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GROUND STATES IN COMPLEX BODIES

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Abstract. A unified framework for analyzing the existence of ground states in wide classes of elastic complex bodies is presented here. The approach makes use of classical semicontinuity results, Sobolev mappings and Cartesian currents. Weak diffeomorphisms are used to represent macroscopic deformations. Sobolev maps and Cartesian currents describe the inner substructure of the material elements. Balance equations for irregular minimizers are derived. A contribution to the debate about the role of the balance of configurational actions follows. After describing a list of possible applications of the general results collected here, a concrete discussion of the existence of ground states in thermodynamically stable quasicrystals is presented at the end.

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1. Introduction

A prominent influence of the material texture (substructure at different low scales) on the macroscopic mechanical behavior of bodies is often registered in common experiments of condensed matter physics. Such an influence is exerted through inner actions conjugated with substructural changes and bodies displaying it are called *complex*.

In the standard format of continuum mechanics, each material element is assigned to a place in space and no direct geometrical information about its inner substructure is given *a priori* (see the treatise [52]). When active material complexity occurs, active in the sense that peculiar actions arise, such a scheme does not permits a direct representation of these actions: they are power-conjugated with morphological changes inside the material elements. For this reason one finds reasonable to consider each material element as a system and to describe its inner geometry at least at coarse grained level. Descriptors of the substructural morphology are selected here as elements of a finite-dimensional differentiable manifold, the manifold of substructural shapes, by following this way the general model-building framework of the mechanics of complex bodies in [7,38,42] (see also [5,6,12,33,41,51]).

Here the basic aim is to present a general framework for analyzing the existence of ground states in wide classes of complex bodies, the ones covered by the multifield modeling sketched above.

Keywords and phrases. Cartesian currents, complex bodies, ground states, multifield theories.

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The attention is focused on bodies admitting energies of the type

$$\mathcal{E}(u,\nu) := \int_{\mathcal{B}_0} e(x, u(x), F(x), \nu(x), N(x)) \, \mathrm{d}x \tag{1.1}$$

where u represents the gross deformation, F its spatial derivative, ν the morphological descriptor of the inner substructure, N its spatial derivative, $\mathcal{B}_0$ the reference gross shape of the body. The approach is characterized by the use of classical semicontinuity results, Sobolev mappings and Cartesian currents. In particular, the macroscopic transplacement field (the gross deformation) is considered as a weak diffeomorphism while the morphological descriptor map as a Sobolev map or a Cartesian current. It is shown that in the case in which there are energetic interactions involving minors of both F and N, then u and ν should be considered as a unique map in the setting of Cartesian currents.

The results extend to complex bodies theorems for simple elastic bodies in [1,11,27,29,45] (see also the critical remarks in [2]).

The structure of the paper is sketched below.

In Section 2, the representation of gross deformation and substructural morphology in complex bodies is briefly discussed. The variational principle governing ground states of non-linear elastic complex bodies is stated in Section 3. The general path leading to existence results is presented in Section 4. The possible occurrence of a Lavrentiev gap phenomenon and the consequences of considering the morphological descriptor maps as Cartesian currents are also discussed. In Section 5, balance equations associated with irregular minimizers are derived: the natural representation of actions associated with horizontal variations is used in absence of tangential derivatives of transplacement fields and morphological descriptor maps. A list of possible applications of the general framework is presented in Section 6. Section 7 includes details about the special case of quasicrystals: the physics suggests the appropriate functional environment in which ground states may be found.

2. Morphology and deformation of complex bodies

In its primary, abstract sense, a *body* is a collection $\mathfrak{B}$ of material elements, each one considered as a patch of matter made of entangled molecules or the characteristic piece of some atomic lattice. In other words it is the smallest piece of matter characterizing the nature of the material constituting a body. The first problem one tackles in thinking of bodies is the representation of their morphology, that is the representation of the set $\mathfrak{B}$. In standard continuum mechanics such a representation is minimalist: Each material element is considered as a structureless box, a *monad* in Leibnitz's words, described only by the place in space of its center of mass so that one has a bijective map $\varphi : \mathfrak{B} \to \mathcal{E}^3$ from $\mathfrak{B}$ into the three-dimensional Euclidean space $\mathcal{E}^3$ and calls $\varphi(\mathfrak{B})$ a *placement* of the body. $\varphi(\mathfrak{B})$ is indicated by $\mathcal{B}$ and is assumed to be a bounded domain with boundary $\partial\mathcal{B}$ of finite two-dimensional measure, a boundary where the outward unit normal is defined to within a finite number of corners and edges. In this way one is 'collapsing' the material element at a point and neglects any information about its internal structure. Of course $\mathcal{E}^3$ can be identified with $\mathbb{R}^3$ once an origin is chosen. A reference place $\mathcal{B}_0 := \varphi_0(\mathfrak{B})$, generic points of which are labeled by x, is accepted by $\mathbb{R}^3$. For technical purposes it is convenient to distinguish between the space containing $\mathcal{B}_0$ and the one in which all other placements of the body are. To this aim an isomorphic copy of $\mathbb{R}^3$, indicated by $\hat{\mathbb{R}}^3$, is selected: it contains each new place $\mathcal{B} := \varphi(\mathfrak{B})$. The generic $\mathcal{B}$ is achieved from $\mathcal{B}_0$ by means of a *transplacement* field (the standard deformation) defined by $u := \varphi \circ \varphi_0^{-1}$, with

$$\mathcal{B}_0 \ni x \mapsto u(x) \in \mathcal{B}.$$

A basic assumption is that u is *one-to-one* and *orientation preserving*, the last requirement meaning that at each x the spatial derivative Du (the standard *gradient of deformation*) has positive determinant: $\det Du(x) > 0$. Commonly the notation $F := Du(x) \in \mathrm{Hom}\left(T_x\mathcal{B}_0, T_{u(x)}\mathcal{B}\right) \simeq \mathbb{R}^3 \otimes \hat{\mathbb{R}}^3 = M_{3\times 3}$ is adopted, with $M_{3\times 3}$ the linear space of 3×3 matrices.

The standard picture of the morphology of a continuum body does not contain any direct information about the morphology of the material texture. However, in complex bodies, the prototype element is a rather

complicated ensemble of entangled molecules, or, more generally, substructures. The direct description of the substructural morphology is necessary when alterations of the substructures generate peculiar inner actions within the body, actions influencing prominently the gross behavior. The representation of these actions follows from the representation of the substructural morphology. To account for the inner shape of the material elements, one may consider a map $\varkappa : \mathfrak{B} \to \mathcal{M}$ assigning *morphological descriptors* selected within a *finite-dimensional differentiable manifold* $\mathcal{M}$, called *manifold of substructural shapes*. Elements of $\mathcal{M}$ furnish, in fact, a rough description of the essential features of the geometry of the substructure. Unless required by the theorems below, at a first glance $\mathcal{M}$ is considered here as abstract as possible so that the results are valid for a wide class of complex bodies, a family possibly restricted only by the peculiar assumptions required by specific analyses.

Geometrical structures over the manifold of substructural shapes have often a precise physical meaning so that they have to be attributed to $\mathcal{M}$ carefully, according to the specific case analyzed. For example, one may consider $\mathcal{M}$ endowed with boundary to model effects such as volumetric transitions. Moreover, when the substructure displays its own peculiar inertia, the related kinetic energy can be represented in its first approximation by means of a quadratic form. In this way, the (quadratic) substructural kinetic energy induces a Riemannian structure on $\mathcal{M}$, the metric being assigned by the coefficients of the quadratic form. In general the substructural kinetic energy may naturally induce only a Finsler structure over $\mathcal{M}$ or some gauge structure (see [10,39,41]).

A *morphological descriptor map* $\nu = \varkappa \circ \varphi_0^{-1}$,

$$\mathcal{B}_0 \ni x \longmapsto \nu(x) \in \mathcal{M},$$

is defined over $\mathcal{B}_0$. It is the Lagrangian representation of the morphological descriptor field and is assumed to be differentiable. Its spatial derivative $D\nu$ is indicated by $N := D\nu(x) \in \mathrm{Hom}\left(T_x\mathcal{B}_0, T_{\nu(x)}\mathcal{M}\right) \simeq \mathbb{R}^3 \otimes T_\nu\mathcal{M} \simeq M_{\dim\mathcal{M}\times 3}$.

The Eulerian (actual) counterpart of the map ν, indicated by ν_a, is given by $\nu_a := \varkappa \circ \varphi^{-1} = \varkappa \circ \varphi_0^{-1} \circ u^{-1}$. Its actual derivative $D_a\nu_a$ is an element of $\mathrm{Hom}\left(T_y\mathcal{B}, T_{\nu_a(x)}\mathcal{M}\right)$ at each $y \in \mathcal{B}$.

The morphological descriptor ν and its derivative N may or may not affect the measures of deformation, depending only on the specific circumstances engaged. Examples clarify the issue. In fact, in the cases in which ν represents a microdisplacement, a microscopic independent rotation of the substructure or it measures a microdeformation, N enters the measures of gross deformation depending on the special case envisaged (see examples in [7,42]). Contrary, when ν represents substructural events not related with changes in length or microdisplacements, the standard measures of deformation are sufficient.

3. Energy and the variational principle

Hyper-elastic complex bodies are considered here. A sufficiently smooth density $e := e(x, u, F, \nu, N)$ describes the states of equilibrium locally. Each material element is then considered as a system closed with respect to the exchange of mass and in energetic contact with the neighboring fellows (the last circumstance being evidenced by the presence of the gradients F and N in the list of entries of e).

Given u and ν, the global energy $\mathcal{E}(u, \nu)$ of $\mathcal{B}_0$ is then simply

$$\mathcal{E}(u, \nu) := \int_{\mathcal{B}_0} e\left(x, u(x), F(x), \nu(x), N(x)\right) \, \mathrm{d}x. \tag{3.1}$$

Ground states are minimizers of $\mathcal{E}(u, \nu)$, *i.e.* fields u and ν, selected in appropriate functional classes, that satisfy the variational principle

$$\min_{u,\nu} \mathcal{E}(u, \nu).$$

In common cases $\mathcal{E}(u,\nu)$ splits naturally in the sum

$$\mathcal{E}(u,\nu)=\int_{\mathcal{B}_0} e^i\left(x,F(x),\nu(x),N(x)\right)\,\mathrm{d}x+\int_{\mathcal{B}_0}\left(e_1^e(u(x))+e_2^e(\nu(x))\right)\,\mathrm{d}x, \tag{3.2}$$

where $e^i(x,F,\nu,N)$ is the *internal 'stored' energy*, $e_1^e(y)$ the potential of standard bulk (gravitational) forces and $e_2^e(\nu)$ the potential of direct bulk actions over the substructure such as electric fields in the case of polarizable substructures.

The requirement of objectivity, that is the invariance with respect to the action of $SO(3)$ (here on both the ambient space $\hat{\mathbb{R}}^3$ and $\mathcal{M}$), implies that in the range of large deformations the energy density $e(x,y,F,\nu,N)$ cannot be convex with respect to F, see pertinent comments in [52]), once one fixes the other arguments, while it may be a convex function of N (see [42]).

A prominent special case of (3.1) is the one of *partially decomposed energies*. They are characterized by two sufficiently smooth functions e_E and e_M such that

$$\mathcal{E}(u,\nu)=\int_{\mathcal{B}_0}\left(e_E(x,u(x),F(x),\nu(x))+e_M(x,\nu(x),N(x))\right)\,\mathrm{d}x. \tag{3.3}$$

Special expressions of the decomposed energy density describe ferroelectrics, spin glasses, liquid crystals, affine bodies, etc. More specifically, the density in (3.3) is a generalized form of the Ginzburg-Landau energy

$$e_E(x,\nu)+\frac{1}{2}\varpi|N|^2,$$

with $e_E(x,\nu)$ a non-homogeneous two-well energy and ϖ an appropriate material constant.

From a physical point of view a constitutive choice of the type (3.3) is like to imagine that the substructural action due to the relative change of the substructural shapes between neighboring material elements (an action called *microstress*) is not influenced directly by the macroscopic deformation, the interplay being only indirect.

