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Formulation of balance relations and configurational fields for continua with microstructure and moving point defects via invariance

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Abstract

The purpose of this work is the formulation of models for the dynamics of continua with microstructure and material inhomogeneity. In particular, attention is focused here on the balance relations and configurational fields for such continua obtained via invariance. To this end, the approach of Capriz (Capriz, G., 1989. Springer Tracts in Natural Philosophy, vol. 37) to the formulation of continua with microstructure as based upon the invariance of the internal power with respect to superimposed rigid-body rotations is extended to one based upon the Euclidean frame-indifference of the total energy balance. This is then combined with an extension of the work of Gurtin (Gurtin, M.E., 1995. Arch. Rat. Mech. Anal. 131, 67–100) on the formulation of static configurational fields to the case of dynamic and microstructure. In this way, one obtains in particular the dependence of the configurational momentum density, configurational or Eshelby stress, as well as the internal and external configurational momentum supply rate, or configurational force, densities, on the corresponding microstructural fields. These can then be used to derive the forms of the balance relations relevant to the case that the continuum contains defects at which the microstructure is discontinuous. As an application of the formulation, this is done here for the case of a continuum with microstructure containing a single defect. © 2001 Elsevier Science Ltd. All rights reserved.

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1. Introduction

In order to apply models for materials with microstructure (e.g., multiphase materials, granular or damaged materials, liquid crystals, polycrystals) to the description of the behaviour of actual such materials, one must in general account as well for the fact that these are fundamentally *heterogeneous* in nature, i.e., contain various kinds of material inhomogeneities such as point defects, dislocations, shear bands,

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microcracks, and so on. Attempts to incorporate this fact into the *continuum* modeling of such materials have led to a number of approaches and viewpoints on the issue, depending in part on the nature of the structure or heterogeneity in question. In the context of field-based approaches, for example, the Ozeen–Zöcher–Frank theory forms the basis of a number of comprehensive models for the equilibrium behaviour of nematic liquid crystals containing point and line defects (e.g., Brinkman and Cladis, 1982; Kléman, 1983; Virga, 1994). Such models have been recently extended, on the basis of the Ericksen–Leslie theory, to the dynamic case by Cermelli and Fried (1999), accounting in particular for the effect of microstructural inhomogeneity on the general behaviour via the approach of Gurtin (1995) to configurational forces. A quite different approach, finding application in the realm of polycrystals containing inclusions, microcracks, and so on, is that offered by homogenization and self-consistent methods (e.g., Suquèt, 1998). Here, both microstructure (e.g., texture, different phases, twins) and defects (e.g., microcracks) fall under the rubic of "material inhomogeneity" in the form of a dependence of material properties (e.g., elasticity or compliance tensors) on material element. As implied by the original work of Eshelby (1951, 1970), a field-based description of such material inhomogeneity, and the corresponding forms taken by configurational fields such as the Eshelby stress, depend crucially on the type of microstructure in question. One purpose of the current work is the formulation of such configurational fields including contributions from a general class of microstructure, including such cases as phase transitions, granular and damaged materials, as well as liquid crystals and other materials such as polycrystals possessing an orientation structure as characterized, e.g., by a director field. In particular, this is done here both for the classical case in which the inhomogeneities are smoothly distributed in the material, as well as for the case of point defects.

The formulation to this end is carried out in a dynamical setting via an extension of the approach of Capriz (1989) for continua with microstructure as based on the invariance of the internal power with respect to superimposed rigid-body rotations to the one based on the invariance of the total energy balance with respect to the change [2] of observer. Such an approach has a long tradition; in the realm of pure continuum mechanics, the insight that such invariance of certain "action integrals" can be used to derive mechanical balance relations goes back at least to the work of the Cosserat brothers (Cosserat and Cosserat, 1909; also see, e.g., Truesdell and Toupin, 1960) on rods and shells, and was extended to continua with general microstructure by Toupin (1964) in his theory of oriented hyperelastic materials (see, e.g., Truesdell and Noll, 1992, Section 123). The extension of this idea to the thermodynamical or thermomechanical context was achieved by Green and Rivlin (1964), who used the invariance of the total energy balance with respect to superimposed rigid-body motions to derive the mass, linear momentum, and angular momentum, balances (see, e.g., Marsden and Hughes, 1983, Chapter 2). This approach has been substantially rigourized, extended and generalized by Šilhavý (see, e.g., Šilhavý, 1997, Chapter 6) for general thermodynamic systems via the transformation properties of working and heating with respect to change of observer. Invariance of the total energy balance with respect to change of observer was used by Capriz et al. (1982) to derive balance relations in the case of affine microstructure, by Pitteri (1990) in the context of a statistical mechanical approach to models for microstructure, and most recently by Capriz and Virga (1994) in the context of continua with general microstructure. Central to this approach are (1), the forms taken by the total energy density, total energy flux density, and total energy (external) supply rate density, as well as (2), the transformation properties of the fields in question with respect to the change of

[2] Note that the balance relations obtained via invariance are independent of whether the invariance involved is with respect to superimposed rigid-body motions or with respect to change of observer (i.e., Euclidean frame-indifference). By contrast, in the context of constitutive relations i.e., relations between the fields of interest, Euclidean frame-indifference and invariance with respect to superimposed rigid-body motions are never equivalent (see, e.g., Svendsen and Bertram, 1999). Indeed, in this context, the latter requirement is stronger, i.e., equivalent to those of Euclidean frame-indifference *plus* form-invariance, which together constitute what is commonly known as material frame-indifference.

Euclidean observer. From the point of view of the treatment of observers and the invariance of the energy balance with respect to change of these, the current approach represents in part an extension to the general microstructure of that found in Capriz et al. (1982) for affine microstructure. Comparison of the current approach with the more recent work of Capriz and Virga (1994) on materials with microstructure shows that basic differences arise in (1), the modeling of the microstructural momentum balance, (2), the transformation properties of certain microfields, and (3), the treatment of the kinetic energy and inertia of the microstructure. Except for the latter aspect, however, the resulting balance relations for the microstructure are in essence the same.

The connection with material inhomogeneity and possible defect structure is achieved via a combination of this approach to microstructure with an extension of the recent balance relation, dissipation-based approach of Gurtin (1995) to the formulation of (static) configurational forces to dynamics, in some ways analogous to that of Cermelli and Fried (1997). In particular, such an approach to configurational forces extends earlier variational- or virtual-power-based formulations of such forces (e.g., Maugin et al., 1992; Maugin, 1993) to a non-equilibrium thermodynamic context. Such a combined approach has been used recently by Cermelli and Fried (1999) to formulate evolution equations and configurational fields for defective nematic fluids. Similarly, Mariano (2000) has combined the approach of Capriz (1989) to microstructure with that of Gurtin (1995) to configurational forces and applied the resulting formulation [3] in particular to two-phase continua and continua with singular surfaces.

To begin, the kinematics of a continuum with microstructure is briefly summarized (Section 2). With this in hand, we turn then to the formulation of balances relations for a continuum with microstructure containing no defects (Section 3) on the basis of the Euclidean frame-indifference of the total energy balance for such a continuum. In preparation for the case of a continuum with microstruture and defects, we derive next the forms taken by the configurational fields for a continuum with microstructure and smoothly varying material inhomogeneity (Section 4). After summarizing basic results from the dissipation principle (Section 5) consistent with the current approach for completeness, we turn finally to application of the basic results to the case of a continuum with microstructure and point defects (Section 6). Before we begin, a word on notation. If $\mathscr{W}$ and $\mathscr{Z}$ represent linear spaces, let $\mathrm{Lin}(\mathscr{W},\mathscr{Z})$ represent the set of all linear mappings from $\mathscr{W}$ to $\mathscr{Z}$. If in addition these are inner product spaces, the corresponding inner products induce the transpose $\mathsf{A}^{\mathrm{T}} \in \mathrm{Lin}(\mathscr{Z},\mathscr{W})$ of any $\mathsf{A} \in \mathrm{Lin}(\mathscr{W},\mathscr{Z})$, as well as the inner product $\mathsf{A}\cdot\mathsf{B} := \mathrm{tr}_{\mathscr{W}}(\mathsf{A}^{\mathrm{T}}\mathsf{B}) = \mathrm{tr}_{\mathscr{Z}}(\mathsf{A}\mathsf{B}^{\mathrm{T}})$ on $\mathrm{Lin}(\mathscr{W},\mathscr{Z})$ for all $\mathsf{A},\mathsf{B} \in \mathrm{Lin}(\mathscr{W},\mathscr{Z})$. In this case, we can also identify the symmetric $\mathrm{sym}(\mathsf{A}) := \frac{1}{2}(\mathsf{A}+\mathsf{A}^{\mathrm{T}})$ and skew-symmetric $\mathrm{skw}(\mathsf{A}) := \frac{1}{2}(\mathsf{A}-\mathsf{A}^{\mathrm{T}})$ parts of any $\mathsf{A} \in \mathrm{Lin}(\mathscr{W},\mathscr{W})$; let $\mathrm{Sym}(\mathscr{W},\mathscr{W})$ and $\mathrm{Skw}(\mathscr{W},\mathscr{W})$, respectively, represent the corresponding subspaces of $\mathrm{Lin}(\mathscr{W},\mathscr{W})$. The principle linear space in this work is of course that of three-dimensional Euclidean vector space $\mathscr{V}$. Other mathematical notations and concepts will be introduced as needed in the sequel.

2. Kinematics

Let E represent a three-dimensional Euclidean point space and $B \subset E$ an arbitrary reference configuration of some material body. The motion of the material body with respect to B and E takes as usual the form

$$\xi : I \times B \to E \,|\, (t,b) \mapsto p = \xi(t,b) \tag{2.1}$$

[3] I thank the editors of this special issue for drawing my attention to the work of Capriz and Virga (1994) and Mariano (2000).

over a time interval I, with $\xi_t = \xi(t,\cdot) : B \to E$ a local diffeomorphism for all $t \in I$, and $\xi_b := \xi(\cdot, b) : I \to E$, a smooth curve in E for all $b \in B$. Basic kinematic quantities of interest obtained from Eq. (2.1) include the material velocity

$$\dot{\xi} : I \times B \to \mathscr{V} \tag{2.2}$$

and the deformation gradient

$$\boldsymbol{F} := \nabla\xi : I \times B \to \mathrm{Lin}^+(\mathscr{V}, \mathscr{V}). \tag{2.3}$$

As usual, we have the split

$$\dot{\boldsymbol{F}}\boldsymbol{F}^{-1} = \dot{\overline{(\nabla\xi)}}(\nabla\xi)^{-1} = (\nabla\dot{\xi})(\nabla\xi)^{-1} = \boldsymbol{D} + \boldsymbol{W} : I \times B \to \mathrm{Lin}(\mathscr{V}, \mathscr{V}) \tag{2.4}$$

of the velocity gradient (i.e., expressed as a time-dependent field on B) into its symmetric $\boldsymbol{D} := \mathrm{sym}(\dot{\boldsymbol{F}}\boldsymbol{F}^{-1})$ and skew-symmetric $\boldsymbol{W} := \mathrm{skw}(\dot{\boldsymbol{F}}\boldsymbol{F}^{-1})$ parts.

