. On strong discontinuity waves

As pointed out in the analysis of the critical time for the weak discontinuity waves, the nonlinearity of the constitutive relation for the intrinsic part of the pressure in the fluid $\wp^F(\varrho_t^F; n_E)$ indicates the possibility of growth of the shock waves, i.e. the waves carrying strong discontinuities. They are not described by the local field equations (2.3)–(2.8) any more. We have to construct weak solutions of those equations. Very little has been done in this respect for the case of multicomponent continua. In this work, we show solely some basic properties of shock waves for the simple model under consideration which follow from the jump conditions (2.9)–(2.14). As before, we assume the body to be undisturbed ahead of the shock wave, i.e. its state is supposed to be $\mathbf{w}^+$ given by (3.14). Bearing in mind the relations

$$
\begin{aligned}
\left[\left[\mathbf{e}^S \cdot \mathbf{1}\right]\right] = \left[\left[\mathbf{e}^S \cdot (\mathbf{n} \otimes \mathbf{n})\right]\right] &= -\frac{1}{c}\left[\left[\mathbf{v}^S \cdot \mathbf{n}\right]\right], \\
\left[\left[\mathbf{e}^S - \mathbf{e}^S \cdot \mathbf{n}\,\mathbf{1}\right]\right]\mathbf{n} &= -\frac{1}{2c}\left[\left[\mathbf{v}^S - \mathbf{v}^S \cdot \mathbf{n}\,\mathbf{n}\right]\right],
\end{aligned} \tag{4.1}
$$

which follow from the jump condition (2.14), the remaining jump conditions yield the following relations:

$$
\begin{aligned}
\left[\left[\mathbf{e}^S \cdot \mathbf{1}\right]\right] &= \varrho^S \left[\left[\frac{1}{\varrho_t^S}\right]\right], \qquad \left[\left[\mathbf{v}^F \cdot \mathbf{n}\right]\right] = -\varrho_0^F \left[\left[\frac{1}{\varrho_t^F}\right]\right]\mathbf{c}, \\
[[\Delta]] &= \frac{\varphi}{c^3}\left[\left[\wp^F\right]\right] + \varphi\left[\left[\mathbf{e}^S \cdot \mathbf{1}\right]\right], \\
\left[\left[\mathbf{e}^S \cdot \mathbf{1}\right]\right] &= \frac{\varphi\beta}{c^3\varrho^S}\left(c^2 - \frac{\lambda^S + 2\mu^S}{\varrho^S} - \frac{\varphi\beta}{c\varrho^S}\right)^{-1}\left[\left[\wp^F\right]\right], \\
\left[\left[\mathbf{v}^F - \mathbf{v}^F \cdot \mathbf{n}\,\mathbf{n}\right]\right] &= 0, \qquad \left(c^2 - \frac{\mu^S}{\varrho^S}\right)\left[\left[\mathbf{v}^S - \mathbf{v}^S \cdot \mathbf{n}\,\mathbf{n}\right]\right] = 0, \\
\varrho_0^{F2} c^2 &= -\frac{\left[\left[\wp^F\right]\right]}{\left[\left[\frac{1}{\varrho_t^F}\right]\right]}.
\end{aligned} \tag{4.2}
$$

These relations should be read in the following way. The formulae (4.1) together with $(4.2)_{1-4}$ determine the jumps of ϱ_t^S, $\mathbf{e}^S \cdot \mathbf{1}$, $\mathbf{v}^S \cdot \mathbf{n}$, $\mathbf{v}^F \cdot \mathbf{n}$ and Δ in terms of the jumps of the mass density of the fluid ϱ_t^F and of the intrinsic pressure p^F which are, in turn, connected by the barotropic constitutive relation (2.16). According to $(4.2)_5$, the admissible discontinuity of the fluid velocity $\mathbf{v}^F$ reduces to the component in the direction of propagation $\mathbf{n}$. The tangential component must be continuous. On the other hand, according to $(4.2)_6$, the tangential component of velocity of the skeleton $\mathbf{v}^S$ can be discontinuous but its discontinuity propagates

with the velocity of transversal sound wave equal to $\sqrt{\mu^S/\varrho^S}$. Hence, it can be solely due to initial conditions and does not grow during the motion of the body.

The last relation $(4.2)_7$ determines the speed of propagation of such waves if the jump of the mass density ϱ_t^F is given. This relation is identical with the classical Rankine–Hugoniot condition for shock waves in gases.

The investigation of the one-dimensional problem of construction of weak solutions accounting for these relations and the analogy to the theory of shock waves in gases is in progress and it shall be presented in a forthcoming paper.

5. Concluding remark

In spite of the practical – in particular, medical – applications of shock waves in porous materials, the theoretical research in this field has not made much progress since many years. This is due to the two following main reasons. First of all, it is very difficult to extend the methods of solutions of one-dimensional hyperbolic problems to higher spatial dimensions. Unfortunately, such an extension is necessary in practical applications of shock waves in porous materials (e.g. in lithotripsy). Secondly, in the case of more than two fields, very little is known about the criteria of choice of a weak solution. It is known that the usual entropy criterion does not yield uniqueness of solution and an alternative is not yet known. This problem was only indicated in the present work.

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WEIERSTRASS-INSTITUT FÜR ANGEWANDTE ANALYSIS UND STOCHASTIC
Mohrenstraße 39, D-10117 Berlin, Germany.
e-mail: wilmansk@wias-berlin.de

Received October 7, 1997.

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Arch. Mech. T. 50, nr 3, str. 341 – 672, Warszawa 1998.