For example, take into account a body in which $\nu(x)$ is a second rank symmetric tensor with components $\nu_{\alpha\beta}$, a tensor measuring a micro-deformation of each material element, a deformation independent of the macroscopic one, as it occurs in soft bodies with families of polymeric chains scattered in a melt (see *e.g.* [44]). The manifold of substructural shapes $\mathcal{M}$ then coincides with the linear space of second rank symmetric tensors over $\mathbb{R}^3$. For the sake of simplicity, one may also make use here of the displacement vector $\mathsf{u}=i^{-1}(u(x))-x$, with i the isomorphism between $\mathbb{R}^3$ and $\hat{\mathbb{R}}^3$. The elastic energy depends on $(D\mathsf{u})_{ij}$, $\nu_{\alpha\beta}$ and $N_{\alpha\beta i}$. Take note that in this example there is no distinction between covariant and contravariant components for the sake of simplicity. Latin indices indicate coordinates in the ambient space while Greek indices label coordinates over $\mathcal{M}$. In infinitesimal deformation and linear elastic setting, the elastic energy density takes the form

$$\begin{aligned}e^i(D\mathsf{u},\nu,N)=&\frac{1}{2}C_{ijhk}(D\mathsf{u})_{ij}(D\mathsf{u})_{hk}\\&+A^1_{ij\alpha\beta}(D\mathsf{u})_{ij}\nu_{\alpha\beta}+A^2_{ij\alpha\beta k}(D\mathsf{u})_{ij}N_{\alpha\beta k}\\&+\frac{1}{2}A^3_{\alpha\beta\gamma\delta}\nu_{\alpha\beta}\nu_{\gamma\delta}+A^4_{\alpha\beta\gamma\delta k}\nu_{\alpha\beta}N_{\alpha\beta k}+\frac{1}{2}A^5_{\alpha\beta i\gamma\delta j}N_{\alpha\beta i}N_{\gamma\delta j},\end{aligned}$$

with the constitutive tensors C and A^k, $k=1,\dots,5$, endowed at least with 'major' symmetries. If the material texture is centrosymmetric, a property that can be assumed commonly for each material element, by standard group calculations one may verify that all odd constitutive tensors vanish, namely $A^2_{ij\alpha\beta k}=0$, $A^4_{\alpha\beta\gamma\delta k}=0$,

so that the energy reduces to a very special case of (3.3), precisely

$$e^i\left(D\mathsf{u},\nu,D\nu\right)=\frac{1}{2}C_{ijhk}\left(D\mathsf{u}\right)_{ij}\left(D\mathsf{u}\right)_{hk}+A^1_{ij\alpha\beta}\left(D\mathsf{u}\right)_{ij}\nu_{\alpha\beta}\\+\frac{1}{2}A^3_{\alpha\beta\gamma\delta}\nu_{\alpha\beta}\nu_{\gamma\delta}+\frac{1}{2}A^5_{\alpha\beta i\gamma\delta j}N_{\alpha\beta i}N_{\gamma\delta j}.$$

Such a reduction does not occur when, for example, the morphological descriptor is a vector with generic component ν_α, a vector belonging to some copy of $\mathbb{R}^3$. In infinitesimal deformation and linear elastic setting, the elastic energy density takes in this case the form

$$e^i\left(D\mathsf{u},\nu,D\nu\right)=\frac{1}{2}C_{ijhk}\left(D\mathsf{u}\right)_{ij}\left(D\mathsf{u}\right)_{hk}+A^1_{ij\alpha}\left(D\mathsf{u}\right)_{ij}\nu_\alpha+A^2_{ij\alpha k}\left(D\mathsf{u}\right)_{ij}N_{\alpha k}\\+\frac{1}{2}A^3_{\alpha\gamma}\nu_\alpha\nu_\gamma+A^4_{\alpha\gamma k}\nu_\alpha N_{\gamma k}+\frac{1}{2}A^5_{\alpha i\gamma j}N_{\alpha i}N_{\gamma j},$$

with the constitutive tensors C and A^k, $k=1,\dots,5$, endowed with 'major' symmetries. If the material is centrosymmetric, then the expression of the energy reduces to

$$e^i\left(D\mathsf{u},\nu,D\nu\right)=\frac{1}{2}C_{ijhk}\left(D\mathsf{u}\right)_{ij}\left(D\mathsf{u}\right)_{hk}+A^2_{ij\alpha k}\left(D\mathsf{u}\right)_{ij}N_{\alpha k}\\+\frac{1}{2}A^3_{\alpha\gamma}\nu_\alpha\nu_\gamma+\frac{1}{2}A^5_{\alpha i\gamma j}N_{\alpha i}N_{\gamma j}.$$

This energy density appears in the mechanics of microcracked bodies (see [42]) and in the one of quasi-periodic alloys (see [40]) in infinitesimal deformation regime and is not a special case of (3.1). A special expression of the energy above is adequate for the mechanics of quasicrystals.

4. Ground states: existence theorems

Two steps are in general necessary for determining existence of minimizers of functionals by the direct methods of calculus of variations: (*i*) the extension of the functional class of competitors to some topological space in such a way that energy bounded sets are compact, and (*ii*) the appropriate extension of the energy functional over this enlarged class as a lower semicontinuous function. The first requirement forces one to introduce a class of competitors which includes non-smooth functions. Once the class of competitors is selected, the extended energy under scrutiny is defined as the relaxed energy. However, even in the setting of finite elasticity of simple bodies, the relaxed energy is not known actually, so that only heuristic choices for (*i*) and (*ii*) can be made.

In the more general context of complex bodies considered here, a similar procedure is followed.

The results do not exclude *a priori* a Lavrentiev gap phenomenon. Moreover, with respect to the non-linear elasticity of simple bodies, the situation tackled is even more intricate for the presence of the interplay between gross and substructural changes.

Take note that the choice of the topology and of the functional extensions mentioned above requires additional assumptions on the structure of the energy and the functional class of competitors. Such assumptions have often a non-trivial physical meaning (a meaning that has to be clarified at least in special cases of prominent physical interest) and, in this sense, they have constitutive nature. The effect of such assumptions becomes prominent when they imply the existence of singular minimizers and/or phenomena of localization of energy.

4.1. **Preliminaries**

Let $I\left(k,n\right)$ be the space of multi-indices of length k. Denote also by 0 the empty multi-index of length 0. For any α, the *complementary* multi-index to α in $(1,2,...,n)$ is denoted by $\bar{\alpha}$ and the sign of the permutation from $(1,2,...,n)$ into $(\alpha_1,...,\alpha_k,\bar{\alpha}_1,...,\bar{\alpha}_{n-k})$ is indicated by $\sigma\left(\alpha,\bar{\alpha}\right)$.

For $(\mathbf{e}_1, ..., \mathbf{e}_n)$ and $(\varepsilon_1, ..., \varepsilon_N)$ bases in $\mathbb{R}^n$ and $\mathbb{R}^N$ respectively, $\Lambda_r\left(\mathbb{R}^n \times \mathbb{R}^N\right)$ indicates the vector space of skew-symmetric tensors over $\mathbb{R}^n \times \mathbb{R}^N$ of the form

$$\xi = \sum_{|\alpha|+|\beta|=r} \xi^{\alpha\beta} \mathbf{e}_\alpha \wedge \varepsilon_\beta = \sum_{\max(0,r-n)}^{\min(r,N)} \xi_{(k)},$$

where

$$\xi_{(k)} = \sum_{\substack{|\alpha|+|\beta|=r \\ |\beta|=k}} \xi^{\alpha\beta} \mathbf{e}_\alpha \wedge \varepsilon_\beta.$$

The decomposition $\xi = \sum_k \xi_{(k)}$ does not depend on the choice of the bases.

For any linear map $G : \mathbb{R}^n \to \mathbb{R}^N$, the notation $M(G)$ is used for the simple n-vector in $\Lambda_n\left(\mathbb{R}^n \times \mathbb{R}^N\right)$ tangent to the graph of G and defined by

$$\begin{aligned} M(G) &:= \Lambda_n (id \times G)(\mathbf{e}_1 \wedge ... \wedge \mathbf{e}_n) \\ &= (\mathbf{e}_1, G(\mathbf{e}_1)) \wedge ... \wedge (\mathbf{e}_n, G(\mathbf{e}_n)). \end{aligned}$$

In coordinates one gets

$$M(G) = \sum_{k=0}^{\min(n,N)} M_{(k)}(G),$$

where

$$M_{(k)}(G) = \sum_{\substack{|\alpha|+|\beta|=n \\ |\beta|=k}} \sigma(\alpha, \bar{\alpha}) M_{\bar{\alpha}}^{\beta}(\mathbf{G}) \mathbf{e}_\alpha \wedge \varepsilon_\beta.$$

$\mathbf{G}$ indicates the matrix associated with G. Moreover, $M_{\bar{\alpha}}^{\beta}(\mathbf{G})$ is the determinant of the submatrix of $\mathbf{G}$ made of the rows and the columns indexed by β and $\bar{\alpha}$ respectively. It is also convenient to put $M_0^0(\mathbf{G}) := 1$. In the special case in which $n = N = 3$, the components of $M(G)$ are the entries of G, $\operatorname{adj} G$ and $\det G$.

For $\mathcal{M}$ a smooth manifold, $\Lambda_r(\mathcal{M})$ can be also defined as $\Lambda_r(\mathcal{M}) := \cup_{\nu \in \mathcal{M}} \Lambda_r(T_\nu \mathcal{M})$. The definition is natural, because $T_\nu \mathcal{M}$ a linear space. Related definitions can be then adapted. The natural vector algebra over the fiber $\Lambda_r(T_\nu \mathcal{M})$ is extended over the fiber bundle $\Lambda_r(T\mathcal{M})$.

Consider the two orthogonal subspaces $\mathbb{R}^3$ and $\mathbb{R}^N$ of the Euclidean space $\mathbb{R}^3 \times \mathbb{R}^N$, select $\mathcal{B}_0$ as a smooth open domain of $\mathbb{R}^3$ and take $u : \mathcal{B}_0 \to \mathbb{R}^N$.

For $u \in W^{1,1}\left(\mathcal{B}_0, \mathbb{R}^N\right)$, let $\tilde{\mathcal{B}}_0$ be the subset of $\mathcal{B}_0$ of Lebesgue points for both u and Du. Let also $\tilde{u}$ be a Lusin representative of u, and $\tilde{u}(x)$ and $D\tilde{u}(x)$ the Lebesgue values of u and Du at $x \in \tilde{\mathcal{B}}_0$. The Lusin-type theorem for $W^{1,1}$ functions implies that the graph of u, namely

$$\mathcal{G}_u := \left\{(x, y) \in \mathcal{B}_0 \times \mathbb{R}^N \mid x \in \tilde{\mathcal{B}}_0,\, y = \tilde{u}(x)\right\},$$

is a 3-rectifiable subset of $\mathcal{B}_0 \times \mathbb{R}^N$ with approximate tangent vector space at $(x, u(x))$ generated by the vectors $(\mathbf{e}_1, Du(x)\mathbf{e}_1), ..., (\mathbf{e}_3, Du(x)\mathbf{e}_3)$.

For any $u \in W^{1,1}\left(\mathcal{B}_0, \mathbb{R}^N\right)$ with $|M(Du(\mathbf{x}))| \in L^1(\mathcal{B}_0)$, the 3-*current integration* over the graph of u is the linear functional on smooth 3-forms with compact support in $\mathcal{B}_0 \times \mathbb{R}^N$ defined by

$$\begin{aligned} G_u &:= \int_{\mathcal{B}_0} (id \times u)^{\#}(\omega) = \int_{\mathcal{B}_0} \left\langle (id \times u)^{\#}(\omega), \mathbf{e}_1 \wedge \mathbf{e}_2 \wedge \mathbf{e}_3 \right\rangle \, \mathrm{d}x \\ &= \int_{\mathcal{B}_0} \langle \omega(x, u(x)), M(Du(x)) \rangle \, \mathrm{d}x, \end{aligned}$$

where # indicates pull-back of forms ω. By the area formula

$$G_u = \int_{\mathcal{G}_u} \langle \omega, \xi \rangle \ \mathrm{d}\mathcal{H}^3 \llcorner \mathcal{G}_u, \tag{4.1}$$

where $\xi(x) := \frac{M(Du(x))}{|M(Du(x))|}$ and $x \in \mathcal{B}_0$. ξ is the unit 3-vector that orients the approximate tangent plane to $\mathcal{G}_u$ at x; moreover, G_u has finite mass $\mathbf{M}(G_u) := \sup_{\|\omega\|_\infty \leq 1} G_u(\omega)$ since

$$\mathbf{M}(G_u) = \int_{\mathcal{B}_0} |M(Du(x))| \ \mathrm{d}x = \mathcal{H}^3(\mathcal{G}_u).$$

In particular, G_u is a vector valued measure on $\mathcal{B}_0 \times \mathbb{R}^N$. It is common usage to say that G_u is an integer rectifiable 3-current with integer multiplicity 1 on $\mathcal{B}_0 \times \mathbb{R}^N$.

For a generic function $u \in W^{1,1}(\mathcal{B}_0, \mathbb{R}^N)$ with $|M(Du(x))| \in L^1(\mathcal{B}_0)$, in general the *boundary current* ∂G_u, defined by

$$\partial G_u(\omega) := G_u(\mathrm{d}\omega), \qquad \omega \in \mathcal{D}^2(\mathcal{B}_0 \times \mathbb{R}^N),$$

does not vanish, although $\partial G_u(\omega) = 0$ for all $\omega \in \mathcal{D}^2(\mathcal{B}_0 \times \mathbb{R}^N)$ if u is smooth. A typical example is the map $u(x) := \frac{x}{|x|}$ that belongs to $W^{1,2}(B^3(0,1), \mathbb{R}^3)$. One computes that $\partial G_u = -\delta_0 \times S^2$ on $\mathcal{D}^2(B^3(0,1) \times \mathbb{R}^3)$, where δ_0 is Dirac delta. However, by approximating a map u in the Sobolev norm by means of C^2 maps, it is easy to prove that $\partial G_u = 0$ on $\mathcal{D}^2(\mathcal{B}_0 \times \mathbb{R}^N)$ if $u \in W^{1,3}(\mathcal{B}_0, \mathbb{R}^N)$.

4.2. **Functional characterization of the gross deformation**

The transplacement field is considered here as a weak diffeomorphism.