As discussed in Section 1, continua with microstructure, e.g., granular materials, or liquid crystals, are of interest in this work. Field models for such materials rely on an idealization of the "kinematics" of the microstructure in the form of, in the referential context, a time-dependent field on B, e.g., the Cosserat rotation field, or the director field for uniaxial liquid crystals. From the mathematical point of view, a formulation sufficiently general to encompass such standard models is obtained when this field is assumed to take values in a submanifold [4] $\mathscr{G}$ of some finite-dimensional inner product space $\mathscr{W}$. Let $\imath : \mathscr{G} \to \mathscr{W} of \mathscr{G}$ represent the smooth inclusion of $\mathscr{G}$ into $\mathscr{W}$, and $\pi : \mathscr{W} \to \mathscr{G}$ the corresponding projection of $\mathscr{W}$ onto $\mathscr{G}$, such that $\pi \circ \imath = 1_{\mathscr{G}}$ holds. To simplify the formulation to follow, it is useful to work with the form

$$\varsigma : I \times B \to \mathscr{W} | (t,b) \mapsto \mathscr{s} = \varsigma(t,b) \tag{2.5}$$

of the structure field included into $\mathscr{W}$; in terms of ς, the actual structure field [5] is given by $\pi \circ \varsigma : I \times B \to \mathscr{G}$. Although not important for the formulation of the balance relations, the distinction between ς and $\pi \circ \varsigma$ becomes so for the constitutive relations, which depend directly on $\pi \circ \varsigma$, not ς (see Section 5). Likewise, they depend in general directly on the corresponding (induced) projections of the kinematic fields $\nabla\varsigma : I \times B \to \mathrm{Lin}(\mathscr{V}, \mathscr{W})$, $\dot{\varsigma} : I \times B \to \mathscr{W}$, and $\nabla\dot{\varsigma} : I \times B \to \mathrm{Lin}(\mathscr{V}, \mathscr{W})$ associated with ς onto the corresponding tensor bundles of $\mathscr{G}$.

Turning next to Euclidean observers, these are characterized as usual by the fact that they measure the same time lapses and spatial distances between events in classical spacetime. Because of this, the motion

$$\lambda : I \times E \to E | (t,p) \mapsto p' = \lambda(t,p) \tag{2.6}$$

of an unprimed Euclidean observer with respect to a primed one represents a Euclidean isometry at each $t \in I$, i.e., $\lambda_t := \lambda(t,\cdot) : E \to E$ is an affine isometry for all $t \in I$. Further, $\lambda_p := \lambda(\cdot, p) \in C^2(I, E)\ \ \forall p \in E$. Being an affine isometry for all $t \in I$, λ can be expressed in the form

$$\lambda(t,p) = \lambda(t,o) + \boldsymbol{Q}(t)(p - o) \quad \forall t \in I \text{ and } \forall p, o \in E, \tag{2.7}$$

with

$$\boldsymbol{Q} : I \to \mathrm{Rot}(\mathscr{V}, \mathscr{V}) | t \mapsto (\nabla\lambda)(t,o) =: \boldsymbol{Q}(t) \tag{2.8}$$

[4] For example, in the case of uniaxial nematic liquid crystals, $\mathscr{G}$ could be the unit sphere S^2, a smooth compact submanifold of three-dimensional Euclidean vector space $\mathscr{V} \mathrel{\widehat{=}} \mathscr{W}$. In this case, we have $\imath(\boldsymbol{e}) = \boldsymbol{e}$ for all $\boldsymbol{e} \in S^2$, and $\pi(\boldsymbol{a}) = \boldsymbol{a}/|\boldsymbol{a}|$ for all non-zero $\boldsymbol{a} \in \mathscr{V}$.

[5] It is the projected form $\pi \circ \varsigma$ of ς which corresponds directly to the generic structure field $\boldsymbol{v}$ of Capriz (1989). On the other hand, the current approach is formally simpler than his in the sense that his $\boldsymbol{v}$ takes values on a general finite-dimensional manifold $\mathscr{M}$ which is not necessarily a submanifold of some linear space. Nevertheless, all special cases considered by him can also formulated as special cases of the current, formally simpler framework.

corresponding rotation of λ (independent of $o \in E$). For simplicity, we assume without loss of (physical) generality in what follows that $\boldsymbol{Q}(0) = \mathbf{1}$.

Let $\boldsymbol{\tau}$ be any time-dependent $\mathscr{V}$-tensor field on B with respect to the unprimed observer, and $\boldsymbol{\tau}'$ its counterpart with respect to the primed one. Central to the formulation of the Euclidean frame-indifference of tensor fields and other quantities in this work is the tensor field

$$\Delta\boldsymbol{\tau}(b) := \{\lambda^*\boldsymbol{\tau}' - \boldsymbol{\tau}\}(0, b) \tag{2.9}$$

on B which represents the deviation of $\boldsymbol{\tau}$ from being Euclidean frame-indifferent at (the arbitrary time) $t = 0$, with $\lambda^*\boldsymbol{\tau}'$ the "pull-back" of $\boldsymbol{\tau}'$ to the unprimed observer via λ. Take for example the material velocity $\dot{\xi}$ and its gradient $\nabla\dot{\xi}$. The usual transformation

$$\xi' = \lambda \diamond \xi = \boldsymbol{Q}(\xi - o) + \lambda_o \tag{2.10}$$

of ξ from Eq. (2.7) with $(\lambda \diamond \xi)(t, b) := \lambda(t, \xi(t, b))$ induces via space and time differentiation those

$$\begin{aligned} \dot{\xi}' &= \dot{\boldsymbol{Q}}(\boldsymbol{r}_o \circ \xi) + \dot{\lambda}_o + \boldsymbol{Q}\dot{\xi}, \\ \nabla\dot{\xi}' &= \dot{\boldsymbol{Q}}(\nabla\xi) + \boldsymbol{Q}(\nabla\dot{\xi}), \end{aligned} \tag{2.11}$$

for $\dot{\xi}$ and $\nabla\dot{\xi}$, respectively, with

$$\boldsymbol{r}_o(p) := p - o, \tag{2.12}$$

the position vector of $p = \xi(t, b) \in E$ relative to $o \in E$. In terms of Eq. (2.9), Eq. (2.11) takes the forms

$$\begin{aligned} \Delta\dot{\xi}(b) &= \{\boldsymbol{Q}^{\mathrm{T}}\dot{\xi}' - \dot{\xi}\}(0, b) = \boldsymbol{\Omega}\boldsymbol{r}_o(\xi(0, b)) + \boldsymbol{t}, \\ \Delta(\nabla\dot{\xi})(b) &= \{\boldsymbol{Q}^{\mathrm{T}}(\nabla\dot{\xi}') - \nabla\dot{\xi}\}(0, b) = \boldsymbol{\Omega}(\nabla\xi)(0, b), \end{aligned} \tag{2.13a, b}$$

via Eq. (2.12), with $\boldsymbol{\Omega} := \dot{\boldsymbol{Q}}(0) \in \mathrm{Skw}(\mathscr{V}, \mathscr{V})$ and $\boldsymbol{t} := \dot{\lambda}_o(0) \in \mathscr{V}$ (recall that $\boldsymbol{Q}(0) = \mathbf{1}$). As such, we have $\nabla(\Delta\dot{\xi})(b) = \Delta(\nabla\dot{\xi})(b) = \boldsymbol{\Omega}(\nabla\xi)(0, b)$.

Next, we turn to the transformation properties of the fields representing the kinematics of the microstructure in the formulation. Such transformation properties are determined in part by the physical interpretation of this kinematic field. This issue has been discussed at length in Capriz (1989) for various kinds of microstructure; here, attention is restricted to the class of microstructure for which the kinematic field ς is considered to be Euclidean frame-indifferent, something applying to all special cases of interest (e.g., the director field for uniaxial nematic liquid crystals). From this point of view, ς, which is sometimes interpreted as a "micro-displacement," can be contrasted with the standard displacement field, which is not Euclidean frame-indifferent. Indeed, from the point of view of Euclidean frame-indifference, ς is more akin to, e.g., $\boldsymbol{F}$. In any case, on this basis, the observer transformation (2.7) induces that

$$\varsigma' = \ell(\boldsymbol{Q}, \varsigma) \tag{2.14}$$

of ς via the left action $\ell : \mathrm{Rot}(\mathscr{V}, \mathscr{V}) \times \mathscr{W} \to \mathscr{W}$ of $\mathrm{Rot}(\mathscr{V}, \mathscr{V})$ on $\mathscr{W}$. Consequently, $\Delta\varsigma(b) = \mathbf{0}$ follows from Eq. (2.9). In turn, Eq. (2.14) induces the transformation relations

$$\begin{aligned} \Delta\dot{\varsigma}(b) &= \mathscr{A}_{\varsigma_0}(b)\,\boldsymbol{\Omega}, \\ \Delta(\nabla\dot{\varsigma})(b) &= (\nabla\mathscr{A}_{\varsigma_0})^S(b)\,\boldsymbol{\Omega} \end{aligned} \tag{2.15a, b}$$

for $\dot{\varsigma}$ and $\nabla\dot{\varsigma}$, respectively, which can be compared to Eq. (2.13a,b) for the material velocity $\dot{\xi}$ and its gradient $\nabla\dot{\xi}$. Here, $\varsigma_0 := \varsigma(0, \cdot)$, $\mathscr{A}_\varsigma := \mathscr{A} \circ \varsigma$, and

