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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

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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 $\nabla_R \theta$)

$$\left.\frac{\partial S}{\partial t}\right|_{\mathbf{X}} + \nabla_R \cdot (\mathbf{Q}/\theta) = \sigma^{\mathrm{th}} + \sigma^{\mathrm{intr}}, \tag{2.5}$$

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].

References

1. J.D. ESHELBY, *Force on an elastic singularity*, Phil. Trans. Roy. Soc. Lond., **244**, 87–112, 1951.
2. M.O. PEACH and J.S. KOEHLER, *Forces exerted on dislocations and the stress field produced by Them*, Phys. Rev., **II-80**, 436–439, 1950.
3. H. ZORSKI, *Theory of discrete defects*, Arch. Mech. Stos., **18**, 301–372, 1966.
4. H. ZORSKI, *Force on a defect in nonlinear elastic medium*, Int. J. Engng. Sci., **19**, 1573–1579, 1981.
5. D. ROGULA, *Forces in material space*, Arch. Mech., **29**, 705–715, 1977.
6. G.A. MAUGIN, *Material inhomogeneities in elasticity*, Chapman and Hall, London 1993.
7. G.A. MAUGIN, *Material forces: Concepts and applications*, Appl. Mech. Rev., **48**, 213–245, 1995.

8. G.A. MAUGIN, *Thermomechanics of inhomogeneous-heterogeneous systems*, ARI, **50**, 41–56, 1997.
9. G.A. MAUGIN and W. MUSCHIK, *Thermodynamics with internal variables*, I-II, J. Non-Equilibr. Thermodynam., **19**, 217–295, 1994.
10. G.A. MAUGIN, *On the structure of the theory of polar elasticity*, Phil. Trans. Roy. Soc. Lond., **A 356**, 1367–1395, 1998.
11. A. FOMETHE and G.A. MAUGIN, *Material forces in thermoelastic ferromagnets*, Cont. Mech. Thermodynam., **8**, 275–292, 1996.
12. C. DASCALU and G.A. MAUGIN, *Material forces and energy-release rate in homogeneous elastic solids with defects*, C.R. Acad. Sci. Paris, **II-317**, 1135–1140, 1993.
13. M. EPSTEIN and G.A. MAUGIN, *Energy-momentum tensor and material uniformity in finite elasticity*, Acta Mechanica, **83**, 127–133, 1990.
14. G.A. MAUGIN, *On shock waves, and phase-transition fronts in continua*, ARI, **50**, 141–149, 1998.
15. P. GERMAIN, *Shock-waves, jump relations and structures*, [in:] Advances in Applied Mechanics, C.S. YIH [Ed.], Vol. 12, pp. 131–194, Academic Press, New York 1972.
16. G.A. MAUGIN and C. TRIMARCO, *The dynamics of configurational forces at phase-transition fronts*, Meccanica, **30**, 605–619, 1995.
17. R.M. BOWEN, *Toward a thermodynamics and mechanics of mixtures*, Arch. Rat. Mech. Anal., **24**, 370–403, 1967.
18. M. GRINFELD, *Thermodynamic methods in the theory of heterogeneous systems*, ISIMM Series, Longman, Harlow, Essex 1991.
19. G.A. MAUGIN and S. CADET, *Existence of solitary waves in martensitic alloys*, Int. J. Engng. Sci., **29**, 243–255, 1991.
20. G.A. MAUGIN and C.I. CHRISTOV, *Nonlinear duality between elastic waves and quasi-particles in microstructured solids*, Proc. Estonian Acad. Sci., **A 46**, 78–94, 1997.
21. G.A. MAUGIN and C.I. CHRISTOV, *Nonlinear wave and conservation laws (Nonlinear duality between elastic waves and quasi-particles)*, [in:] Nonlinear Wave Phenomena, D. INMAN and A. GURAN [Eds.], World Scientific, Singapore [to be published].
22. L.M. TRUSKINOWSKY, *About the "normal growth" approximation in the dynamical theory of phase transitions*, Cont. Mech. and Thermodynam., **6**, 195–208, 1994.

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