Definition 4.1. Let $u \in W^{1,1}(\mathcal{B}_0, \hat{\mathbb{R}}^3)$. u is said a *weak diffeomorphism* (one writes $u \in \mathrm{dif}^{1,1}(\mathcal{B}_0, \mathbb{R}^3)$) if

(1) $|M(Du(x))| \in L^1(\mathcal{B}_0)$;
(2) $\partial G_u = 0$ on $\mathcal{D}^2(\mathcal{B}_0, \hat{\mathbb{R}}^3)$;
(3) $\det Du(x) > 0$ a.e. $x \in \mathcal{B}_0$;
(4) for any $f \in C_c^\infty(\mathcal{B}_0 \times \mathbb{R}^3)$

$$\int_{\mathcal{B}_0} f(x, u(x)) \det Du(x) \ \mathrm{d}x \leq \int_{\mathbb{R}^3} \sup_{x \in \mathcal{B}_0} f(x, y) \, \mathrm{d}y. \tag{4.2}$$

The requirement 3 above is the standard condition assuring that the map $\tilde{u}$ be orientation preserving. Condition 4 is a global one-to-one condition, while items 1 and 2 provide the necessary uniformity. For instance, the norm of the minors of Du, namely $|M(Du)|$, is simply the standard square norm.

Condition 4 has been introduced in the form

$$\int_{\mathcal{B}_0} (\det Du(x)) \ \mathrm{d}x \leq \mathrm{vol}(u(\mathcal{B}_0)) \tag{4.3}$$

in [11] where the discussion is limited to the macroscopic deformation of (simple) bodies in the setting of $W^{1,3}(\mathcal{B}_0, \hat{\mathbb{R}}^3)$ maps. It allows frictionless contact of parts of the boundary of the body while still prevents the penetration of matter. Condition (4.3) is equivalent to (4.2) with $u(\mathcal{B}_0)$ substituted by $u(\tilde{\mathcal{B}}_0)$, with $\tilde{\mathcal{B}}_0$ the subset of $\mathcal{B}_0$ of Lebesgue points of u and Du. The version (4.2) is more useful for the analysis presented here.

Essential properties of weak diffeomorphisms are collected in the theorem below, the proof of which can be found in [27], where such a class of diffeomorphisms has been introduced.

Theorem 4.1.

(1) (Closure) *Let* $\{u_k\}$ *be a sequence with* $u_k \in \mathrm{dif}^{1,1}(\mathcal{B}_0, \hat{\mathbb{R}}^3)$ *for any* k. *If*

$$u_k \rightharpoonup u \quad \text{and} \quad M(Du_k) \rightharpoonup v$$

weakly in L^1, *then* $v = M(Du)$ *a.e. and, if* $\det Du > 0$ *a.e., then* $u \in \mathrm{dif}^{1,1}(\mathcal{B}_0, \hat{\mathbb{R}}^3)$.

(2) (Compactness) *Let* $\{u_k\}$ *be a sequence with* $u_k \in W^{1,r}(\mathcal{B}_0, \hat{\mathbb{R}}^3)$, $r > 1$, *and* u_k*'s weak diffeomorphisms. Assume that there exists a constant* $C > 0$ *and a convex function* $\vartheta : [0, +\infty) \to \mathbb{R}^+$ *such that* $\vartheta(t) \to +\infty$ *as* $t \to 0^+$, *and*

$$\|M(Du_k)\|_{L^r(\mathcal{B}_0)} \leq C, \qquad \int_{\mathcal{B}_0} \vartheta(\det Du_k(x))\ \mathrm{d}x \leq C.$$

Then, by taking subsequences $\{u_j\}$ *with* $u_j \rightharpoonup u$ *in* $W^{1,r}(\mathcal{B}_0, \hat{\mathbb{R}}^3)$, *one gets* $u_j \to u$ *in* $L^r(\mathcal{B}_0)$, $M(Du_j) \rightharpoonup M(Du)$ *in* L^r *and* $\int_{\mathcal{B}_0} \vartheta(\det Du(x))\ \mathrm{d}x \leq C$. *In particular,* u *is a weak diffeomorphism.*

In particular, below it is assumed that the gross deformation is an element of

$$\mathrm{dif}^{r,1}(\mathcal{B}_0, \hat{\mathbb{R}}^3) := \left\{ u \in \mathrm{dif}^{1,1}(\mathcal{B}_0, \hat{\mathbb{R}}^3) | \, |M(Du)| \in L^r(\mathcal{B}_0) \right\},$$

for some $r > 1$.

4.3. **Functional characterization of the morphological descriptor maps**

Above it has been emphasized that at each $x \in \mathcal{B}_0$ one gets $N \in \mathrm{Hom}\left(T_x\mathcal{B}_0, T_{\nu(x)}\mathcal{M}\right) \simeq \mathbb{R}^3 \otimes T_\nu \mathcal{M}$. When the energy density e admits derivative with respect to N, such a derivative describes the weakly non-local (gradient-conjugated) interactions between neighboring material elements, interactions (the so-called microstresses) due to relative changes in the substructural shapes. When one wants to compute in covariant way N explicitly, a connection over $\mathcal{M}$ is necessary. Its choice determines the representation of the microstress and, in this sense, it has constitutive nature. Physics may suggest also that a connection on $\mathcal{M}$ has no physical meaning as in the case of liquids with 'dispersed' bubbles. Moreover, even when $\mathcal{M}$ is selected to be Riemannian, in some circumstances the gauge needed for N might not be the Levi-Civita one (see, *e.g.*, [10]). In this case, if no prevalent role is given to the Levi-Civita connection, the parallel transport over geodetics may be non-isometric in general and also it can be even unbounded as a consequence of topological features of $\mathcal{M}$ itself. The metric $g_{\mathcal{M}}$ generating the Levi-Civita connection has also non-trivial physical meaning. In fact, as already mentioned in Section 3, when the material substructure admits its own kinetic energy, its first approximation is quadratic in the rates of the morphological descriptors, a quadratic form with coefficients given by $g_{\mathcal{M}}$. Conversely, if the quadratic substructural kinetic energy is prescribed by experimental data, its coefficients determine the metric itself. In this case, the related Levi-Civita connection brings information from substructural kinetics. Consequently, if the covariant gradient of ν is calculated by making use of the natural Levi-Civita connection, in dynamic setting the substructural kinetics may directly determine the representation of the microstress.

By Nash theorem, $\mathcal{M}$ is considered as a *submanifold* in $\mathbb{R}^N$ for some appropriate dimension. In addition it is assumed that $\mathcal{M}$ is closed. The covariant derivative of the map ν is in agreement with the differential of ν as a map from $\mathcal{B}_0$ into $\mathbb{R}^N$.

With the premises above it is assumed that ν belongs to the Sobolev space $W^{1,s}(\mathcal{B}_0, \mathcal{M})$, $s > 1$, defined by

$$W^{1,s}(\mathcal{B}_0, \mathcal{M}) := \left\{ \nu \in W^{1,s}\left(\mathcal{B}_0, \mathbb{R}^N\right) \ | \ \nu(x) \in \mathcal{M} \text{ for a.e. } x \in \mathcal{B}_0 \right\}.$$

Remarkably, since the isometric embedding of $\mathcal{M}$ in $\mathbb{R}^N$ by Nash's theorem is not unique, its choice (then the choice of the appropriate space $W^{1,s}(\mathcal{B}_0, \mathcal{M})$) is an additional constitutive prescription.

4.4. **Boundary conditions**

Boundary data have to be assigned for both the fields u and ν. As regards the macroscopic deformation u, place, traction or mixed data can be prescribed. As regards Dirichlet data, the ones considered here, since the deformation u is assumed to be an element of a Sobolev space, its value along the boundary $\partial\mathcal{B}_0$ or along an open part $\partial\mathcal{B}_{0,u}$ of it has to be assigned in the sense of traces. If Du admits summable minors, there is also the possibility to fix the value of the current ∂G_u as a functional on $\mathcal{D}^2(\mathbb{R}^3 \times \hat{\mathbb{R}}^3)$, a condition called *strong anchoring*. Notice that $\partial G_{u_k} \rightharpoonup \partial G_u$ if $M(Du_k) \to M(Du)$ in L^1. The assignment of ∂G_u is, in fact, stronger than prescribing the sole trace of u and reduces to it if $u \in W^{1,r}(\mathcal{B}_0, \hat{\mathbb{R}}^3)$, $r \geq 3$, or $u \in W^{1,2}(\mathcal{B}_0, \hat{\mathbb{R}}^3)$ and $\operatorname{adj} Du \in L^{\frac{3}{2}}$.

Boundary data of Dirichlet type are naturally admissible also for ν and they should be intended in the sense of traces. In fact, in some physical circumstances one may prescribe the shape of the substructure at the boundary of a complex body. The prototype example is the one of liquid crystals in nematic phase. In this case, the substructure is made of stick molecules with end-to-tail symmetry embedded in a ground liquid. For example, in a channel the orientation of the stick molecules along the walls of the channel can be prescribed by means of the use of surfactants spread along the walls themselves (see, *e.g.*, [9]). However, when shrewdness of this type are not available, a natural choice is to imagine that the material elements at the boundary do not undergo substructural changes so that one may prescribe that ν vanishes identically if the null value is included in $\mathcal{M}$.

In special circumstances one may think of the material elements on the boundary as made of simple material and that the complexity of the matter vanishes in a boundary layer: the relevant theory is not yet developed.

Moreover, one could consider the boundary as a sort of membrane coating the body. This point of view is helpful when one would like to assign data in terms of substructural tractions given by the conormal derivative $\partial_{D\nu} e\ n$, with n the normal to the boundary in the points in which it is defined. In fact, devices able to assign along the external boundary of the body contact direct actions on the substructure inside each material element seem to be not available, so that the natural boundary condition for substructural tractions is $\partial_{D\nu} e\ n = 0$. Such a condition makes always sense because at each x the conormal derivative $\partial_{D\nu} e\ n$ is an element of the cotangent space $T^*_{\nu(x)}\mathcal{M}$, a linear space indeed, containing the null value. The external boundary of the body can be also considered as a structured surface endowed with a surface energy depending on the normal (if the boundary is anisotropic), the surface gradient of deformation, the curvature tensor, the morphological descriptor and its surface gradient. In this case, the derivative of the surface energy with respect to the gradient of the morphological descriptor, applied to the normal, is the boundary datum in term of substructural action [40]. Of course, the choice of an explicit expression of the surface energy is strictly of constitutive nature.

4.5. **Existence results**

The portions $\partial\mathcal{B}_{0,u}$ and $\partial\mathcal{B}_{0,\nu}$ of the boundary where Dirichlet data are prescribed, may or may not coincide with the whole $\partial\mathcal{B}_0$. On $\partial\mathcal{B}_0 \backslash \partial\mathcal{B}_{0,u}$ and $\partial\mathcal{B}_0 \backslash \partial\mathcal{B}_{0,\nu}$ it is assumed that macroscopic and microscopic tractions satisfy the natural homogeneous null condition.

Define the space $\mathcal{W}_{r,s}$ by

$$\mathcal{W}_{r,s} := \left\{ (u,\nu) \,|\, u \in \operatorname{dif}^{r,1}(\mathcal{B}_0, \hat{\mathbb{R}}^3),\ \nu \in W^{1,s}(\mathcal{B}_0, \mathcal{M}) \right\}.$$

Imagine also that the energy functional (3.1) is extended to $\mathcal{W}_{r,s}$ as

$$\mathcal{E}(u,\nu) = \int_{\mathcal{B}_0} e(x, u(x), Du(x), \nu(x), D\nu(x))\ \mathrm{d}x,$$

where $u(x)$, $Du(x)$, $\nu(x)$ and $D\nu(x)$ are the Lebesgue values of u, ν and their weak derivatives.

Constitutive assumptions about the structure of the energy density e are also necessary. They are additional to the ones described in the previous sections concerning the functional nature of the fields involved.

Consider the energy density e as a map

$$e : \mathcal{B}_0 \times \hat{\mathbb{R}}^3 \times \mathcal{M} \times M^+_{3\times 3} \times M_{N\times 3} \to \bar{\mathbb{R}}^+$$

with values $e\,(x, u, F,\nu, N)$. The assumptions below about e apply.

(H1): e is polyconvex in F and convex in N. More precisely, there exists a Borel function

$$Pe : \mathcal{B}_0 \times \hat{\mathbb{R}}^3 \times \mathcal{M} \times \Lambda_3(\mathbb{R}^3 \times \hat{\mathbb{R}}^3) \times M_{N\times 3} \to \bar{\mathbb{R}}^+,$$

with values $Pe\,(x, u, \nu, \xi, N)$, which is

(a) l.s.c. in (u, ν, ξ, N) for a.e. $x \in \mathcal{B}_0$;

(b) convex in (ξ, N) for any (x, u, ν);

(c) such that $Pe\,(x, u, \nu, M\,(F)\,, N) = e\,(x, u, \nu, F, N)$ for any list of entries (x, u, ν, F, N) with $\det F > 0$.

In terms of Pe, the energy functional becomes

$$\mathcal{E}\,(u, \nu) = \int_{\mathcal{B}_0} Pe\,(x, u\,(x)\,, \nu\,(x)\,, M\,(F)\,, N)\ \mathrm{d}x. \tag{4.4}$$

(H2): The energy density e satisfies the growth condition

$$e\,(x, u, \nu, F, N) \geq C_1\,(|M\,(F)|^r + |N|^s) + \vartheta\,(\det F) \tag{4.5}$$

for any (x, u, ν, F, N) with $\det F > 0$, $r, s > 1$, $C_1 > 0$ constants and $\vartheta : (0, +\infty) \to \mathbb{R}^+$ a convex function such that $\vartheta\,(t) \to +\infty$ as $t \to 0^+$.