$$\mathscr{A}(\mathscr{s}) := D_1\ell_{\mathscr{s}} \in \mathrm{Lin}(\mathrm{Skw}(\mathscr{V}, \mathscr{V}), \mathscr{W}) \tag{2.16}$$

represents the action of the Lie algebra $\mathrm{Skw}(\mathscr{V},\mathscr{V})$ of $\mathrm{Rot}(\mathscr{V},\mathscr{V})$ on $\mathscr{W}$ induced by that ℓ of $\mathrm{Rot}(\mathscr{V},\mathscr{V})$ on $\mathscr{W}$, $D_1\ell_{\jmath}$ being the Fréchet derivative of $\ell_{\jmath} := \ell(\cdot,\jmath) : \mathrm{Rot}\ (\mathscr{V},\mathscr{V}) \to \mathscr{W}$ at the identity $\mathbf{1} \in \mathrm{Rot}(\mathscr{V},\mathscr{V})$. Further, the notation $(\nabla\mathscr{A}_{\varsigma_0})^S$ has been introduced for the linear transformation $(\nabla\mathscr{A}_{\varsigma_0})^S(b) \in \mathrm{Lin}(\mathrm{Skw}\ (\mathscr{V},\mathscr{V}),\mathrm{Lin}(\mathscr{V},\mathscr{W}))$ induced by $(\nabla\mathscr{A}_{\varsigma_0})(b) \in \mathrm{Lin}(\mathscr{V},\mathrm{Lin}(\mathrm{Skw}(\mathscr{V},\mathscr{V}),\mathscr{W}))$. In addition, that $\mathscr{A}(\jmath)$ for $D_1\ell_{\jmath}$ reflects the formal correspondence of this mapping with the "infinitesimal generator" mapping [6] introduced by Capriz (1989, Section 3) in this context.

3. Euclidean frame-indifference and balance relations

The formulation of the balance relations for a material with microstructure to follow is caried out in a referential setting. As such, all time-dependent fields to follow will be the ones on B unless otherwise indicated. For simplicity, attention is restricted here to thermomechanical processes that are smooth in time. In this sense, the formulation of the total energy balance pursued here is consistent with, e.g., the more general thermomechanical history-based approach of Šilhavý (1997, Chapter 6). Further, assume for the moment that all fields of interest on B are smooth, i.e., that B contains no singular points, lines or surfaces, i.e., defects.

As already discussed briefly in Section 1, the approach being pursued here to the formulation of balance relations for materials with microstructure is based on the invariance of the total energy balance with respect to Euclidean observer. We begin then with the formulation of this relation. To this end, let [7]

$$\int_P \boldsymbol{h}\cdot\boldsymbol{n} : I \to \mathbb{R} \tag{3.1}$$

represent the total energy flux, and

$$\int_P s : I \to \mathbb{R} \tag{3.2}$$

the total energy supply rate, to the material from its environment (i.e., external) during its motion ξ in E with respect to any $P \subset B$. As usual, $\boldsymbol{h}$ represents the total energy flux density, and s the corresponding supply rate density. Combining Eqs. (3.1) and (3.2) with the total energy [8]

$$\int_P e : I \to \mathbb{R} \tag{3.3}$$

of the system yields the quantity

$$\mathscr{E}(P) := \dot{\overline{\int_P e}} - \int_{\partial P} \boldsymbol{h}\cdot\boldsymbol{n} - \int_P s = \int_P \dot{e} - \operatorname{div}\boldsymbol{h} - s \tag{3.4}$$

measuring the total energy balance of, or in, the system. In particular, the total energy of the system is *balanced* when $\mathscr{E}(P)$ vanishes for all $P \subset B$.

[6] To be precise, Capriz (1989, Section 3) defined this mapping on the axial vectors of the elements of $\mathrm{Skw}(\mathscr{V},\mathscr{V})$.

[7] We leave the volume $\mathrm{d}v$ and surface $\mathrm{d}a$ measures out of the corresponding integral notations in this work for simplicity. In addition, the unit vector field $\boldsymbol{n}$ normal to boundaries of three-dimensional regions is as usual assumed to be *outwardly* directed unless otherwise indicated.

[8] As discussed by Šilhavý (1997, Section 5.3), in the context of the energy balance, the existence of $\int_P e$, and so e, is based upon the so-called accessibility assumption, i.e., that any two thermomechanical states of the material can be connected by some process.

The formulation of the invariance of $\mathscr{E}(P)$ as given in Eq. (3.4) with respect to change of observer is based on the decompositions

$$\begin{aligned} e &= \varrho\varepsilon + \varrho k, \\ \boldsymbol{h} &= -\boldsymbol{q} + \boldsymbol{l}, \\ s &= r + m, \end{aligned} \tag{3.5}$$

of the densities e, $\boldsymbol{h}$ and s into their Euclidean frame-indifferent and observer-dependent parts. In particular, the Euclidean frame-indifferent or "internal" parts of these, i.e., $\varrho\varepsilon$, $\boldsymbol{q}$ and r, represent as usual the internal energy, heat flux, and internal energy supply rate, densities, respectively, with ϱ the mass density. The observer-dependent parts ϱk, $\boldsymbol{l}$ and m represent the kinetic energy, mechanical energy flux, and mechanical external supply rate, densities, respectively. Being Euclidean frame-indifferent, the transformation relations

$$\Delta\varrho = 0, \qquad \Delta\varepsilon = 0, \qquad \Delta\boldsymbol{q} = \boldsymbol{0}, \qquad \Delta r = 0 \tag{3.6a–d}$$

follow via Eq. (2.9) for ϱ, ε, $\boldsymbol{q}$, and r, respectively. In turn, these induce those

$$\Delta e = \varrho\Delta k, \qquad \Delta\boldsymbol{h} = \Delta\boldsymbol{l}, \qquad \Delta s = \Delta m \tag{3.7}$$

for total energy, total energy flux, and total energy external supply rate, density, respectively.

Being of a kinematic or mechanical nature, the class of microstructure under consideration here contributes to the specific kinetic energy k, the total mechanical energy flux density $\boldsymbol{l}$, and corresponding external supply rate density m of the system. Accordingly, we have the generalized forms

$$\begin{aligned} k &= \tfrac{1}{2}\,\dot{\xi}\cdot\dot{\xi} + k_s, \\ \dot{k} &= \ddot{\xi}\cdot\dot{\xi} + \dot{\boldsymbol{\mu}}\cdot\dot{\varsigma}, \\ \boldsymbol{l} &= \boldsymbol{P}^{\mathrm{T}}\dot{\xi} + \boldsymbol{\Sigma}^{\mathrm{T}}\dot{\varsigma}, \\ m &= \boldsymbol{b}\cdot\dot{\xi} + \boldsymbol{\beta}\cdot\dot{\varsigma} \end{aligned} \tag{3.8a–d}$$

for k, $\dot{k}$, $\boldsymbol{l}$ and m, respectively. Here, $\dot{\xi}$ represents the continuum specific momentum, $\boldsymbol{\mu}$ that of the microstructure, $\boldsymbol{P}$ the first Piola-Kirchhoff tress, $\boldsymbol{\Sigma}$ the microstructural stress or momentum flux, $\boldsymbol{b}$ the continuum momentum external supply rate density, $\boldsymbol{\beta}$ the microstructural momentum external supply rate density, and k_s the contribution to k from the microstructure, i.e., from ς and $\dot{\varsigma}$. The form (3.8b) for $\dot{k}$, in particular that $\dot{k}_s = \dot{\boldsymbol{\mu}}\cdot\dot{\varsigma}$ for $\dot{k}_s$, generalizes the "Lagrangian" approach to the formulation of $\dot{k}$ considered by Capriz (1989, Section 7) and Capriz and Virga (1994). In the case of the ubiquitous quadratic form $k_s(\varsigma,\dot{\varsigma}) = \frac{1}{2}\dot{\varsigma}\cdot\boldsymbol{\Theta}(\varsigma)\dot{\varsigma}$ for k_s, for example, $\dot{\boldsymbol{\mu}}$ takes the form $\dot{\boldsymbol{\mu}} = \boldsymbol{\Theta}\ddot{\varsigma} + \frac{1}{2}\dot{\boldsymbol{\Theta}}\dot{\varsigma}$, the specific microinertia tensor $\boldsymbol{\Theta}$ being as usual symmetric and positive-definite.

Now, on the basis of Eqs. (3.5) and (3.8a–d), $\mathscr{E}(P)$ as given in Eq. (3.4) reduces to

$$\mathscr{E}(P) = \overline{\int_P \varrho\varepsilon}^{\,\cdot} + \int_{\partial P}\boldsymbol{q}\cdot\boldsymbol{n} - \int_P r + \int_P ck + \boldsymbol{z}\cdot\dot{\xi} + \boldsymbol{\pi}\cdot\dot{\varsigma} - \boldsymbol{P}\cdot\nabla\dot{\xi} - \boldsymbol{\Sigma}\cdot\nabla\dot{\varsigma} \tag{3.9}$$

in terms of the fields

$$c := \dot{\varrho}, \tag{3.10a}$$

$$\boldsymbol{z} := \varrho\ddot{\xi} - \mathrm{div}\boldsymbol{P} - \boldsymbol{b}, \tag{3.10b}$$

$$\boldsymbol{\pi} := \varrho\dot{\boldsymbol{\mu}} - \mathrm{div}\boldsymbol{\Sigma} - \boldsymbol{\beta}, \tag{3.10c}$$

on B, representing production-like quantities for mass, continuum momentum, and microstructural [9] momentum, respectively. Together with Eq. (3.6a–d), then, the transformation relations

$$\Delta \boldsymbol{P} = \boldsymbol{0}, \qquad \Delta \boldsymbol{\Sigma} = \boldsymbol{0} \tag{3.11a, b}$$

for $\boldsymbol{P}$ and $\boldsymbol{\Sigma}$, as well as those [10]

$$\Delta \boldsymbol{z} = \boldsymbol{0}, \qquad \Delta \boldsymbol{\pi} = \boldsymbol{0} \tag{3.12a, b}$$

for the internal supply rate densities induce in turn the transformation relation

$$\begin{aligned}\Delta \mathscr{E}(P) &:= (\lambda^* \mathscr{E}')(P) - \mathscr{E}(P) \\ &= \int_P \frac{1}{2} c_0 \, \Delta\dot{\xi} \cdot \Delta\dot{\xi} + c_0 \, \Delta k_s + (\boldsymbol{z}_0 + c_0 \dot{\xi}_0) \cdot \Delta\dot{\xi} + \int_P \boldsymbol{\pi}_0 \cdot \Delta\dot{\boldsymbol{\varsigma}} - \boldsymbol{P}_0 \cdot \Delta(\nabla\dot{\xi}) - \boldsymbol{\Sigma}_0 \cdot \Delta(\nabla\dot{\varsigma})\end{aligned} \tag{3.13}$$

for $\mathscr{E}(P)$ via Eqs. (3.8a) and (3.9) with respect to any $P \subset B$. Note that Eq. (3.6a) implies $\Delta c = 0$ via Eq. (3.10a) and the Euclidean frame-indifference of the material time derivative. Consequently, $\mathscr{E}(P)$ will be Euclidean frame-indifferent, or independent of Euclidean observer, iff $\Delta\mathscr{E}(P)$ vanishes. Note that this condition generalizes similar considerations based on the invariance of the internal power worked with by Capriz (1989, Section 9) and Segev (1994) to the context of total energy balance (see also Capriz and Virga (1994), in this regard).

Of all the transformations appearing in Eq. (3.13), only that Δk_s for the contribution of the microstructure to the specific kinetic energy is yet to be determined. To this end, assume that the form $k_s(\varsigma, \dot{\varsigma})$ of the dependence of k_s on ς and $\dot{\varsigma}$ is observer-invariant. In this case,

$$\{\lambda^*[k_s'(\varsigma', \dot{\varsigma}')]\}|_{t=0} = k_s'(\varsigma_0, \dot{\varsigma}_0 + \Delta\dot{\varsigma}) = k_s(\varsigma_0, \dot{\varsigma}_0 + \Delta\dot{\varsigma}), \tag{3.14}$$

and so

$$\Delta k_s = k_s(\varsigma_0, \dot{\varsigma}_0 + \Delta\dot{\varsigma}) - k_s(\varsigma_0, \dot{\varsigma}_0) \tag{3.15}$$

follow from Eqs. (2.9), (2.14) and $\boldsymbol{Q}(0) = \boldsymbol{1}$. So, as long as $k_s(\cdot,\cdot)$ is continuous in its second argument, Δk_s vanishes when $\Delta\dot{\varsigma}$ does. In particular, this can be verified for special cases, e.g., for the quadratic form $k_s = \frac{1}{2}\dot{\varsigma} \cdot \boldsymbol{\Theta}(\varsigma)\dot{\varsigma}$. Since $\Delta\dot{\varsigma}$ is not zero in general (i.e., from Eq. (2.15a)), Eq. (3.15) implies that k_s is in general not Euclidean frame-indifferent.

Now, Eq. (3.13) clearly holds for all Euclidean observer transformations. Consequently, $\mathscr{E}(P)$ will be observer-invariant if and only if Eq. (3.13) vanishes for all possible such transformations. In particular, consider the special observer transformation of a pure translation, i.e., $\boldsymbol{\Omega} = \boldsymbol{0}$. Then,

$$\begin{aligned}\Delta\dot{\xi} &= \boldsymbol{t}, \qquad \Delta(\nabla\dot{\xi}) = \boldsymbol{0}, \\ \Delta\dot{\varsigma} &= \boldsymbol{0}, \qquad \Delta(\nabla\dot{\varsigma}) = \boldsymbol{0}\end{aligned} \tag{3.16}$$

follow from Eqs. (2.13a,b) and (2.15a,b), leading in turn to the reduced form

$$\Delta\mathscr{E}(P) = \frac{1}{2}(\boldsymbol{t} \cdot \boldsymbol{t}) \int_P c_0 + \boldsymbol{t} \cdot \int_P \boldsymbol{z}_0 + c_0 \dot{\xi}_0 \tag{3.17}$$

[9] The microstructural internal momentum supply rate density $\boldsymbol{\pi}$ appearing in Eq. (3.10c) corresponds to the field $-\boldsymbol{\zeta}$ in the approach Capriz (1989, Section 8) and that of Capriz and Virga (1994) when we model $\varrho\dot{\boldsymbol{\mu}}$ via a "Lagrangian" form for this quantity in terms of the kinetic (co)energy.

[10] On the basis of Eqs. (3.6a), (3.10b), and (3.11a), the assumption (3.12a) is equivalent to the standard result $\varrho\Delta\dot{v} = \Delta\boldsymbol{b}$ (e.g., Marsden and Hughes, 1983; see also Šilhavý, 1997, Chapter 6). Similarly, Eq. (3.12b) is equivalent to $\varrho\Delta\dot{\boldsymbol{\mu}} = \Delta\boldsymbol{\beta}$. Note that this latter transformation is qualitatively different from that for the external supply rate density formulated by Capriz et al. (1982) for affine microstructure with the help of mass-point considerations, and from that of Capriz and Virga, who assume $\Delta\boldsymbol{\beta} = \boldsymbol{0}$.

of Eq. (3.13) via Eq. (3.15) and the assumed continuity of $k_s(\cdot,\cdot)$ in its second argument. This last result represents a polynomial in $\boldsymbol{t}$. For this polynomial to vanish for all $\boldsymbol{t}$, the corresponding coefficients must vanish identically, yielding

$$\int_P c_0 = 0 \Rightarrow c = \dot{\varrho} = 0 \tag{3.18}$$

via Eq. (3.10a), as well as

$$\int_P \boldsymbol{z}_0 = \boldsymbol{0} \Rightarrow \boldsymbol{z} = \varrho\ddot{\xi} - \operatorname{div}\boldsymbol{P} - \boldsymbol{b} = \boldsymbol{0} \tag{3.19a, b}$$

from Eq. (3.10b). The second form of these last two expressions results from the fact that $t = 0$ is physically arbitrary, as well as the assumed continuity of the integrands. On account of Eqs. (3.18) and (3.19a,b), then, Eq. (3.13) reduces to

$$\Delta\mathscr{E}(P) = \boldsymbol{\Omega} \cdot \int_P \mathscr{A}_{\varsigma_0}^{\mathrm{T}}\boldsymbol{\pi}_0 - \boldsymbol{P}_0\boldsymbol{F}_0^{\mathrm{T}} - (\nabla\mathscr{A}_{\varsigma_0})^{\mathrm{ST}}\boldsymbol{\Sigma}_0 \tag{3.20}$$

via the transformation relations (2.13a,b) and (2.15a,b). Since the first and third terms appearing in the integrand of Eq. (3.20) take values in $\mathrm{Skw}(\mathscr{V},\mathscr{V})$, $\Delta\mathscr{E}(P)$ as given by Eq. (3.20) vanishes for all $\boldsymbol{\Omega} \in \mathrm{Skw}(\mathscr{V},\mathscr{V})$ iff

$$\mathrm{skw}(\boldsymbol{P}\boldsymbol{F}^{\mathrm{T}}) = \mathscr{A}_{\varsigma}^{\mathrm{T}}\boldsymbol{\pi} - (\nabla\mathscr{A}_{\varsigma})^{\mathrm{ST}}\boldsymbol{\Sigma} \tag{3.21}$$

holds identically. This represents in the current context the important result [11] obtained by Capriz (1989, Eq. (9.4)) on the basis of the invariance of the internal power with respect to superimposed rigid-body rotations. As noted by him, the combination of Eq. (3.21) with the evolution relation (3.10c) for the microstructural specific momentum yields the "standard" local form

$$\varrho\mathscr{A}_{\varsigma}^{\mathrm{T}}\dot{\boldsymbol{\mu}} = \mathrm{skw}(\boldsymbol{P}\boldsymbol{F}^{\mathrm{T}}) + \operatorname{div}(\mathscr{A}_{\varsigma}^{\mathrm{T}}\boldsymbol{\Sigma}) + \mathscr{A}_{\varsigma}^{\mathrm{T}}\boldsymbol{\beta} \tag{3.22}$$

of moment of momentum balance taking values in $\mathrm{Skw}(\mathscr{V},\mathscr{V})$ in which $\mathrm{skw}(\boldsymbol{P}\boldsymbol{F}^{\mathrm{T}})$ appears as a source term. Finally, Eq. (3.10c), as well as the results (3.18) and (3.19), lead to the reduced form

$$\mathscr{E}(P) = \int_P \varrho\dot{\varepsilon} + \operatorname{div}\boldsymbol{q} - r + \boldsymbol{\pi}\cdot\dot{\varsigma} - \boldsymbol{P}\cdot\nabla\dot{\xi} - \boldsymbol{\Sigma}\cdot\nabla\dot{\varsigma} \tag{3.23}$$

for $\mathscr{E}(\xi)$ from Eq. (3.9) via the divergence theorem. Assuming then there exists at least one observer with respect to which $\mathscr{E}(P)$ in fact vanishes, it does so with respect to all, and yields the localized form

$$\varrho\dot{\varepsilon} = \boldsymbol{P}\cdot\nabla\dot{\xi} + \boldsymbol{\Sigma}\cdot\nabla\dot{\varsigma} - \boldsymbol{\pi}\cdot\dot{\varsigma} - \operatorname{div}\boldsymbol{q} + r \tag{3.24}$$

of total energy balance via the assumed continuity of the integrand. Incorporating Eq. (3.21) into Eq. (3.24) yields the alternative form

$$\varrho\dot{\varepsilon} = \mathrm{sym}(\boldsymbol{P}\boldsymbol{F}^{\mathrm{T}})\cdot\boldsymbol{D} + \boldsymbol{\Sigma}\cdot\nabla(\dot{\varsigma} - \mathscr{A}_{\varsigma}\boldsymbol{W}) + \mathscr{A}_{\varsigma}^{\mathrm{T}}\boldsymbol{\Sigma}\cdot\nabla\boldsymbol{W} - \boldsymbol{\pi}\cdot(\dot{\varsigma} - \mathscr{A}_{\varsigma}\boldsymbol{W}) - \operatorname{div}\boldsymbol{q} + r \tag{3.25}$$

of reduced local energy balance via Eq. (2.4) in terms of the "Jaumann" objective time derivative $\dot{\varsigma} - \mathscr{A}_{\varsigma}\boldsymbol{W}$ of ς. In particular, since $\nabla\boldsymbol{W}$ is Euclidean frame-indifferent, Eq. (3.25) shows that the energy balance is indeed so.