The convexity of Pe in (ξ, N) for any (x, y, ν) is in essence an assumption of stability which is more subtle than usual. In fact, in standard elasticity the condition involves only $M\,(F)$. Here there is an interplay between the gross deformation and the substructure: the former must contribute to the stability of the latter and *vice versa*.

The growth condition imposes that the set of admissible energies has a lower bound which is a decomposed energy of Ginzburg-Landau type that generates only interactions between neighboring material elements. Such actions are of gradient type, and generate the so-called microstress. In other words, the assumption (4.5) means that, in a conservative setting, substructural events within the generic material element, events that generate self-actions, may only increase the energy.

If there is a pair $(u_0, \nu_0) \in \mathcal{W}_{r,s}$ such that $\mathcal{E}\,(u_0, \nu_0) < +\infty$, from the closure theorem for weak diffeomorphisms above and Ioffe's classical semicontinuity result, the following theorem holds:

Theorem 4.2. *Under the hypotheses* (H1) *and* (H2) *the functional* $\mathcal{E}$ *achieves the minimum value in the classes*

$$\mathcal{W}^d_{r,s} := \{(u, \nu) \in \mathcal{W}_{r,s} | u = u_0 \ \textit{on}\ \partial\mathcal{B}_{0,u},\ \nu = \nu_0 \ \textit{on}\ \partial\mathcal{B}_{0,\nu}\}$$

and

$$\mathcal{W}^c_{r,s} := \left\{(u, \nu) \in \mathcal{W}_{r,s} \mid \partial G_u = \partial G_{u_0} \ \textit{on}\ \mathcal{D}^2(\mathbb{R}^3 \times \hat{\mathbb{R}}^3),\ \nu = \nu_0 \ \textit{on}\ \partial\mathcal{B}_{0,\nu}\right\}.$$

This theorem extends traditional existence results for simple elastic bodies and also the results for the minimizers of material substructures existing in special cases when gross deformations are neglected. Moreover, it indicates a path to characterize ground states in classes of bodies that have been not investigated so far.

Several variants are possible.

(H3): Assume that the energy density satisfies the growth condition

$$e\,(x, u, \nu, F, N) \geq C_2(|F|^2 + |Adj\ F|^{3/2} + |N|^s) + \vartheta\,(\det F) \tag{4.6}$$

for any (x, u, ν, F, N) with $\det F > 0$, $C_2 > 0$ a constant and $\vartheta : (0, +\infty) \to \mathbb{R}^+$ as above.

The growth condition (4.6) has the same physical meaning of (4.5), differences relying only in the explicit dependence of the lower bound on the macroscopic deformation.

Define now the class $\mathcal{W}_{2,\frac{3}{2},s}$ as

$$\begin{aligned}\mathcal{W}_{2,\frac{3}{2},s} \quad :\quad = \Big\{ &(u,\nu)\,|u \in W^{1,2}(\mathcal{B}_0,\hat{\mathbb{R}}^3),\, Adj(Du) \in L^{3/2},\\ &(4) \text{ in Definition 4.11 holds},\ \nu \in W^{1,s}\big(\mathcal{B}_0,\mathcal{M}\big)\Big\}.\end{aligned}$$

If the energy functional $\mathcal{E}$ is defined now on the class $\mathcal{W}_{2,\frac{3}{2},s}$, and there is a pair $(u_0,\nu_0) \in \mathcal{W}_{2,\frac{3}{2},s}$ such that $\mathcal{E}\,(u_0,\nu_0) < +\infty$, on account of the $L\log L$ estimate in [45], the new existence result below follows.

Theorem 4.3. *Under assumptions* (H1) *and* (H3)*, the functional* $\mathcal{E}$ *achieves its minimum value in the class*

$$\mathcal{W}^d_{2,\frac{3}{2},s} := \Big\{(u,\nu) \in \ \mathcal{W}_{2,\frac{3}{2},s} \mid u = u_0 \ \textit{on}\ \partial\mathcal{B}_{0,u}, \nu = \nu_0 \ \textit{on}\ \partial\mathcal{B}_{0,\nu}\Big\}.$$

The special case of partially decomposed free energies (3.3) falls, of course, within the theorems above. Moreover, in the setting justifying Theorem 2, the additive decomposition of the energy density e in its *macroscopic* and *microscopic* parts e_E and e_M allows one to separate the growth condition (4.5) in two parts, namely

$$e_E\,(x,u,\nu,F) \geq C_1\,|M\,(F)|^r + \vartheta\,(\det F)\,, \tag{4.7}$$

$$e_M\,(x,u,\nu,N) \geq C_1\,|N|^s\,. \tag{4.8}$$

By fixing ν in (4.7), one recovers a growth condition rather standard in finite elasticity of simple bodies where it is imposed only that $e_E\,(x,u,F) \geq C_1\,|M\,(F)|^r + \vartheta\,(\det F)$ (see, *e.g.*, [52]). This last requirement is tantamount to affirm that one is able to find ground states for bodies with a content of energy greater or equal to the one of a 'fictitious' elastic simple body with energy given by $C_1\,|M\,(F)|^r + \vartheta\,(\det F)$. In using (4.7), however, one is saying something more because of the presence of the morphological descriptor ν. With (4.7) it is prescribed that the standard lower bound for simple bodies be also valid for the macroscopic part of the energy of complex bodies admitting partially decomposed structure. The presumption is that substructural events accruing within each material element do not alter the lower bound, roughly speaking, substructural changes within the material element may only increase the global energy in conservative setting, at least with respect to $C_1\,|M\,(F)|^r + \vartheta\,(\det F)$. No matter about weakly non-local substructural interactions measured by the microstress, namely by the derivative of the energy with respect to $D\nu$. The energetics of such interactions is described by e_M. The condition (4.8) indicates that the energy accounting for both substructural changes and weakly non-local interactions of gradient type admits as lower bound the energy of a 'fictitious' rigid complex material for which the energy stored within each material element is negligible with respect to the one associated with weakly non-local interactions. Specifically, the energy of such a 'fictitious' complex material is an extension of the Dirichlet energy and reduces to it when $s = 2$. In conservative case, the requirement (4.8) is quite natural because substructural activity within the material element may only increase the energy density, being the energy density of all events non-negative.

Analogous physical interpretations hold in the setting justifying Theorem 3 where (4.7) and (4.8) become respectively

$$e\,(x,u,\nu,F) \geq C_2(|F|^2 + |Adj\ F|^2) + \vartheta\,(\det F)\,,$$

$$e_M\,(x,u,\nu,N) \geq C_2\,|N|^2\,,$$

being e_M in this case a Dirichlet energy when $C_2 = \frac{1}{2}$.

4.6. **Remarks about the possible presence of a Lavrentiev gap phenomenon**

There is no evidence that the energy functional

$$\mathcal{E}(u,\nu)=\int_{\mathcal{B}_0} Pe\left(x,u(x),\nu(x),M(F),N\right)\,\mathrm{d}x$$

defined over the class $\mathcal{W}_{r,s}$ is the relaxed version of the same functional defined on regular pairs (u,ν), namely there is no evidence that

$$\mathcal{E}(u,\nu):=\inf\left\{\liminf_{j\to\infty}\mathcal{E}(u_j,\nu_j)\ \mid\ (u_j,\nu_j)\rightharpoonup(u,\nu)\ \text{ in } L^1,(u_j,\nu_j)\in C^1\right\}$$

for any $(u,\nu)\in\mathcal{W}_{r,s}$. In other words, a Lavrentiev gap phenomenon, namely

$$\mathcal{E}(u,\nu)<\inf\left\{\liminf_{j\to\infty}\mathcal{E}(u_j,\nu_j)\ \mid\ (u_j,\nu_j)\rightharpoonup(u,\nu)\ \text{ in } L^1,(u_j,\nu_j)\in C^1\right\},$$

is not excluded *a priori*. Examples of special cases of the one treated here are known from the scientific literature. For instance, in two-dimensional ambient space there are examples of non-linear elastic simple materials admitting a gap between the infimum of the energy over admissible continuous deformations belonging to a Sobolev space $W^{1,r}$ and the analogous infimum over admissible continuous deformations belonging to a Sobolev space $W^{1,s}$ with $s<r$ [20].

A gap phenomenon driven this time by the topology of the substructural manifold $\mathcal{M}$ can also arise. When the manifold of substructural shapes $\mathcal{M}$ has a non trivial homology, then defects may arise.

In particular, for example, a gap phenomenon appears for the Dirichlet integral

$$\mathcal{D}(\nu):=\frac{1}{2}\int_{\mathcal{B}_0}|D\nu(x)|^2\,\mathrm{d}x \tag{4.9}$$

involving maps $\nu:\mathcal{B}_0\to S^2$, with S^2 the unit sphere, and for Dirichlet boundary data (see results in [23,25,26]). Take note that the exponent 2 and the circumstance that the manifold of substructural shapes is S^2 is crucial for the remarks in what follows. The energy above, in absence of gross deformations, describes cases of spin glasses, magnetostrictive materials in conditions of magnetic saturation and soft composites reinforced with a dense family of microfibers not endowed with end-to-tail symmetry.

The gap phenomenon appears when the degree of the boundary datum is different from zero (because regular maps satisfying it are absent) and even for some boundary data with zero degree [32]. However, it is possible to find an explicit form for the relaxed version of (4.9) on $W^{1,2}$ which gives rise to a non-local functional [4].

A further difference between the maps in $W^{1,2}$ and the regular ones relies in the behavior of the current

$$\mathbf{D}_\nu(\eta):=\int_{\mathcal{B}_0}\eta\wedge\nu^{\#}\omega_{S^2},\qquad \eta\in\mathcal{D}^1(\mathcal{B}_0),$$

with ω_{S^2} the volume form over S^2, a current which can be considered as integration along the field $D(x)$ defined by duality by $D_\nu(x):=*\omega_{S^2}$, with $*$ the Hodge star operator. Take note that, whereas $D_\nu(x)\neq 0$, $D_\nu(x)$ generates $\ker D\nu(x)$ at x. Since the outward flux across the boundary $\partial B(x_0,r)$ of a ball $B(x_0,r)$, centered at x_0 and with radius r, is the degree of the map $\nu\big|_{\partial B(\mathbf{x}_0,r)}$, it follows that $\operatorname{Div}D_\nu=0$ for any $\nu\in C^1(\mathcal{B}_0)$. In contrast, and for the same reason, for the map $\nu(x):=\frac{x}{|x|}\in W^{1,2}\left(\mathcal{B}_0,S^2\right)$ one gets $\operatorname{Div}D_\nu=4\pi\delta_0$ in distributional sense.

By following results in [24,30,31], a way to link the loss of energy in the Dirichlet integral and the 'bad' behavior of some functions in $W^{1,2}$ in pulling-back 2-forms, is to associate with each map $\nu\in W^{1,2}\left(\mathcal{B}_0,S^2\right)$

the current integration over its graph

$$G_\nu(\omega) = \int_{\mathcal{B}_0} \omega(x, \nu(x), M(D\nu(x))) \, \mathrm{d}x.$$

In particular, it is proved that if $\{\nu_j\}$ is a sequence of S^2-valued maps with equibounded Dirichlet energies and T is a current such that $G_{\nu_j} \rightharpoonup T$, then T has finite mass and there exists a map $\nu_T \in W^{1,2}(\mathcal{B}_0, S^2)$ and a one-dimensional integer rectifiable current L_T, both map and current individuated uniquely by T, such that

$$T = G_{\nu_T} + L_T \times S^2 \text{ on } \mathcal{D}^3(\mathcal{B}_0 \times S^2).$$

Moreover, $L_T = 0$ if $M(D\nu_j)$ weakly converges in $L^1(\mathcal{B}_0, \Lambda_3(\mathbb{R}^3, \hat{\mathbb{R}}^3))$.

The meaning of the concentration line L_T is clear from the point of view of weak convergence. In fact, if $G_{\nu_j} \rightharpoonup T = G_{\nu_T} + L_T \times \mathcal{M}$, then on two-dimensional sections orthogonal to the support of L_T in a thin tube wrapped around the support itself, for j sufficiently large, ν_j assumes as value the entire sphere, point by point. L_T is then a line (a line defect) in which there is 'fusion' of the substructure, fusion in the sense of complete disorder so that the concept of prevailing direction loses its meaning. Moreover, the currents D_{ν_j}, associated with the elements of the sequence $\{\nu_j\}$, converge (in the sense of currents) to the current $D_T = D_{\nu_T} + 4\pi L_T$; in particular $\partial D_T = 0$ on $\mathcal{B}_0 \times S^2$. If $L_T = 0$, the graph of ν_T has no boundary and $\mathrm{Div}\, D_{\nu_T} = 0$. In this case, if ν_T would have point singularities, all singularities would have zero degree.

It could be possible to extend the previous discussion by substituting S^2 with a generic two dimensional compact manifold $\mathcal{M}$, but $L_T = 0$ if $\mathcal{M}$ is not homologically a sphere.