[11] Also obtained by Capriz and Virga (1994).

4. Configurational fields and microstructure

Now, we turn to the formulation of the configurational fields for a continuum with microstructure of the type considered in the last section. To this end, we follow Gurtin (1995) and Cermelli and Fried (1997) in dealing first with the case in which the material inhomogeneity is smoothly varying, i.e., no defects. The formulation of these fields is based on the notion of an evolving control region in B, i.e., one into, or out of, which elements of the material body, may flow during some process. Let $R \subset B$ represent this set at some arbitrary time (e.g., $t = 0$). The evolution of this region due to mass flux into or out of it in can be represented with the help of a time-dependent mapping

$$\kappa : I \times R \to B \tag{4.1}$$

of R into B *formally* (but not physically) analogous to the motion (2.1) of B in E. In this case,

$$\xi \diamondsuit \kappa : I \times R \to E \tag{4.2}$$

represents the motion of the evolving control region in question with respect to E. Let

$$v_\kappa \diamondsuit \kappa := \dot{\kappa} \tag{4.3}$$

represent the specific mass flux corresponding to κ. In particular, $v_\kappa|_{\partial\kappa_t[R]} \cdot \boldsymbol{n}_{\partial\kappa_t[R]}$ represents the rate at time t at which mass enters or leaves the control region at its boundary $\partial\kappa_t[R]$ with unit normal $\boldsymbol{n}_{\partial\kappa_t[R]}$.

To formulate configurational fields in this framework, consider first the generic balance relation

$$\mathscr{B}(\kappa) := \overline{\int_\kappa \psi}^{\,\cdot} - \int_\kappa \pi - \int_{\partial\kappa} \boldsymbol{\phi}_\kappa \cdot \boldsymbol{n} - \int_\kappa \sigma = 0 \tag{4.4}$$

for mass, continuum momentum, microstructural momentum, or entropy [12] relative to κ. Here, we use the notation

$$\left(\int_\kappa \psi\right)(t) := \int_{\kappa_t[R]} \psi_t \tag{4.5}$$

for volume integrals defined on κ; boundary integrals are defined similarly. In Eq. (4.4) appear, the referential density ψ, the internal supply or "production" rate density π, and the external supply rate density σ, associated with the balance in question. Further,

$$\boldsymbol{\phi}_\kappa := \boldsymbol{\phi} + \psi_c v_\kappa \tag{4.6}$$

represents the form of the corresponding flux density $\boldsymbol{\phi}$ relative to κ, i.e., taking into account the additional process of addition or deletion of mass at $\partial\kappa$ via the "configurational" form ψ_c of ψ. With the help of the transport relation

$$\overline{\int_\kappa \psi}^{\,\cdot} = \int_\kappa \grave{\psi} + \int_{\partial\kappa} \psi v_\kappa \cdot \boldsymbol{n} \tag{4.7}$$

via Eq. (4.3), $\grave{\psi}$ representing the partial time derivative of ψ, one obtains the form

$$\mathscr{B}(\kappa) = \int_\kappa \grave{\psi} - \int_\kappa \pi - \int_{\partial\kappa} \boldsymbol{\phi} \cdot \boldsymbol{n} - \int_\kappa \sigma + \int_{\partial\kappa} v_\kappa \cdot (\psi - \psi_c)\boldsymbol{n} \tag{4.8}$$

[12] The case of total energy balance is a bit more involved, and so dealt with separately below.

for $\mathscr{B}(\kappa)$ from Eqs. (4.4) and (4.6). Adapting next the argument of Gurtin (1995) to the current context, assume that $\mathscr{B}(\kappa)$ is in fact independent of the choice, the evolving control region, i.e., if $\chi : I \times R \to B$ is a second such choice, then $\mathscr{B}(\kappa) = \mathscr{B}(\chi)$. From Eq. (4.8), this can be the case for all such κ only if

$$\psi_c = \psi \tag{4.9}$$

holds identically, with $\psi \in \{\varrho, \varrho\grave{\xi}, \varrho\boldsymbol{\mu}, \varrho\eta\}$, η being the specific entropy. As such, Eq. (4.8) reduces to

$$\mathscr{B}(\kappa) = \int_\kappa \grave{\psi} \; - \; \int_\kappa \pi \; - \; \int_{\partial\kappa} \boldsymbol{\phi} \cdot \boldsymbol{n} - \; \int_\kappa \sigma = \overline{\int_\kappa \psi}^{\,\cdot} - \int_\kappa \pi \; - \; \int_{\partial\kappa} \boldsymbol{\phi}_\kappa \cdot \boldsymbol{n} \; - \; \int_\kappa \sigma \tag{4.10}$$

for all κ, while Eqs. (4.6) and (4.9) imply in particular the forms

$$\begin{aligned} \boldsymbol{P}_\kappa &= \boldsymbol{P} + \varrho\grave{\xi} \otimes v_\kappa, \\ \boldsymbol{\Sigma}_\kappa &= \boldsymbol{\Sigma} + \varrho\boldsymbol{\mu} \otimes v_\kappa, \\ \boldsymbol{q}_\kappa &= \boldsymbol{q} - \theta\varrho\eta\, v_\kappa, \end{aligned} \tag{4.11}$$

for the corresponding flux fields relative to κ; in particular, that for $\boldsymbol{q}$ follows from the entropy balance and Clausius–Duhem constitutive forms

$$\begin{aligned} \boldsymbol{k} &= \theta^{-1}\boldsymbol{q}, \\ \sigma &= \theta^{-1} r, \end{aligned} \tag{4.12}$$

for the entropy flux and external supply rate densities, θ being the absolute temperature.

Turning now to the energy balance, this is based in the dynamic configurational context in part on the forms

$$\begin{aligned} \boldsymbol{l}_\kappa &= \boldsymbol{P}_\kappa^{\mathrm{T}}\dot{\xi}_\kappa + \boldsymbol{\Sigma}_\kappa^{\mathrm{T}}\dot{\varsigma}_\kappa + \boldsymbol{E}_\kappa^{\mathrm{T}} v_\kappa, \\ m_\kappa &= \boldsymbol{b} \cdot \dot{\xi}_\kappa + \boldsymbol{\beta} \cdot \dot{\varsigma}_\kappa + \boldsymbol{s} \cdot v_\kappa \end{aligned} \tag{4.13}$$

for mechanical energy flux and external supply rate densities, respectively, with respect to κ. Here,

$$\begin{aligned} \dot{\xi}_\kappa \diamond \kappa &:= \overline{\xi \diamond \kappa}^{\,\cdot} = [\grave{\xi} + (\nabla\xi)v_\kappa] \diamond \kappa, \\ \dot{\varsigma}_\kappa \diamond \kappa &:= \overline{\varsigma \diamond \kappa}^{\,\cdot} = [\grave{\varsigma} + (\nabla\varsigma)v_\kappa] \diamond \kappa, \end{aligned} \tag{4.14}$$

represent the referential velocity of the control region with respect to E, and the rate of change of ς relative to κ, respectively. Further,

$$\boldsymbol{E}_\kappa = \boldsymbol{E} + \varrho\boldsymbol{c} \otimes v_\kappa \tag{4.15}$$

represents the form of the configurational or Eshelby stress $\boldsymbol{E}$ relative to κ, $\boldsymbol{c}$ being the corresponding momentum density, and $\boldsymbol{s}$ the corresponding supply-rate density. From Eqs. (4.11), (4.13) and (4.15), then, one obtains the form

$$\begin{aligned} \mathscr{E}(\kappa) &= \overline{\int_\kappa e}^{\,\cdot} \; - \; \int_{\partial\kappa} \boldsymbol{h}_\kappa \cdot \boldsymbol{n} \; - \; \int_\kappa s_\kappa \\ &= \int_\kappa \grave{e} \; - \; \int_{\partial\kappa} \boldsymbol{h} \cdot \boldsymbol{n} \; - \; \int_\kappa s \; + \; \int_{\partial\kappa} v_\kappa \cdot (\boldsymbol{A} + \varrho\boldsymbol{m} \otimes v_\kappa)\boldsymbol{n} \; + \; \int_\kappa v_\kappa \cdot \boldsymbol{d} \end{aligned} \tag{4.16}$$

for $\mathscr{E}(\kappa)$, analogous to Eq. (4.8) for the other balance relations, where

$$\begin{aligned} \boldsymbol{m} &:= -(\nabla\xi)^{\mathrm{T}}\grave{\xi} - (\nabla\varsigma)^{\mathrm{T}}\boldsymbol{\mu} - \boldsymbol{c}, \\ \boldsymbol{A} &:= \varrho\{\varphi - \tfrac{1}{2}\grave{\xi}\cdot\grave{\xi} + (k_s - \boldsymbol{\mu}\cdot\grave{\varsigma})\}\mathbf{1} - (\nabla\xi)^{\mathrm{T}}\boldsymbol{P} - (\nabla\varsigma)^{\mathrm{T}}\boldsymbol{\Sigma} - \boldsymbol{E}, \\ \boldsymbol{d} &:= -(\nabla\xi)^{\mathrm{T}}\boldsymbol{b} - (\nabla\varsigma)^{\mathrm{T}}\boldsymbol{\beta} - \boldsymbol{s}, \end{aligned} \tag{4.17}$$

and

$$\varphi = \varepsilon - \theta\eta \tag{4.18}$$

represents the specific free energy. As above for Eq. (4.8), we now adapt the approach of Gurtin (1995) to the case of total energy balance. To this end, assume that energy balance is independent of the choice of evolving control region, i.e., that $\mathscr{E}(\kappa) = \mathscr{E}(\chi)$ holds for all evolving control regions κ, χ. In other words, a change of evolving control region results in no energy production. From Eq. (4.16), this can only be the case when $\boldsymbol{m}$, $\boldsymbol{A}$ and $\boldsymbol{d}$ vanish identically, yielding

$$\begin{aligned} \boldsymbol{c} &= -(\nabla\xi)^{\mathrm{T}}\grave{\xi} - (\nabla\varsigma)^{\mathrm{T}}\boldsymbol{\mu}, \\ \boldsymbol{E} &= \varrho\{\varphi - \tfrac{1}{2}\grave{\xi}\cdot\grave{\xi} - \boldsymbol{\mu}\cdot\grave{\varsigma} - k_s\}\mathbf{1} - (\nabla\xi)^{\mathrm{T}}\boldsymbol{P} - (\nabla\varsigma)^{\mathrm{T}}\boldsymbol{\Sigma} \\ \boldsymbol{s} &= -(\nabla\xi)^{\mathrm{T}}\boldsymbol{b} - (\nabla\varsigma)^{\mathrm{T}}\boldsymbol{\beta}, \end{aligned} \tag{4.19}$$

for the specific configurational momentum, configurational stress, and configuration external supply rate density. With these results, the total energy balance (4.16) reduces to

$$\mathscr{E}(\kappa) = \int_{\kappa} \grave{e} \; - \int_{\partial\kappa} \boldsymbol{h}\cdot\boldsymbol{n} \; - \int_{\kappa} s \tag{4.20}$$

for all κ.

Having obtained the configurational fields (4.19), we are now in a position to formulate the so-called configurational force balance. In the context of smooth inhomogeneity, this can be obtained from the corresponding translational invariance of $\mathscr{E}(\kappa)$ as given by Eq. (4.20), with the time-dependent translation involved acting on κ. As is well-known from, e.g., the continuum theory of dislocations, loss of translational invariance in the material is associated with the presence of dislocations and may be characterized, e.g., by the torsion of the corresponding material connection (e.g., Bilby et al., 1955; Noll, 1967). In the current case of smooth inhomogeneity, however, such invariance applies. Let

$$v_{\kappa}^{*} = v_{\kappa} + \boldsymbol{a} \tag{4.21}$$

represent the corresponding induced transformation of v_{κ} for $\boldsymbol{a} \in \mathscr{V}$. Being independent of velocity, the "internal" energy fields ε, $\boldsymbol{q}$ and r are invariant with respect to such a transformation, i.e.,

$$\varepsilon^{*} = \varepsilon, \qquad \boldsymbol{q}^{*} = \boldsymbol{q}, \qquad r^{*} = r. \tag{4.22}$$

This is not the case, however, for the "mechanical" energy fields k, $\boldsymbol{l}$ and m; indeed, Eq. (4.21) induces the transformations

$$\grave{k}^{*} = \grave{k} + \grave{\boldsymbol{c}}\cdot\boldsymbol{a}, \qquad \boldsymbol{l}^{*} = \boldsymbol{l} + \boldsymbol{E}^{\mathrm{T}}\boldsymbol{a}, \qquad m^{*} = m + \boldsymbol{s}\cdot\boldsymbol{a}. \tag{4.23}$$

In addition, it induces that

$$\pi^{*} = \pi + \boldsymbol{f}\cdot\boldsymbol{a} = 0 + \boldsymbol{f}\cdot\boldsymbol{a} \tag{4.24}$$

for the energy internal supply, or production, rate density, $\boldsymbol{f}$ being the corresponding configurational quantity. Requiring $\mathscr{E}^{*}(\kappa) = \mathscr{E}(\kappa)$ then yields the configurational momentum or force balance

$$\overline{\int_{\kappa} \varrho\boldsymbol{c}}^{\,\cdot} = \int_{\kappa} \boldsymbol{f} \; + \int_{\partial\kappa} \boldsymbol{E}_{\kappa}\boldsymbol{n} \; + \int_{\kappa} \boldsymbol{s} \tag{4.25}$$

relative to κ from Eq. (4.20). This generalizes the derivation of this balance given by Cermelli and Fried (1997) for the standard case on the basis of the invariance of the disspation rate with respect to change of *referential or material* observer. Clearly, this balance is in essence of material, rather than spatial, character. Combining lastly Eq. (4.19) and the localized form of the configurational momentum or force balance (4.25) yields that

$$\boldsymbol{f} = \{\tfrac{1}{2}\dot{\xi} \cdot \dot{\xi} + \boldsymbol{\mu} \cdot \dot{\varsigma} - k_s - \varphi\}\nabla\varrho + \varrho\{(\nabla\boldsymbol{\mu})^{\mathrm{T}}\dot{\varsigma} - \nabla k_s - \nabla\varphi\} + (\nabla(\nabla\xi))^{\mathrm{ST}}\boldsymbol{P} + (\nabla(\nabla\varsigma))^{\mathrm{ST}}\boldsymbol{\Sigma} - (\nabla\varsigma)^{\mathrm{T}}\boldsymbol{\pi} \tag{4.26}$$

for the configurational momentum internal supply rate density or internal configurational "force" via Eqs. (2.3), (3.10c) and (3.19a,b). Clearly, on the basis of Eq. (4.26), then, configurational momentum is "produced," among other things, by an inhomogeneous mass density, specific free energy φ, and deformation gradient $\boldsymbol{F} = \nabla\xi$, as in the classical case. Additional contributions to $\boldsymbol{f}$ arise in the current context due to the inhomogeneity of ς, $\boldsymbol{\mu}$ and k_s. These results reduce to those of Gurtin (1995) when inertia, external supplies and microstructure are neglected, and to those of Cermelli and Fried (1997) when external supplies and microstructure are neglected. They also reduce to those of Cermelli and Fried (1999) for uniaxial nematic liquid crystals when external supplies are neglected, when k_s is assumed to take the quadratic form $\frac{1}{2}l^2\dot{\varsigma} \cdot \dot{\varsigma}$ (l being a lengthscale), and when the microstructure in question is represented by a Euclidean unit vector field, i.e., the director.

5. Dissipation principle

Although not the main thrust of the current work, the basic thermodynamic results for the class of materials being considered here following from the Coleman–Noll dissipation principle as based on the Clausius–Duhem inequality consistent with the current approach are summarized briefly in this section for completeness and comparison with other approaches. To begin, the form of the dissipation rate relevant to the current constitutive class is obtained via combination of the reduced local energy balance with the corresponding form of the entropy balance and the constitutive relations (4.12). This results in the local form

$$\delta = \boldsymbol{P}_a \cdot \dot{\boldsymbol{F}} + \boldsymbol{\Sigma}_a \cdot \nabla\dot{\varsigma} - \boldsymbol{\pi}_a \cdot \dot{\varsigma} - \theta^{-1}\boldsymbol{q} \cdot \nabla\theta - \varrho\eta\dot{\theta} - \varrho\dot{\varphi} \tag{5.1}$$

of the dissipation rate density via Eq. (1), the split

$$\begin{aligned} \boldsymbol{P} &= \boldsymbol{P}_a + \boldsymbol{P}_r, \\ \boldsymbol{\Sigma} &= \boldsymbol{\Sigma}_a + \boldsymbol{\Sigma}_r, \\ \boldsymbol{\pi} &= \boldsymbol{\pi}_a + \boldsymbol{\pi}_r, \end{aligned} \tag{5.2}$$

of the constitutive fields into active and reactive parts, and Eq. (2), the assumption

$$\boldsymbol{P}_r \cdot \dot{\boldsymbol{F}} + \boldsymbol{\Sigma}_r \cdot \nabla\dot{\varsigma} - \boldsymbol{\pi}_r \cdot \dot{\varsigma} = 0 \tag{5.3}$$

(e.g., Capriz, 1989) that the constraints are "perfect." In other words, they do no work.

Consider now the case of viscous, elastic material behaviour for the class of materials with microstructure and moving defects under consideration, something that would apply to, e.g., liquid crystals, or granular materials. In this case, we have the basic constitutive form

$$\mathscr{C}(\theta, \boldsymbol{F}, \varsigma, \nabla\theta, \nabla\varsigma, \dot{\boldsymbol{F}}, \dot{\varsigma}) = \mathscr{C}(\theta, \boldsymbol{F}, \pi(\varsigma), \nabla\theta, \pi_{*\varsigma}(\nabla\varsigma), \dot{\boldsymbol{F}}, \pi_{*\varsigma}\dot{\varsigma}) \tag{5.4}$$

for the dependent constitutive fields $\boldsymbol{P}_a$, $\boldsymbol{\Sigma}_a$, $\boldsymbol{\pi}_a$, $\boldsymbol{q}$, η and φ; recall that $\pi : \mathscr{W} \to \mathscr{G}$ represents the projection of $\mathscr{W}$ onto the structure submanifold; further, $\pi_{*\mathscr{s}} : \mathscr{W} \to T_{\pi(\mathscr{s})}\mathscr{G}$ represents the induced projection at $\mathscr{s} \in \mathscr{W}$.

For example, in the case of uniaxial nematic liquid crystals, we would have $\mathscr{W} = \mathscr{V}$, $\mathscr{G} = S^2$, $\pi(\boldsymbol{a}) = \boldsymbol{a}/|\boldsymbol{a}|$, and so $\pi_{*\boldsymbol{a}} = 1 - \pi(\boldsymbol{a}) \otimes \pi(\boldsymbol{a})$, for all non-zero $\boldsymbol{a} \in \mathscr{V}$. One then obtains in the standard way the restrictions

$$\begin{aligned} \eta &= -\varphi_{,\theta}, \\ \mathbf{0} &= \varphi_{,\nabla\theta}, \\ \boldsymbol{\Sigma}_a &= \varrho\,\varphi_{,\nabla\varsigma} = \varrho\,\pi_{*\varsigma}^{\mathrm{T}}\,\varphi_{,\pi_{*\varsigma}(\nabla\varsigma)}, \\ \mathbf{0} &= \varphi_{,\dot{\boldsymbol{F}}}, \\ \mathbf{0} &= \varphi_{,\dot{\varsigma}} = \pi_{*\varsigma}^{\mathrm{T}}\,\varphi_{,\pi_{*\varsigma}\dot{\varsigma}}, \end{aligned} \tag{5.5}$$

on the constitutive parts of the dependent constitutive fields from the dissipation inequality $\delta \geqslant 0$ in the context of the Coleman–Noll dissipation principle for all thermodynamically admissible processes. Consequently, the specific free energy takes on the reduced constitutive form

$$\varphi(\theta, \boldsymbol{F}, \varsigma, \nabla\varsigma) = \varphi(\theta, \boldsymbol{F}, \pi(\varsigma), \pi_*(\nabla\varsigma)). \tag{5.6}$$

Likewise, δ reduces to

$$\delta = \{\boldsymbol{P}_a - \varrho\varphi_{,\boldsymbol{F}}\}\boldsymbol{F}^{\mathrm{T}} - (\boldsymbol{\pi}_a + \varrho\varphi_{,\varsigma}) \cdot \dot{\varsigma} - \theta^{-1}\boldsymbol{q} \cdot \nabla\theta \tag{5.7}$$

from Eq. (5.1). In particular, this implies the equilibrium forms

$$\begin{aligned} \boldsymbol{P}_{ae} &= \varrho\varphi_{,\boldsymbol{F}}, \\ \boldsymbol{\pi}_{ae} &= -\varrho\varphi_{,\varsigma}, \end{aligned} \tag{5.8}$$

for the constitutive parts of $\boldsymbol{P}$ and $\boldsymbol{\pi}$, respectively. Detailed examples of all of these in particular cases, and in particular that of liquid crystals, can be found in Capriz (1989, parts II and III). Now we turn to the case that the inhomogeneity of the material with microstructure in question is no longer smooth, i.e., to the case that this materials contains moving point defects.