4.7. **Cartesian currents and the special case of spin substructures**

Dirichlet energies involving S^2-valued maps describe essential aspects of the mechanical behavior of bodies with spin structure that does not suffer deformation. Basic results have been obtained in the current literature. Essential aspects are reviewed here first, then it is shown how they can be extended to energies more general that the Dirichlet one, that is to the description of the mechanical behavior or deformable bodies with spin substructure. Basically the analysis is essentially the same, the physics of the phenomena covered is enlarged drastically.

A current $T \in \mathcal{D}_3(\mathcal{B}_0 \times \hat{\mathbb{R}}^3)$ is in $\mathrm{cart}^{2,1}(\mathcal{B}_0 \times S^2)$ if there exist a map $\nu_T \in W^{1,2}(\mathcal{B}_0, S^2)$ and an integer rectifiable current L_T on $\mathcal{D}^1(\mathcal{B}_0)$ such that $T = G_{\nu_T} + L_T \times S^2$ over $\mathcal{D}^3(\mathcal{B}_0 \times \hat{\mathbb{R}}^3)$. If $T \in \mathrm{cart}^{2,1}(\mathcal{B}_0 \times S^2)$, then ν_T and L_T are uniquely defined by T (see [24,30,31]).

The extension of the Dirichlet energy associated with S^2-valued morphological descriptor maps to $\mathrm{cart}^{2,1}(\mathcal{B}_0 \times S^2)$ can be obtained by defining the energy on the space $cart^{2,1}(\mathcal{B}_0 \times S^2)$ as

$$\mathcal{D}(T) := \int_{\mathcal{B}_0} F(n, \vec{T}) \, \mathrm{d}\|T\|,$$

where $F(n, \xi)$ is the polyconvex extension of the integrand

$$f(n, N) := \begin{cases} \frac{1}{2}|N|^2 & \text{if } N^* n = 0 \\ +\infty & \text{otherwise} \end{cases}$$

to the space of 3-vectors in $\Lambda_3(\mathbb{R}^3 \times S^2)$, while $\vec{T} := \frac{\mathrm{d}T}{\mathrm{d}\|T\|}$ is the Radon-Nykodim derivative of T with respect to its total variation. Precisely, $F(n, \xi)$ is defined by

$$\begin{aligned} F(n, \xi) \quad : \quad & = \sup\{\phi(\xi) \mid \phi : \Lambda_3(\mathbb{R}^3 \times S^2) \to \mathbb{R}, \\ & \phi \text{ linear}, \ \phi(M(N)) \le f(n, N), \ \forall (n, N)\}. \end{aligned}$$

One shows (see [24,31]) that

***(i)*:**

$$\mathcal{D}(T) := \frac{1}{2}\int_{\mathcal{B}_0} |D\nu_T|^2 \ \mathrm{d}x + 4\pi \mathbf{M}(L_T) \tag{4.10}$$

if $T = G_{\nu_T} + L_T \times S^2 \in cart^{2,1}\left(\mathcal{B}_0 \times S^2\right)$;

***(ii)*:** $\mathcal{D}(T)$ is lower semicontinuous due to the convergence of currents with equibounded Dirichlet energies and

***(iii)*:** $\mathcal{D}(T)$ is the relaxed counterpart of the Dirichlet integral for the convergence above.

***(iii)*:** (Closure) The class $cart^{2,1}\left(\mathcal{B}_0 \times S^2\right)$ is closed with respect to the convergence of currents with equibounded masses and norms $\|\nu_{Tj}\|_{W^{1,2}}$.

Existence of minimizers for (4.10) in $cart^{2,1}\left(\mathcal{B}_0 \times S^2\right)$ under Dirichlet boundary conditions and absence of gap then follows. Such minimizers describe ground states of bodies with spin structure in which the gross deformation is neglected.

The results described above extend to an existence theorem of minimizers for an elastic body with spin structure admitting a decomposed energy of the type

$$\mathcal{E}(u, \nu_T) = \int_{\mathcal{B}_0} e_E(x, u, \nu_T, Du) \ \mathrm{d}x + \frac{1}{2}\int_{\mathcal{B}_0} |D\nu_T|^2 \ \mathrm{d}x + 4\pi \mathbf{M}(L_T). \tag{4.11}$$

Theorem 4.4. *If e_E satisfies* (H1) *and either* (H2) *or* (H3)*, then the functional* (4.11) *admits minimizers in $W^{r,s}(\mathcal{B}_0, \hat{\mathbb{R}}^3) \times cart^{2,1}(\mathcal{B}_0 \times S^2)$ under Dirichlet conditions.*

The theorem above is the main result of the present section, the details of the proof are not specified here because they are implied directly. The presence of the term $4\pi\mathbb{M}(L_T)$ in (4.11) is a constitutive choice. It takes into account the energetic contribution of the overall behavior of the regions of the body in which the disorder is so high that the identification of a local orientation becomes meaningless, regions that are here described by the one dimensional current L_T.

4.8. **The general case**

Here, previous remarks are generalized. The aim is to obtain existence results allowing (i) the interactions between the substructural changes and gross deformation even at level of first gradients (taking also into account the minors involving elements of *both* F and N) and, contemporarily, (ii) the possible localization of substructural activity along lines, with a possible generation of local substructural disorder.

Note that the energy density e does not depend (at least as far as one may imagine in common cases) on the product $u(x)\, D\nu(x)$. In fact, the derivative of e with respect to u is the representative of standard external body forces and it is not natural to presume that the standard body forces depend on the relative changes in material substructure from place to place.

Below it is convenient to consider the pair deformation-morphological descriptor as a unique map $(u, \nu) : \mathcal{B}_0 \to \hat{\mathbb{R}}^3 \times \mathcal{M}$.

All minors of the matrix

$$\begin{pmatrix} F \\ N \end{pmatrix}$$

are collected in $M\left(\begin{pmatrix} F \\ N \end{pmatrix}\right)$. Define the set

$$\mathcal{I} := \left\{ (\alpha, \beta) \,|\alpha \in I(k,3),\ \beta \in I(k, 3+N),\ 0 \le k \le 3 \text{ s.t.} \right.$$

$$\left. \left| M^{\alpha}_{\beta}\begin{pmatrix} F \\ N \end{pmatrix}\right| \le e(x, u, F, \nu, N),\ \forall (x, u, F, \nu, N) \right\}$$

and let $\mathcal{J} \subset \mathcal{I}$ be defined by

$$\mathcal{J} := \left\{ (\alpha,\beta) \,|\alpha \in I(k,3)\,,\ \beta \in I(k,3+N)\,,\ 0 \le k \le 3 \text{ s.t. } \exists\, r>1 \text{ s.t.} \right.$$
$$\left. \left| M^{\alpha}_{\beta} \begin{pmatrix} F \\ N \end{pmatrix} \right|^{r} \le e(x,u,F,\nu,N)\,,\ \forall (x,u,F,\nu,N) \right\}.$$

As an additional constitutive assumption on the energy, it is assumed here that the energy density e is such that

$$(\alpha,\beta) \in \mathcal{I} \Longrightarrow (\alpha',\beta') \in \mathcal{J},\ \ \forall (\alpha',\beta')\,,\ \alpha' < \alpha, \quad \beta' < \beta.$$

If (u_j,ν_j) is a sequence of pairs deformation-morphological descriptor which are equibounded in energy, then for any α and β the sequence

$$\left\{ M^{\alpha}_{\beta} \begin{pmatrix} Du_j \\ D\nu_j \end{pmatrix} \right\}$$

is equibounded in $L^1(\mathcal{B}_0)$ if $(\alpha,\beta) \in \mathcal{I}$ and equibounded in some $L^r(\mathcal{B}_0)$, $r>1$, if $(\alpha',\beta') \in \mathcal{J}$. Consequently, by taking subsequences, $(u_j,\nu_j) \to (u,\nu)$ in L^1 and there exist measures μ^{α}_{β} in $\mathcal{B}_0 \times \hat{\mathbb{R}}^3 \times \mathbb{R}^N$ such that for any $\phi \in C^0(\mathcal{B}_0 \times \hat{\mathbb{R}}^3 \times \mathbb{R}^N)$ one gets

$$\int_{\mathcal{B}_0} \phi(x,u_j(x),\nu_j(x)) M^{\alpha}_{\beta} \begin{pmatrix} Du_j \\ D\nu_j \end{pmatrix} \mathrm{d}x \to \int_{\mathcal{B}_0 \times \hat{\mathbb{R}}^3 \times \mathbb{R}^N} \phi(x,u(x),\nu(x))\ \mathrm{d}\mu^{\alpha}_{\beta}(x,y,\nu)$$

for any $(\alpha,\beta) \in \mathcal{I}$. Moreover, if $(\alpha,\beta) \in \mathcal{J}$, one also gets

$$\int_{\mathcal{B}_0 \times \hat{\mathbb{R}}^3 \times \mathbb{R}^N} \phi(x,u(x),\nu(x))\ \mathrm{d}\mu^{\alpha}_{\beta}(x,y,\nu) == \int_{\mathcal{B}_0} \phi(x,u(x),\nu(x)) M^{\alpha}_{\beta} \begin{pmatrix} Du \\ D\nu \end{pmatrix} \mathrm{d}x.$$

For each j, the previous measures can be collected in a vector-valued measure, or, better, in the *semi-currents*

$$G_{(u_j,\nu_j)} := \int_{\mathcal{B}_0} \left\langle \omega(x,u_j(x),\nu_j(x)), M \begin{pmatrix} Du_j \\ D\nu_j \end{pmatrix} \right\rangle \mathrm{d}x,$$

and

$$G_{(u,\nu)} := \int_{\mathcal{B}_0} \left\langle \omega(x,u(x),\nu(x)), M \begin{pmatrix} Du \\ D\nu \end{pmatrix} \right\rangle \mathrm{d}x,$$

defined over the space

$$\mathcal{D}^{3,\mathcal{I}} := \left\{ \omega = \sum_{\substack{\beta:=(\beta_1,\beta_2) \\ (\alpha,\beta)\in\mathcal{I}}} \omega_{\alpha,\beta_1,\beta_2}(x,u,\nu)\ \mathrm{d}x^{\alpha} \wedge \mathrm{d}u^{\beta_1} \wedge \mathrm{d}z^{\beta_2} \right\},$$

of 3-forms on $\mathcal{B}_0 \times \hat{\mathbb{R}}^3 \times \mathbb{R}^N$. It follows that

***(i)*:** the $G_{(u_j,\nu_j)}$'s have equibounded masses;
***(ii)*:** $G_{(u_j,\nu_j)} \to T := G_{(u,\nu)} + S$, over $\mathcal{D}^{3,\mathcal{I}}$;
***(iii)*:** the component $S^{\alpha\beta}(\phi) := S\left(\phi(x,u,\nu)\ \mathrm{d}x^{\alpha} \wedge \mathrm{d}u^{\beta_1} \wedge \mathrm{d}z^{\beta_2}\right)$ is identically zero if $(\alpha,\beta) \in \mathcal{J}$.

As appropriate extension of the energy $e = e(x,y,\nu,F,N)$, one considers its polyconvex form

$$Pe(x,u,\nu,\xi) = \sup \left\{ \phi(\xi) \,|\phi \in \mathrm{Hom}(\Lambda_3(\mathbb{R}^3 \times \hat{\mathbb{R}}^3 \times \mathbb{R}^N), \mathbb{R}),\ \text{s.t.} \right.$$
$$\left. \phi\left(M \begin{pmatrix} F \\ N \end{pmatrix} \right) \le e(x,u,F,\nu,N)\,,\ \forall (x,u,F,\nu,N) \right\}.$$

Note that, differently from the existence results in previous sections, here the polyconvexification of the energy accounts for all minors of the matrix $\begin{pmatrix} F \\ N \end{pmatrix}$.

It is rather simple to show that Pe is (i) l.s.c. in ξ for any fixed (x,u,ν), (ii) positively homogeneous of degree 1 in ξ and (iii) $Pe\,(x,u,\nu,\xi) \geq \|\xi\|$. Then it is possible to extend the energy functional to vector-valued measures $T = \left\{T^{\alpha}_{\beta}\right\}_{(\alpha,\beta)\in\mathcal{I}}$ in the direct product $\mathbb{R}^3 \times \hat{\mathbb{R}}^3 \times \mathbb{R}^N$ by putting

$$\mathcal{F}\,(T) := \int Pe(x,u,\nu,\vec{T})\ \mathrm{d}\,\|T\|\,.$$

A classical semicontinuity result of Reshetnyak [47–49] states that $\mathcal{F}$ is semicontinuous with respect to the weak convergence of measures under the further assumption

$$Pe\,(x,u,\nu,\xi) \text{ is l.s.c. in } (x,u,\nu,\xi)\,.$$

Then, existence of minimizers in a class of semi-currents closed under the weak convergence of measures follows trivially.

Such a general program has to be completed by analyzing the current S in the item (ii) above, by computing explicitly the integral functional and then discussing the possible absence of gap phenomenon. This program as been developed in [24,31] in the special case of the Dirichlet energy $\frac{1}{2}\int_{\mathcal{B}_0} |D\nu|^2\ \mathrm{d}x$, with $\nu : \mathcal{B}_0 \to \mathcal{M}$, where $\mathcal{M}$ is a compact, oriented, Riemannian manifold $\mathcal{M}$ of dimension ≥ 2. The general case is still open.