6. The case of point defects

The purpose of this section is to touch briefly on the extension of the results of the previous section to the case when the material contains (non-smooth) inhomogeneities which are point-like, e.g., defect cores in liquid crystals. In a particle, these are represented in the model as isolated singularities in the microstructural field $\varsigma_{\mathrm{t}} := \varsigma(t, \cdot) : B \to \mathscr{W}$ at each $t \in I$. On the other hand, continuum fields such as the material velocity $\dot{\xi}_{\mathrm{t}} : B \to \mathscr{V}$ are smooth in all points of $B \subset E$ by assumption. A complete formulation of this case depends as well on particular forms for the constitutive relations for the material in question, something beyond the scope of the current work. As such, attention is restricted here to the basic forms taken by the balance relations in this case; for a complete formulation along these lines in the case of defective nematic fluids, the interested reader is refered to Cermelli and Fried (1999). For simplicity, the formulation in this section is carried out for the case of a single defect, and all external supply rate densities are neglected. Since singularities may arise in the remaining fields of the formulation, the balance relations must be reformulated to accomodate this possibility.

To this end, let $D_\epsilon \subset B$ represent a ball of radius ϵ about the defect core in the reference configuration B at some arbitrary time (e.g., $t = 0$). Further, let $\delta_\epsilon : I \times D_\epsilon \to B$ represent the evolution of D_ϵ with respect to the material, such that $\xi \diamond \delta_\epsilon : I \times D_\epsilon \to E$ represents that of D_ϵ relative to E. In this case, the curve $\delta_0 : I \to B$, which we identify with $\lim_{\epsilon\to 0} \delta_\epsilon$, represents the evolution of this core with respect to the material. Adapting then, the approaches of Gurtin and Podio-Guidugli (1996) and Cermelli and Fried (1999) to the current context, balance relations along κ containing δ_ϵ (i.e., $\delta_\epsilon \subset \kappa$) are first formulated outside the defect zone, i.e., for $\kappa \setminus \delta_\epsilon$, and then evaluated as ϵ tends to zero. In particular, to this end, consider the integral over $\partial(\kappa\setminus\delta_\epsilon)$ of a flux density $\boldsymbol{\phi}$. Since $\partial(\kappa\setminus\delta_\epsilon)=\partial\kappa\cup\partial\delta_\epsilon$, this integral can be expressed in the form

$$\int_{\partial(\kappa\setminus\delta_\epsilon)}\boldsymbol{\phi}\cdot\boldsymbol{n}=\int_{\partial\kappa}\boldsymbol{\phi}\cdot\boldsymbol{n}_{\partial(\kappa\setminus\delta_\epsilon)}+\int_{\partial\delta_\epsilon}\boldsymbol{\phi}\cdot\boldsymbol{n}_{\partial(\kappa\setminus\delta_\epsilon)}=\int_{\partial\kappa}\boldsymbol{\phi}\cdot\boldsymbol{n}-\int_{\partial\delta_\epsilon}\boldsymbol{\phi}\cdot\boldsymbol{n}, \tag{6.1}$$

with

$$\boldsymbol{n}_{\partial(\kappa\setminus\delta_\epsilon)}|_{\partial\kappa}=\boldsymbol{n}_{\partial\kappa},\qquad \boldsymbol{n}_{\partial(\kappa\setminus\delta_\epsilon)}|_{\partial\delta_\epsilon}=-\boldsymbol{n}_{\partial\delta_\epsilon}. \tag{6.2}$$

In addition, the transport theorem for $\kappa\setminus\delta_\epsilon$ takes the form

$$\begin{aligned}\overline{\int_{\kappa\setminus\delta_\epsilon}\psi}^{\cdot}&=\int_{\kappa\setminus\delta_\epsilon}\grave{\psi}+\int_{\partial(\kappa\setminus\delta_\epsilon)}\psi\, v_{\kappa\setminus\delta_\epsilon}\cdot\boldsymbol{n}_{\partial(\kappa\setminus\delta_\epsilon)}\\&=\int_{\kappa\setminus\delta_\epsilon}\grave{\psi}+\int_{\partial\kappa}\psi\, v_{\kappa\setminus\delta_\epsilon}\cdot\boldsymbol{n}_{\partial(\kappa\setminus\delta_\epsilon)}+\int_{\partial\delta_\epsilon}\psi\, v_{\kappa\setminus\delta_\epsilon}\cdot\boldsymbol{n}_{\partial(\kappa\setminus\delta_\epsilon)}\\&=\int_{\kappa\setminus\delta_\epsilon}\grave{\psi}+\int_{\partial\kappa}\psi\, v_{\kappa}\cdot\boldsymbol{n}-\int_{\partial\delta_\epsilon}\psi\, v_{\delta_\epsilon}\cdot\boldsymbol{n},\end{aligned} \tag{6.3}$$

again from $\partial(\kappa\setminus\delta_\epsilon)=\partial\kappa\cup\partial\delta_\epsilon$, Eq. (6.2) and the results

$$v_{\kappa\setminus\delta_\epsilon}|_{\partial\kappa}=v_\kappa|_{\partial\kappa},\qquad v_{\kappa\setminus\delta_\epsilon}|_{\partial\delta_\epsilon}=v_{\delta_\epsilon}|_{\partial\delta_\epsilon}. \tag{6.4}$$

Combining Eqs. (6.1) and (6.3) yields

$$\int_{\kappa\setminus\delta_\epsilon}\grave{\psi}\;-\;\int_{\partial(\kappa\setminus\delta_\epsilon)}\boldsymbol{\phi}\cdot\boldsymbol{n}=\overline{\int_{\kappa\setminus\delta_\epsilon}\psi}^{\cdot}\;-\;\int_{\partial\kappa}\boldsymbol{\phi}_\kappa\cdot\boldsymbol{n}\;+\;\int_{\partial\delta_\epsilon}\boldsymbol{\phi}_{\delta_\epsilon}\cdot\boldsymbol{n} \tag{6.5}$$

via Eqs. (4.6) and (4.9). Assume next that ψ is regular in the sense of Gurtin and Podio-Guidugli (1996). In particular, this implies that ψ is (i) smooth away from δ_0 (ii) integrable on B uniformly for t in a compact interval (iii), $t\mapsto\int_{\kappa_t[R]}\psi_t$ is differentiable for all κ, and (iv), $\lim_{\epsilon\to 0}\int_{\partial\delta_\epsilon}\psi\boldsymbol{n}$ exists. In this case, one obtains

$$\overline{\int_{\kappa}\psi}^{\cdot}=\lim_{\epsilon\to 0}\int_{\kappa\setminus\delta_\epsilon}\grave{\psi}\;+\;\int_{\partial\kappa}\psi\, v_\kappa\cdot\boldsymbol{n}\;-\;\lim_{\epsilon\to 0}\int_{\partial\delta_\epsilon}\psi\, v_{\delta_\epsilon}\cdot\boldsymbol{n} \tag{6.6}$$

from Eq. (6.3), as well as

$$\overline{\int_{\kappa}\psi}^{\cdot}=\lim_{\epsilon\to 0}\int_{\kappa\setminus\delta_\epsilon}\pi\;+\;\int_{\partial\kappa}\boldsymbol{\phi}_\kappa\cdot\boldsymbol{n}\;-\;\lim_{\epsilon\to 0}\int_{\partial\delta_\epsilon}\boldsymbol{\phi}_{\delta_\epsilon}\cdot\boldsymbol{n} \tag{6.7}$$

from Eq. (6.5) for a balance relation in the absence of external supplies and the presence of a defect in B. In particular, assuming that ϱ is continuous, and that $\dot{\xi}$ is regular, Eqs. (6.6) and (6.7) imply in particular the forms

$$\overline{\int_{\kappa}\varrho}^{\cdot}=\int_{\partial\kappa}\varrho v_\kappa\cdot\boldsymbol{n}+m_{\mathrm{D}},\;\overline{\int_{\kappa}\varrho\grave{\xi}}^{\cdot}=\int_{\partial\kappa}\boldsymbol{P}_\kappa\boldsymbol{n}+\boldsymbol{t}_{\mathrm{D}}, \tag{6.8}$$

for mass and continuum momentum balance in a region with defect from Eq. (3.19a,b), with

$$m_{\mathrm{D}}:=-\lim_{\epsilon\to 0}\int_{\partial\delta_\epsilon}\varrho v_{\delta_\epsilon}\cdot\boldsymbol{n}, \tag{6.9}$$

the relative mass flux at the defect, and

$$\boldsymbol{t}_{\mathrm{D}} := -\lim_{\epsilon\to 0}\int_{\partial\delta_\epsilon} \boldsymbol{P}_{\delta_\epsilon}\boldsymbol{n} = -\lim_{\epsilon\to 0}\int_{\partial\delta_\epsilon} (\boldsymbol{P} + \varrho\dot{\xi}\otimes v_{\delta_\epsilon})\boldsymbol{n}, \tag{6.10}$$

the stress vector relative to the motion of the defect at the defect. More generally, we have the forms

$$\lim_{\epsilon\to 0}\overline{\int_{\kappa\backslash\delta_\epsilon}\varrho\boldsymbol{\mu}}^{\cdot} = \lim_{\epsilon\to 0}\int_{\kappa\backslash\delta_\epsilon}\boldsymbol{\pi} + \int_{\partial\kappa}\boldsymbol{\Sigma}_\kappa\boldsymbol{n} + \boldsymbol{\sigma}_{\mathrm{D}}, \qquad \lim_{\epsilon\to 0}\overline{\int_{\kappa\backslash\delta_\epsilon}\varrho\boldsymbol{c}}^{\cdot} = \lim_{\epsilon\to 0}\int_{\kappa\backslash\delta_\epsilon}\boldsymbol{f} + \int_{\partial\kappa}\boldsymbol{E}_\kappa\boldsymbol{n} + \boldsymbol{e}_{\mathrm{D}} + \boldsymbol{g}_{\mathrm{D}} \tag{6.11}$$

for microstructural and configuration momentum balances, respectively, in such a region, on the basis of Eqs. (3.10a–c) and (4.25), respectively, with

$$\begin{aligned}\boldsymbol{\sigma}_{\mathrm{D}} &:= -\lim_{\epsilon\to 0}\int_{\partial\delta_\epsilon}\boldsymbol{\Sigma}_{\delta_\epsilon}\boldsymbol{n} = -\lim_{\epsilon\to 0}\int_{\partial\delta_\epsilon}(\boldsymbol{\Sigma} + \varrho\boldsymbol{\mu}\otimes v_{\delta_\epsilon})\boldsymbol{n},\\ \boldsymbol{e}_{\mathrm{D}} &:= -\lim_{\epsilon\to 0}\int_{\partial\delta_\epsilon}\boldsymbol{E}_{\delta_\epsilon}\boldsymbol{n} = -\lim_{\epsilon\to 0}\int_{\partial\delta_\epsilon}(\boldsymbol{E} + \varrho\boldsymbol{c}\otimes v_{\delta_\epsilon})\boldsymbol{n}.\end{aligned} \tag{6.12a, b}$$