5. Balance of standard and substructural actions

The deduction of Euler-Lagrange equations for (3.1) points out the nature of the interactions involved in the mechanical behavior of complex bodies and also the nature of their integral versions (see discussions in [12,38, 40,41]). Here the meaning of Euler-Lagrange equations associated with irregular minimizers of the energy of complex bodies and the conditions under which they exist are discussed.

5.1. Euler-Lagrange equation: C^1-minimizers

The condition

$$\delta\mathcal{E}\,(u,\nu) = 0, \tag{5.1}$$

where δ indicates first variation, characterizes the equilibrium.

For evaluating the first variation of $\mathcal{E}\,(u,\nu)$ it is not necessary to embed the manifold of substructural shapes in some linear space. $\mathcal{M}$ is then considered abstract as in the original format of the mechanics of complex bodies.

Assume first that $\mathcal{E}$ admits minimizers of class C^1. To define variations over $\mathcal{M}$, it is useful to make use of fields of the type $\upsilon : \mathcal{B}_0 \to T\mathcal{M}$, with $\upsilon\,(x) \in T_{\nu(x)}\mathcal{M}$, belonging to the class $C^1_c\,(\mathcal{B}_0, T\mathcal{M})$. For any $x \in \mathcal{B}_0$, here υ is taken such that $\upsilon = \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\nu_\varepsilon\,|_{\varepsilon=0} := \upsilon\,(x)$ in any local chart, being ν_ε a generic smooth curve $(-1,1) \ni \varepsilon \mapsto \nu_\varepsilon \in \mathcal{M}$ crossing ν when $\varepsilon = 0$.

Define

$$C^1_{\bar{u}}(\mathcal{B}_0,\hat{\mathbb{R}}^3) := \left\{u \in C^1_{\bar{u}}(\mathcal{B}_0,\hat{\mathbb{R}}^3) | u = \bar{u} \text{ on } \partial\mathcal{B}_0\right\},$$

$$C^1_{\bar{\nu}}\,(\mathcal{B}_0,\mathcal{M}) := \left\{\nu \in C^1_{\bar{\nu}}\,(\mathcal{B}_0,\mathcal{M})\,|\nu = \bar{\nu} \text{ on } \partial\mathcal{B}_0\right\},$$

where $\bar{u}$ and $\bar{\nu}$ are the boundary data in the Dirichlet problem considered here.

If the energy $\mathcal{E}\,(u,\nu)$ attains a minimum at the pair $(u,\nu) \in C^1_{\bar{u}}(\mathcal{B}_0,\hat{\mathbb{R}}^3) \times C^1_{\bar{\nu}}\,(\mathcal{B}_0,\mathcal{M})$, for $\varepsilon \in (-1,1)$ and each $h \in C^1_c(\mathcal{B}_0,\hat{\mathbb{R}}^3)$, the function $\varepsilon \mapsto \mathcal{E}\,(u+\varepsilon h,\nu_\varepsilon)$ attains a minimum at $\varepsilon = 0$.

The *first variation* $\delta_{h,\upsilon}\mathcal{E}$ of $\mathcal{E}$ *from the ground state along the direction* (h,υ) is then defined naturally by

$$\delta_{h,\upsilon}\mathcal{E}\left(u,\nu\right):=\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\mathcal{E}\left(u+\varepsilon h,\nu_{\varepsilon}\right)|_{\varepsilon=0}\,.$$

At (u,ν) the first variation of the energy then vanishes along any direction (h,υ). Euler-Lagrange equations then follows from the calculation of the first variation:

Theorem 5.1. *Let the pair* (u,ν) *be a minimizer for* $\mathcal{E}$. *Then, (i) for any* $h\in C_c^1\left(\mathcal{B}_0,\mathbb{R}^3\right)$ *and for any* $\upsilon\in C_c^1\left(\mathcal{B}_0,T\mathcal{M}\right)$, *with* $\upsilon\left(x\right)\in T_{\nu(x)}\mathcal{M}$, *the map* $\varepsilon\mapsto\mathcal{E}\left(u+\varepsilon h,\nu_{\varepsilon}\right)$ *is differentiable and the pair* (u,ν) *satisfies the weak form of Euler-Lagrange equations*

$$\int_{\mathcal{B}_0}\left(-b\cdot h+P\cdot Dh+\zeta\cdot\upsilon+\mathcal{S}\cdot D\upsilon\right)\,\mathrm{d}x=0;\tag{5.2}$$

(ii) if $(u,\nu)\in C^2\left(\mathcal{B}_0,\mathbb{R}^3\right)\times C^2\left(\mathcal{B}_0,\mathcal{M}\right)$, *then* (5.2) *is equivalent to the strong form*

$$\mathrm{Div}P+b=0,\tag{5.3}$$

$$\mathrm{Div}\mathcal{S}-\zeta=0\quad\textit{in }T_{\nu}^{*}\mathcal{M}.\tag{5.4}$$

In the equations above, $P\left(x\right):=\partial_F e\in\mathrm{Hom}(T_x^*\mathcal{B}_0,T_{u(x)}^*\mathcal{B})\simeq\mathbb{R}^3\otimes\hat{\mathbb{R}}^3$ is the first Piola-Kirchhoff stress, $b\left(x\right):=-\partial_u e\in T_x^*\mathcal{B}\simeq\mathbb{R}^3$ the vector of standard body forces, $\mathcal{S}\left(x\right):=\partial_{D\nu}e\in\mathrm{Hom}(T_x^*\,\mathcal{B}_0,T_{\nu(x)}^*\mathcal{M})\simeq\mathbb{R}^3\otimes T_{\nu(x)}^*\mathcal{M}$ the microstress measuring constant interactions between neighboring material elements due to substructural changes, $\zeta\left(x\right):=\partial_\nu e\in T_{\nu(x)}^*\mathcal{M}$. In particular, by considering e decomposed additively in internal $e^i\left(x,Du,\nu,D\nu\right)$ and external $e^e\left(u,\nu\right)$ components, ζ splits in the sum $\zeta=z-\beta$, where $z\left(x\right):=\partial_\nu e^i\in T_{\nu(x)}^*\mathcal{M}$ is the self-action within the generic material element due to substructural changes inside it while $\beta\left(x\right):=-\partial_\nu e^e\in T_{\nu(x)}^*\mathcal{M}$ represents external direct body actions on the substructure (a paradigmatic example is the one of electric fields acting on the polarization structure in ferroelectrics). Take note that the term $\partial_{D\nu}e\cdot D\upsilon$ can be considered as the derivative $\frac{\mathrm{d}}{\mathrm{d}\varepsilon}e\left(x,u+\varepsilon h,F+\varepsilon Dh,\nu_{\varepsilon},N+\varepsilon D\upsilon\right)|_{\varepsilon=0}$ since $N:=D\nu\left(x\right)$ belongs to a linear space. The same meaning cannot be attributed to the term $\partial_\nu e\cdot\upsilon$ because $\mathcal{M}$ is not a linear space. The dot denotes the natural pairing between dual spaces.

5.2. **Direct representation of standard and substructural actions: invariance and balance**

Really the balance of actions involved in the mechanics of complex bodies has the same structure of (5.3), (5.4), independently of constitutive issues introduced in specifying the functional dependence of the energy on the state variables in the variational setting considered here. Equation (5.3) is Cauchy balance of standard forces while (5.4) is Capriz balance of substructural actions. A special case of (5.4) is Ginzburg-Landau equation.

To obtain balance equations from the sole direct representation of standard and substructural actions two tools are necessary: (i) a class $\mathfrak{P}$ of subsets $\mathfrak{b}$ of $\mathcal{B}_0$ with non-vanishing volume and the same geometrical regularity of $\mathcal{B}_0$ itself, subsets called *parts*, and (ii) vector fields $h\in C(\mathcal{B}_0,\hat{\mathbb{R}}^3)$ and $\upsilon\in C\left(\mathcal{B}_0,T\mathcal{M}\right)$. Only the power of actions is defined here, without paying attention to constitutive issues.

Given the pair $\tau:=(u,\nu)$, any *power* along (u,ν) is such a map $\mathcal{P}:\mathfrak{P}\left(\mathcal{B}_0\right)\times T\mathfrak{G}\to\mathbb{R}^+$ that $\mathcal{P}\left(\cdot,\tau,\dot{\tau}\right)$ is additive over disjoint parts and $\mathcal{P}\left(\mathfrak{b},\tau,\cdot\right)$ is linear.

The basic point is the explicit representation of $\mathcal{P}$, that is the representation of actions over the generic $\mathfrak{b}$. The usual assumption is that the actions be of volume and contact nature, the latter represented by means of appropriate stresses that are in this case the first Piola-Kirchhoff stress P and the microstress $\mathcal{S}$, no matter about their possible constitutive structure. External bulk actions are represented by the standard covector b of body forces and, at each x, by an element of the cotangent space $T_{\nu(x)}^*\mathcal{M}$, indicated by β. In this way,

the power $\mathcal{P}^{\text{ext}}_{\mathfrak{b}}(h,v)$ exchanged by the generic $\mathfrak{b}$ with the rest of the body and the external environment, a power measured over (h,v) along (u,ν), is represented by

$$\mathcal{P}^{\text{ext}}_{\mathfrak{b}}(h,v) := \int_{\mathfrak{b}} (b\cdot h+\beta\cdot v)\ \mathrm{d}x + \int_{\partial\mathfrak{b}} (Pn\cdot h+\mathcal{S}n\cdot v)\ \mathrm{d}\mathcal{H}^2, \tag{5.5}$$

where $\mathrm{d}\mathcal{H}^2$ is the two-dimensional Hausdorff measure on $\partial\mathfrak{b}$, n the normal to $\partial\mathfrak{b}$ in all places in which it is defined, that is everywhere except a closed subset of $\partial\mathfrak{b}$ with vanishing $\mathcal{H}^2$ measure. Here b, β, P and $\mathcal{S}$ are not defined *a priori* as the derivatives of the energy as energy does not come into play. Once u and ν are given, one says only that, at each x, fields taking values $b(x)\in T^*_{u(x)}\mathcal{B}\simeq\hat{\mathbb{R}}^3$, $\beta(x)\in T^*_{\nu(x)}\mathcal{M}$ (bulk actions) and $P(x)\in \mathrm{Hom}(T^*_x\mathcal{B}_0, T^*_{u(x)}\mathcal{B})\simeq\mathbb{R}^3\otimes\hat{\mathbb{R}}^3$, $\mathcal{S}(x)\in\mathrm{Hom}(T^*_x\mathcal{B}_0, T^*_{\nu(x)}\mathcal{M})\simeq\mathbb{R}^3\otimes T^*_{\nu(x)}\mathcal{M}$ (contact interactions) are defined.

Observers are *representations of the geometrical environments necessary to describe the morphology of a body and its subsequent changes of morphology* (see [41] for a series of questions related with this definition).

Attention is focused here on semi-classical changes in observers, the ones leaving invariant $\mathcal{B}_0$ and changing isometrically both $\hat{\mathbb{R}}^3$ and $\mathcal{M}$. The attribute 'semi' refers to the circumstance that $\mathcal{M}$ is taken into account in addition to the ambient space. By considering the infinitesimal generators of the action of $\hat{\mathbb{R}}^3\ltimes SO(3)$ over $\hat{\mathbb{R}}^3$ and of the same copy of $SO(3)$ over $\mathcal{M}$, one defines $h^*:=h+c+q\times(u-u_0)$, with $c\in\hat{\mathbb{R}}^3$ and $q\times\in SO(3)$ u_0 an arbitrary point in space, and $v^*:=v+\mathcal{A}q$, where $\mathcal{A}(\nu)\in\mathrm{Hom}(\hat{\mathbb{R}}^3, T_\nu\mathcal{M})$ so that $\mathcal{A}^*(\nu)\in\mathrm{Hom}(T^*_\nu\mathcal{M},\hat{\mathbb{R}}^3)$. Here h and v play the role of virtual rates.

Axiom. *At equilibrium the power of external actions is invariant under semi-classical changes in observers, that is* $\mathcal{P}^{\text{ext}}_{\mathfrak{b}}(h,v)=\mathcal{P}^{\text{ext}}_{\mathfrak{b}}(h^*,v^*)$ *for any choice of* $\mathfrak{b}$, c *and* q.

The following theorem is immediate (see [38,40] for further remarks):

Theorem 5.2. *(i) If for any* $\mathfrak{b}$ *the vector fields* $x\mapsto Pn$ *and* $x\mapsto\mathcal{A}^*\mathcal{S}n$ *are defined over* $\partial\mathfrak{b}$ *and are integrable there, the integral balances of actions on* $\mathfrak{b}$ *hold:*

$$\int_{\mathfrak{b}} b\ \mathrm{d}x+\int_{\partial\mathfrak{b}} Pn\ \mathrm{d}\mathcal{H}^2=0,$$

$$\int_{\mathfrak{b}}((u-u_0)\times b+\mathcal{A}^*\beta)\ \mathrm{d}x+\int_{\partial\mathfrak{b}}((u-u_0)\times Pn+\mathcal{A}^*\mathcal{S}n)\ \mathrm{d}\mathcal{H}^2=0.$$

(ii) Moreover, if the tensor fields $x\mapsto P$ *and* $x\mapsto\mathcal{S}$ *are of class* $C^1(\mathcal{B}_0)\cap C^0(\bar{\mathcal{B}}_0)$ *then*

$$\mathrm{Div}P+b=0$$

and there exist a covector field $x\mapsto z\in T_{\nu(x)}\mathcal{M}$ *such that*

$$skw(PF^*)=\frac{1}{2}\mathsf{e}(\mathcal{A}^*z+(D\mathcal{A}^*)\mathcal{S})$$

and

$$\mathrm{Div}\mathcal{S}-z+\beta=0,$$

with $z=z_1+z_2$, $z_2\in Ker\mathcal{A}^*$.

Above e is Ricci's tensor.

The integral balances in the theorem above are associated with the Killing fields of the standard metric in the ambient space $\hat{\mathbb{R}}^3$. In general, a pure integral balance of substructural actions does not make sense because it would involve integrands taking values on $T^*\mathcal{M}$ which is not a linear space.

Substructural interactions appear in the integral balance of moments which is not standard. Their appearances do not imply that they are couples (specifically micro-couples) due to the presence of the operator $\mathcal{A}^*$. In fact, only the products $\mathcal{A}^*\beta$ and $\mathcal{A}^*\mathcal{S}n$ are properly couples while $\mathcal{S}$ and $\mathcal{S}n$ do not.

5.3. **Irregular minimizers: horizontal variations**

Consider local minimizers in $\mathcal{W}^d_{r,s}$ of $\mathcal{E}(u,\nu)$ (see Th. 2). For the sake of simplicity, the lower bound

$$Pe(x,u,\nu,M(F),N) \geq c_1\left(|M(F)|^r + \frac{|M(F)|^{\bar{r}}}{(\det F)^{\bar{r}-1}} + |N|^s\right)$$

for some $r,\bar{r},s>1$ and $c_1>0$, is assumed to be satisfied by the energy density. Consequently, the energy functional

$$\mathcal{E}(u,\nu) := \int_{\mathcal{B}_0} Pe(x,u,\nu,M(F),N)\ \mathrm{d}x,$$

is coercive over $\mathrm{dif}^{r,\bar{r}}(\mathcal{B}_0,\hat{\mathbb{R}}^3)\times W^{1,s}(\mathcal{B}_0,\mathcal{M})$, where

$$\mathrm{dif}^{r,\bar{r}}(\mathcal{B}_0,\hat{\mathbb{R}}^3) := \left\{u\in \mathrm{dif}^{r,1}(\mathcal{B}_0,\hat{\mathbb{R}}^3)\mid M(D\hat{u})\in L^{\bar{r}}(\tilde{u}(\mathcal{B}_0))\right\}.$$

Take note that $\frac{|M(F)|^{\bar{r}}}{(\det F)^{\bar{r}-1}}$ is equal to $|M(D\hat{u})|^r$ where $\hat{u}:=u^{-1}$ in the sense of Lusin representatives.

Basically, the lower bound above means that the energy of the complex body under examination is greater than the one of a fictious body in which self-actions are absent so that substructural actions are only of contact type (microstress).

Let $\phi\in C^1_0\left(\mathcal{B}_0,\mathbb{R}^3\right)$ and consider for ε sufficiently small, the diffeomorphism $\Phi_\varepsilon(x):=x+\varepsilon\phi(x)$ from $\mathcal{B}_0$ into itself, diffeomorphisms that leave unchanged $\partial\mathcal{B}_0$. Consequently, for $|\varepsilon|<\varepsilon_0$, with ε_0 fixed, one gets

$$u_\varepsilon(x) := u\left(\Phi^{-1}_\varepsilon(x)\right)\in \mathrm{dif}^{r,\bar{r}}(\mathcal{B}_0,\hat{\mathbb{R}}^3),$$

$$\nu_\varepsilon(x) := \nu\left(\Phi^{-1}_\varepsilon(x)\right)\in W^{1,s}(\mathcal{B}_0,\mathcal{M}).$$

The map Φ_ε implies also the transformations

$$F\to F_\varepsilon = F_\varepsilon(x) := FD\Phi^{-1}_\varepsilon \quad\text{and}\quad N\to N_\varepsilon = N_\varepsilon(x) := ND\Phi^{-1}_\varepsilon.$$

In this way, one constructs a map

$$\varepsilon\to\mathcal{E}(u_\varepsilon,\nu_\varepsilon) := \int_{\mathcal{B}_0} Pe(x,u_\varepsilon,\nu_\varepsilon,M(F_\varepsilon),N_\varepsilon)\ \mathrm{d}x. \tag{5.6}$$

For the sake of simplicity, assume that Pe is differentiable and

$$|Pe|,\quad |\partial_x Pe|\leq c\left(|M(F)|^r + \frac{|M(F)|^{\bar{r}}}{(\det F)^{\bar{r}-1}} + |N|^s\right), \tag{5.7}$$

$$\left|\partial_{M(F)}Pe\right| \leq c\left(|M(F)|^{r-1} + \frac{|M(F)|^{\bar{r}-1}}{(\det F)^{\bar{r}-1}} + |N|^{\left(1-\frac{1}{\bar{r}}\right)s}\right), \tag{5.8}$$

$$|\partial_N Pe| \leq c\left(|M(F)|^{\left(1-\frac{1}{s}\right)r} + \left(\frac{|M(F)|^{\bar{r}}}{(\det F)^{\bar{r}-1}}\right)^{\left(1-\frac{1}{s}\right)} + |N|^{s-1}\right). \tag{5.9}$$

Then, by Lebesgue's differentiation theorem, the map $\varepsilon\to\mathcal{E}(u_\varepsilon,\nu_\varepsilon)$ is differentiable at zero with derivatives bounded in L^1. As a consequence, the theorem below follows.

Theorem 5.3. *If* $Pe\left(x,u,\nu,M\left(F\right),N\right)$ *satisfies* (5.7)–(5.9) *above, for a local minimizer* (u,ν) *of* $\mathcal{E}\left(u,\nu\right)$ *in* $\mathcal{W}^{d}_{r,s}$ *one gets*

$$F^{*}\partial_{F}e\left(x,u,\nu,F,N\right)\in L^{1}\left(\mathcal{B}_{0}\right),$$

$$N^{*}\partial_{N}e\left(x,u,\nu,F,N\right)\in L^{1}\left(\mathcal{B}_{0}\right),$$

$$\int_{\mathcal{B}_{0}}\mathbb{P}\cdot D\phi\ \mathrm{d}x+\int_{\mathcal{B}_{0}}\partial_{x}e\cdot\phi\ \mathrm{d}x=0\quad\forall\phi\in C^{1}_{0}\left(\mathcal{B}_{0},\mathbb{R}^{3}\right),\tag{5.10}$$

where $\mathbb{P}\left(x\right)\in Aut\left(\mathbb{R}^{3}\right)$ *is the extended Hamilton-Eshelby tensor defined by*

$$\mathbb{P}:=eI-F^{*}P-N^{*}\mathcal{S},\tag{5.11}$$

that is

$$\mathrm{Div}\,\mathbb{P}-\partial_{x}e=0,$$

in distributional sense.

In fact, by using Binet formula and Young inequality (namely $ab\leq\frac{a^{r}}{r}+\frac{b^{\bar{r}}}{\bar{r}}$, $\frac{1}{r}+\frac{1}{\bar{r}}=1$), it is easy to prove that

$$\sup_{|\varepsilon|<\varepsilon_{0}}\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left(Pe\left(\phi\left(x\right),u_{\varepsilon},\nu_{\varepsilon},M\left(F_{\varepsilon}\right),N_{\varepsilon}\right)\det D\Phi_{\varepsilon}\right)\in L^{1}\left(\mathcal{B}_{0}\right).$$

Precisely, Binet formula

$$M^{\beta}_{\alpha}\left(F_{\varepsilon}\right)=\sum_{|\gamma|=|\beta|}M^{\beta}_{\gamma}\left(F_{\varepsilon}\right)M^{\gamma}_{\alpha}\left(D\Phi^{-1}_{\varepsilon}\right)$$

yields

$$\left|M\left(F_{\varepsilon}\right)\right|,\ \left|\frac{\mathrm{d}}{\mathrm{d}\varepsilon}M\left(F_{\varepsilon}\right)\right|\leq c\left|M\left(F\right)\right|.$$

Moreover, one has

$$\left|N_{\varepsilon}\right|,\ \left|\frac{\mathrm{d}}{\mathrm{d}\varepsilon}N_{\varepsilon}\right|\leq c\left|N\right|,$$

so that

$$\left|\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left(Pe\left(\phi\left(x\right),u_{\varepsilon},\nu_{\varepsilon},M\left(F_{\varepsilon}\right),N_{\varepsilon}\right)\det D\Phi_{\varepsilon}\right)\right|\leq$$

$$c\left\{\left|\partial_{x}Pe\right|+\left|\partial_{M(F)}Pe\cdot\frac{\mathrm{d}}{\mathrm{d}\varepsilon}M\left(F_{\varepsilon}\right)\right|+\left|\partial_{N}Pe\cdot\frac{\mathrm{d}}{\mathrm{d}\varepsilon}N_{\varepsilon}\right|\right\}$$

$$\leq c(\left|M\left(F\right)\right|^{r}+\frac{\left|M\left(F\right)\right|^{\bar{r}}}{\left(\det F\right)^{\bar{r}-1}}+\left|N\right|^{s})$$

$$+c(\left|M\left(F\right)\right|^{r-1}+\frac{\left|M\left(F\right)\right|^{\bar{r}-1}}{\left(\det F\right)^{\bar{r}-1}}+\left|N\right|^{\left(1-\frac{1}{\bar{r}}\right)s})\left|M\left(F\right)\right|$$

$$+c(\left|M\left(F\right)\right|^{\left(1-\frac{1}{s}\right)r}+\left(\frac{\left|M\left(F\right)\right|^{\bar{r}}}{\left(\det F\right)^{\bar{r}-1}}\right)^{\left(1-\frac{1}{s}\right)}+\left|N\right|^{s-1})\left|N\right|$$

$$\leq c\left(\left|M\left(F\right)\right|^{r}+\frac{\left|M\left(F\right)\right|^{\bar{r}}}{\left(\det F\right)^{\bar{r}-1}}+\left|N\right|^{s}\right)$$

for all ε, $|\varepsilon|\leq\varepsilon_{0}$.

Then, it follows that

$$\begin{aligned} 0 &= \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\mathcal{E}\left(u_\varepsilon,\nu_\varepsilon\right)=\int_{\mathcal{B}_0}\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left(Pe\left(\phi\left(x\right),u_\varepsilon,\nu_\varepsilon,M\left(F_\varepsilon\right),N_\varepsilon\right)\det D\Phi_\varepsilon\right)|_{\varepsilon=0}\ \mathrm{d}x \\ &= \int_{\mathcal{B}_0}\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left(e\left(\phi\left(x\right),u_\varepsilon,\nu_\varepsilon,F_\varepsilon,N_\varepsilon\right)\det D\Phi_\varepsilon\right)|_{\varepsilon=0}\ \mathrm{d}x. \end{aligned} \tag{5.12}$$

The derivative at $\varepsilon=0$ under the integral sign remains to be computed. Since

$$\Phi_\varepsilon\left(x\right)=x+\varepsilon\phi\left(x\right),$$

$$D\Phi_\varepsilon^{-1}\left(\Phi_\varepsilon\left(x\right)\right)=I-\varepsilon D\phi\left(x\right)+o\left(\varepsilon^2\right)\quad\text{as }\varepsilon\to 0,$$

$$\det D\Phi_\varepsilon\left(x\right)=1+\varepsilon\mathrm{Div}\Phi_\varepsilon\left(x\right)+o\left(\varepsilon^2\right)\quad\text{as }\varepsilon\to 0,$$

uniformly with respect to x (I indicates the unit second rank tensor), the derivative in (5.12) implies (5.10).

Theorem 7 extends to complex bodies a companion result for simple elastic bodies in [31]. The extended Hamilton-Eshelby tensor $\mathbb{P}$ has been introduced in [38] (see also [12]) with reference to smooth minimizers. Here the configurational balance involving $\mathbb{P}$ is extended to irregular minimizers.

Actually, as pointed out by [2] for non-linear elasticity of simple bodies, the differentiability of the map $\varepsilon\longmapsto\mathcal{E}\left(u_\varepsilon,\nu_\varepsilon\right)$ in (5.6) holds actually under the weaker energetic estimate

$$|\partial_x e|+|F^*\partial_F e|+|N^*\partial_N e|\leq c_1 e+c_2,$$

where e and its derivatives are calculated in (x,u,ν,F). Such an estimate has been used in [21] for a delicate analysis of evolution problems in rate-independent models of non-conservative processes in classes of bodies.