The additional configurational field $\boldsymbol{g}_{\mathrm{D}}$ appears due to the loss of translational invariance in the material upon which Eq. (4.25) is based.

The evaluation of the limits appearing in Eqs. (6.9)–(6.11) is contingent on the behaviour of the field densities appearing in the balance relations of the previous section at the defect. This in turn is crucially dependent on the particular forms taken by the constitutive relations of the model. In particular, assuming that the mechanical, non-mechanical and configurational forces acting on the defect remain bounded there, the constitutive fluxes $\boldsymbol{P}_{\delta_\epsilon}$, $\boldsymbol{\Sigma}_{\delta_\epsilon}$, $\boldsymbol{E}_{\delta_\epsilon}$ and $\boldsymbol{q}_{\delta_\epsilon}$ satisfy estimates such as

$$\begin{aligned}&\lim_{\epsilon\to 0}\int_{\partial\delta_\epsilon}|\boldsymbol{P}_{\delta_\epsilon}\boldsymbol{n}| = O(1), \qquad \lim_{\epsilon\to 0}\int_{\partial\delta_\epsilon}\epsilon^{2(p-1)}|\boldsymbol{\Sigma}_{\delta_\epsilon}\boldsymbol{n}|^p = O(1),\\ &\lim_{\epsilon\to 0}\int_{\partial\delta_\epsilon}|\boldsymbol{E}_{\delta_\epsilon}\boldsymbol{n}| = O(1), \qquad \lim_{\epsilon\to 0}\int_{\partial\delta_\epsilon}|\boldsymbol{q}_{\delta_\epsilon}\cdot\boldsymbol{n}| = O(1),\end{aligned} \tag{6.13}$$

respectively (e.g., Cermelli and Fried (1999), in the case of defective nematic fluids). Given physically reasonable constitutive relations for the fluxes, and assuming that any constraint fields (e.g., pressure in the case of incompressibility) are integrable about the defect, one can show via straightforward generalization of the results of Cermelli and Fried (1999) for the case of defective nematic fluids to the current context that Eq. (6.13) follows from those $\lim_{\epsilon\to 0}\dot{\varsigma}|_{\delta_\epsilon} = O(\epsilon^{-1})$ and $\lim_{\epsilon\to 0}\nabla\varsigma\,|_{\delta_\epsilon} = O(\epsilon^{-1})$ of the derivatives of ς. In particular, these latter estimates are based on the physical assumption that the structure field experience no pathological oscillation near the defect.

Finally, consider the form

$$\lim_{\epsilon\to 0}\overline{\int_{\kappa\backslash\delta_\epsilon} e}^{\cdot} = \int_{\partial\kappa}\boldsymbol{h}_\kappa\cdot\boldsymbol{n} + h_{\mathrm{D}} \tag{6.14}$$

for the total energy balance via Eq. (4.16), with

$$h_{\mathrm{D}} := -\lim_{\epsilon\to 0}\int_{\partial\delta_\epsilon}\boldsymbol{h}_{\delta_\epsilon}\cdot\boldsymbol{n}, \tag{6.15}$$

the total energy flux at the defect core; we also work with

$$q_{\mathrm{D}} := -\lim_{\epsilon\to 0}\int_{\partial\delta_\epsilon}\boldsymbol{q}_{\delta_\epsilon}\cdot\boldsymbol{n} \tag{6.16}$$

in what follows. On the basis of the estimates (6.13), both of these exist. To deal with the singularity of the microstructural field ς at the defect core in the context of h_{D}, assume that there exists a field $\mathsf{v} : I\times S^2 \to \mathscr{W}$ on the unit sphere S^2 such that

$$\mathsf{v}(t,\boldsymbol{n}) := \lim_{\epsilon\to 0} \{[\dot{\varsigma} + (\nabla\varsigma)v_\kappa](t,\delta_0(t)+\epsilon\boldsymbol{n})\} \tag{6.17}$$

holds. On this basis, $\mathsf{v}(t,\boldsymbol{n})$ represents, in an asymptotic sense, the rate at which the microstructural field ς is changing at the defect in the direction $\boldsymbol{n}\in S^2$ at time $t\in I$. As with the estimates (6.13), the existence of v can be derived on the basis of the specific, physically reasonable constitutive relations for these fluxes when one assumes in particular that ς does not experience pathological oscillations near the defect. Consequently, then, h_{D} takes the form

$$h_{\mathrm{D}} = -q_{\mathrm{D}} + \dot{\delta}_0\cdot\boldsymbol{t}_{\mathrm{D}} + (\dot{\delta}_0 - \dot{\xi}_{\mathrm{D}})\cdot\boldsymbol{e}_{\mathrm{D}} + \int_{S^2}\mathsf{v}\cdot\boldsymbol{\varphi}_{\mathrm{D}} \tag{6.18}$$

via the results [13]

$$\begin{aligned}
\dot{\delta}_0\cdot\boldsymbol{t}_{\mathrm{D}} &:= -\lim_{\epsilon\to 0}\int_{\partial\delta_\epsilon} v_{\delta_\epsilon}\cdot\boldsymbol{P}_{\delta_\epsilon}\boldsymbol{n},\\
\int_{S^2}\mathsf{v}\cdot\boldsymbol{\varphi}_{\mathrm{D}} &:= -\lim_{\epsilon\to 0}\int_{\partial\delta_\epsilon}[\dot{\varsigma} + (\nabla\varsigma)v_{\delta_\epsilon}]\cdot\boldsymbol{\Sigma}_{\delta_\epsilon}\boldsymbol{n},\\
(\dot{\delta}_0 - \dot{\xi}_{\mathrm{D}})\cdot\boldsymbol{e}_{\mathrm{D}} &:= -\lim_{\epsilon\to 0}\int_{\partial\delta_\epsilon}(v_{\delta_\epsilon} - \dot{\xi})\cdot\boldsymbol{E}_{\delta_\epsilon}\boldsymbol{n},
\end{aligned} \tag{6.19}$$

where

$$\dot{\xi}_{\mathrm{D}}(t) := \dot{\xi}_{\mathrm{t}}(\delta_0(t)) = \dot{\xi}(t,\delta_0(t)) \tag{6.20}$$

represents the continuum velocity at the defect core, and

$$\boldsymbol{\varphi}_{\mathrm{D}}(t,\boldsymbol{n}) := -\lim_{\epsilon\to 0}\{\epsilon^2(\boldsymbol{\Sigma}_{\delta_\epsilon}\boldsymbol{n})(t,\delta_0(t)+\epsilon\boldsymbol{n})\}, \tag{6.21}$$

the microstructural stress "vector" at the defect core in the direction $\boldsymbol{n}\in S^2$ away from the defect core at time $t\in I$. With the help of the regularity of $\dot{\xi}$ and the corresponding result

$$\lim_{\epsilon\to 0}\int_{\partial\delta_\epsilon}\tfrac{1}{2}\varrho(\dot{\xi}\cdot\dot{\xi})\boldsymbol{n} = \boldsymbol{0}, \tag{6.22}$$

one obtains the alternative form

$$h_{\mathrm{D}} = -q_{\mathrm{D}} + \dot{\xi}_{\mathrm{D}}\cdot\boldsymbol{t}_{\mathrm{D}} + (\dot{\delta}_0 - \dot{\xi}_{\mathrm{D}})\cdot\boldsymbol{e}^{\mathrm{str}}_{\mathrm{D}} + \int_{S^2}\mathsf{v}\cdot\boldsymbol{\varphi}_{\mathrm{D}} \tag{6.23}$$

of h_{D} via Eqs. (4.11) and (4.13) in terms of the microstructural part

$$\boldsymbol{E}^{\mathrm{str}}_{\delta_\epsilon} := \varrho\{\varphi - \boldsymbol{\mu}\cdot\dot{\varsigma} - k_s\}1 - (\nabla\varsigma)^{\mathrm{T}}\boldsymbol{\Sigma} - (\nabla\varsigma)^{\mathrm{T}}\varrho\boldsymbol{\mu}\otimes v_{\delta_\epsilon} \tag{6.24}$$

of $\boldsymbol{E}_{\delta_\epsilon}$, where

$$\boldsymbol{e}^{\mathrm{str}}_{\mathrm{D}} := -\lim_{\epsilon\to 0}\int_{\partial\delta_\epsilon}\boldsymbol{E}^{\mathrm{str}}_{\delta_\epsilon}\boldsymbol{n} \tag{6.25}$$

is defined analogous to Eq. (6.12b).

This completes the basic formulation of the balance relations in the presence of a point defect. Further, more detailed result can be obtained in the context of specific constitutive models for the microstructure in question, and are beyond the scope of this work. For further details on the application to the crack

[13] These follow from the integrability assumptions (6.13) and Lemma A1 of Cermelli and Fried (1999).

propagation, the reader is refered to Gurtin and Podio-Guidugli (1996), and for the case of defective nematic fluids to the work of Cermelli and Fried (1999).

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