In the case of bodies with spin structure described by $\nu:\mathcal{B}_0\to S^2$ and admitting a partially decomposed energy with concentration on a line, precisely an energy of the form

$$\mathcal{E}\left(u,\nu_T\right)=\int_{\mathcal{B}_0}e_E\left(x,u,\nu_T,F\right)\ \mathrm{d}x+\frac{1}{2}\int_{\mathcal{B}_0}\left|D\nu_T\right|^2\ \mathrm{d}x+4\pi\mathbf{M}\left(L_T\right),$$

with L_T a one-dimensional integer rectifiable current on $\mathcal{D}^1\left(\mathcal{B}_0\right)$, by using the technique adopted in the proof of the theorem above, a special version of (5.10) follows. It accounts for the contribution of the concentration of energy on the line $L_T=\overrightarrow{T}\wedge\|L_T\|$, namely

$$\int_{\mathcal{B}_0}\mathbb{P}\cdot D\phi\ \mathrm{d}x+\int_{\mathcal{B}_0}\partial_x e\cdot\phi\ \mathrm{d}x=4\pi\int\overrightarrow{T}\otimes\overrightarrow{T}\cdot D\phi\ \mathrm{d}\left\|L_T\right\| \tag{5.13}$$

for any $\phi\in C_0^1\left(\mathcal{B}_0,\mathbb{R}^3\right)$. The integral balance (5.13) is unusual. In the case of homogeneous bodies, (5.13) implies the the internal 'power' of the extended Hamilton-Eshelby stress is determined only by the interactions along the line of concentration of energy. Equation (5.13) extends also a theorem in [26] to the case in which macroscopic deformations occur.

Consider maps $\bar{\phi}\in C_c^1(\hat{\mathbb{R}}^3,\hat{\mathbb{R}}^3)$ with $\bar{\phi}=0$ in a neighborhood of $u\left(\partial\mathcal{B}_0\right)$. For $|\varepsilon|<\varepsilon_0$, with ε_0 fixed, the map $\Phi_\varepsilon\left(y\right)=y+\varepsilon\bar{\phi}\left(y\right)$ is then a diffeomorphism from $\hat{\mathbb{R}}^3$ into $\hat{\mathbb{R}}^3$, so the map $u_\varepsilon\left(x\right):=u\left(x\right)+\varepsilon\bar{\phi}\left(u\left(x\right)\right)$ is a weak diffeomorphism in $\mathrm{dif}^{r,\bar{r}}(\mathcal{B}_0,\hat{\mathbb{R}}^3)$. Since $\bar{\phi}=0$ in a neighborhood of $\tilde{u}\left(\partial\mathcal{B}_0\right)$, all the u_ε agree on $\partial\mathcal{B}_0$; moreover by chain rule it follows that $F_\varepsilon=F_\varepsilon\left(x\right)=F\left(x\right)+\varepsilon D_{u(x)}\bar{\phi}\left(u\left(x\right)\right)F\left(x\right)$.

Define the Cauchy stress tensor as usual by

$$\sigma\left(y\right):=\left(\left(\det F\right)^{-1}\partial_F e\left(x,u,\nu,F,N\right)F^*\right)\left(y\right)\in\mathrm{Hom}(T_y^*\mathcal{B},\hat{\mathbb{R}}^{3*})\simeq\hat{\mathbb{R}}^3\otimes\hat{\mathbb{R}}^3.$$

Assume also that the energy density satisfies the inequality

$$|\partial_u Pe| \leq c(|M(F)|^r + \frac{|M(F)|^{\bar{r}}}{(\det F)^{\bar{r}-1}} + |N|^s). \tag{5.14}$$

Under this additional assumption and (5.7), (5.8), the map

$$\varepsilon \to \mathcal{E}(u_\varepsilon, \nu) := \int_{\mathcal{B}_0} Pe(x, u_\varepsilon, \nu, M(F_\varepsilon), N)\ \mathrm{d}x$$

is differentiable at $\varepsilon = 0$.

Theorem 5.4. *Under conditions* (5.7), (5.8) *and* (5.14) *above, for* (u, ν) *a minimizer in* $W^d_{r,s}$ *of* $\mathcal{E}(u, \nu)$,

$$\sigma \in L^1_{loc}(\tilde{u}(\mathcal{B}_0), \hat{\mathbb{R}}^3 \otimes \hat{\mathbb{R}}^3)$$

and

$$\int_{\tilde{u}(\mathcal{B}_0)} \sigma(y) \cdot D\bar{\phi}(y)\ \mathrm{d}y + \int_{\tilde{u}(\mathcal{B}_0)} b(y) \cdot \bar{\phi}(y)\ \mathrm{d}y = 0,$$

for every $\bar{\phi} \in C^1_0(\hat{\mathbb{R}}^3, \hat{\mathbb{R}}^3)$ *with* $\bar{\phi} = 0$ *in a neighborhood of* $\tilde{u}(\partial\mathcal{B}_0)$, *with* $\tilde{u}$ *the Lusin representative of* u.

The proof follows by direct calculation.

Finally, consider smooth curves $\varepsilon \to \bar{\varphi}_\varepsilon \in Aut(\mathcal{M})$, $\bar{\varphi} \in C^1(\mathcal{M})$, and define

$$\nu_\varepsilon := \bar{\varphi}_\varepsilon(\nu), \quad \nu \in \mathcal{M}.$$

Call also ξ the derivative

$$\xi := \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\nu_\varepsilon\,|_{\varepsilon=0}\,.$$

Assume that the energy density satisfies the inequality

$$|\partial_\nu Pe| \leq c\left(|M(F)|^r + \frac{|M(F)|^{\bar{r}}}{(\det F)^{\bar{r}-1}} + |N|^s\right). \tag{5.15}$$

Under the assumptions (5.7), (5.9) and (5.15) the map

$$\varepsilon \to \mathcal{E}(u, \nu_\varepsilon) := \int_{\mathcal{B}_0} Pe(x, u, \nu_\varepsilon, M(F), N_\varepsilon)\ \mathrm{d}x$$

is differentiable at $\varepsilon = 0$.

Theorem 5.5. *Under conditions* (5.7), (5.9) *and* (5.15) *above, for* u *and* ν *minimizers in* $W^d_{r,s}$ *of* $\mathcal{E}(u, \nu)$,

$$\mathcal{S} \in L^1\left(\mathcal{B}_0, \mathbb{R}^{3*} \otimes T^*\mathcal{M}\right)$$

and

$$\int_{\mathcal{B}_0} \mathcal{S}(x) \cdot D\xi(x)\ \mathrm{d}x + \int_{\mathcal{B}_0} (\beta - z)(x) \cdot \xi(x)\ \mathrm{d}x = 0,$$

for every $\xi \in C^0(T\mathcal{M})$, *with* $(\beta - z)(x) \in T^*_{\nu(x)}\mathcal{M}$.

6. Taxonomy of special cases

Without having the presumption to be a theory of everything, the framework discussed above unifies, in fact, a very large class of models of condensed matter physics. A list of special examples is presented below. It is not exhaustive, of course, but an idea of the potentialities of thinking of complex bodies in terms of maps between manifolds is given.

- **Liquid crystals in nematic phase:** In liquid crystals stick molecules are dispersed in a ground fluid. They may arrange themselves in various manners that characterize different phases. In nematic phase, the stick molecules are ordered along prevailing directions but they do not have distinct head and tail so that $\mathcal{M}$ is identified with the unit sphere in $\mathbb{R}^3$, with the projective plane P^2. The generic material element can be interpreted here as a patch of matter including a family of stick molecules. The morphological descriptor ν is then an indicator of the 'prevailing' direction of the molecules. This point of view has been introduced in [16,17] (see also [13,36]). Oseen-Frank potential, recalled above, is the energy appropriate when one forgets the gross motion. A second-rank tensor $\zeta\left(n\otimes n-\frac{1}{3}I\right)$, with $n\in S^2$, and $\zeta\in\left[-\frac{1}{2},1\right]$, can be also used to account for details of the distribution of the stick molecules. The scalar ζ indicates the *degree of orientation* (as defined in [18]). In this case, then, $\mathcal{M}=S^2\times\left[-\frac{1}{2},1\right]$. Optical biaxiality can emerge so that the symmetry of the molecules becomes that of a rectangular box and two other scalar morphological descriptors are necessary: the *degree of prolation* and the *degree of triaxiality* (see [9]). Alternatively, one may select $\mathcal{M}$ coincident with the quotient between the special unitary group $SU(2)$ and the group of quaternions.
- **Liquid crystals in smectic phase:** In the smectic-A phase a layered structure appears and the stick molecules tend to be aligned orthogonally to the layer interface unless tilt occurs. Natural ingredients for describing the smectic-A phase are the unit vector n representing at each point the local orientational order and a scalar function ℓ parameterizing the layers through its level sets. When tilt is absent and single layers are compressible but at the gross scale there is incompressibility, the energy density can be written as
$$e\left(\ell,\operatorname{grad}\ell\right)=\frac{1}{2}k_1\left(|\operatorname{grad}\ell|-1\right)^2+\frac{1}{2}k_2\left(\operatorname{div}n\right)^2,$$
with k_1 and k_2 material constants. The operators grad and div imply derivatives with respect to u. The term $\left(|\operatorname{grad}\ell|-1\right)^2$ accounts for the compression of layers while $\left(\operatorname{div}n\right)^2$ describes the nematic phase and is the first addendum of (three constant) Frank's potential (see [8]).
- **Liquid crystals in cholesteric phase:** In cholesteric phase, liquid crystals loose in a sense reflection symmetry (the one under the action of $O(3)\setminus SO(3)$) and maintain $SO(3)$-symmetry. An appropriate form of the energy density can be found in [18].
- **Cosserat materials:** In the Cosserat's scheme each material element is considered as a (small) *rigid body* which can rotate independently of the neighboring fellows. The manifold of substructural shapes can be then identified with the unit sphere S^2 or the special orthogonal group $SO(3)$. Local contact couples exchanged between adjacent parts of the body are power conjugated with local rotations and are described by a couple stress tensor. The scheme of Cosserat materials is a special case of multifield theories often used for direct models of structural elements like beams, plates or shells [19] or for composites reinforced with diffused small rigid fibers.
- **Superfluid liquid helium:** The analysis of ground states of ^{3}He falls within the setting discussed above. The energy density is of Ginzburg-Landau type. For ^{3}He in the dipole locked phase, $\mathcal{M}$ coincides simply with $SO(3)$ (thus with S^2) and Cosserat's scheme applies.
- **Ferroelectrics:** To describe the local polarization of crystalline cells in ferroelectrics, a vector is commonly selected within a ball B_p in $\mathbb{R}^3$, the radius of which is the maximum polarization available in the material [50]. In presence of an external electric field acting over the body, the relevant polarization energy has to be added to a Ginzburg-Landau-type decomposed energy density for matter fields.
- **Bodies with polymeric chains:** Various types of materials are made of polymeric linear chains scattered in a melt (see, *e.g.*, [37]). A simple natural descriptor of each single chain is an end-to-end

stretchable vector $\mathbf{r}$. To preserve a natural symmetry under the transformation $\mathbf{r} \to -\mathbf{r}$, the dyad $\mathbf{r} \otimes \mathbf{r}$ is used as morphological descriptor. Then, the manifold of substructural shapes $\mathcal{M}$ coincides with the (linear) space of symmetric tensors with positive determinant $\mathrm{Sym}^+\left(\mathbb{R}^3, \mathbb{R}^3\right)$. In this sense the representation falls within the class of affine bodies mentioned below. The energy may be selected in various manners; in particular, if the linear chains are 'dilute', the energy does not depend on $D\nu$ while, when their are 'dense' up to interacting through van der Walls forces and/or entanglements, the dependence on $D\nu$ appears.

- **Polyelectrolyte polymers and polymer stars:** Polyelectrolyte polymers are characterized by the possible polarization of chains. In this case, by adopting the notation above, the manifold of substructural shapes can be selected as $\mathcal{M} = \mathrm{Sym}^+\left(\mathbb{R}^3, \mathbb{R}^3\right) \times B_p$. Moreover the chains may link with each other up to form a star. In this case we may imagine to have $\mathcal{M} = \mathrm{Sym}^+\left(\mathbb{R}^3, \mathbb{R}^3\right) \times B_{p_m} \times (0, c)$, with $c > 0$. Numbers in $(0, c)$ describe the *radius of gyration* of the star.
- **Bodies with affine structure:** In the special case in which the manifold of substructural shape coincides with the linear space of second-rank tensors, the substructure is called affine [44,53]. The scheme is suitable to cover various cases such as the one of bodies with dense polymeric linear chains discussed above or fullerene-reinforced composites. A basic interest to mention this special model is that when there is an internal constraint of the type $\nu = f(F)$, so that the substructure becomes *latent* in the sense of Capriz [6]. In this case the energy density reduces to the one of a second-grade Cauchy body, namely $e = e(x, F, \nabla F)$.
- **Porous and multi-phase bodies:** When pores are finely scattered throughout a body, we may imagine that the generic material element is a patch of matter with spherical voids and we can select the morphological descriptor as a scalar indicating the *void volume fraction*. In this case $\mathcal{M}$ reduces to the interval of the real axis $[0, 1]$ (see [46]). The scheme of porous materials is useful when multiple phases (for example m phases) coexist within a body and phase transitions occur [22]. The description can be refined to account for deeper details in the rearrangement of phases. The combined use of scalar and second-order tensor valued morphological descriptor fields allows one to account for the re-orientation of martensitic variants, as proposed in [3].
- **Quasi-periodic alloys:** Quasi-periodic atomic arrangements exist in nature and characterize some specific classes of metallic alloys. For example, in the prominent case of quasicrystals, the formation and annihilation of atomic rearrangements is necessary to assure quasi-periodicity, so that internal degrees of freedom appear within the crystalline cells and describe the local atomic rearrangements (a process called *phason activity*). In all cases, the appropriate morphological descriptor of the degrees of freedom inside 'atomic cells' is a vector so that $\mathcal{M}$ coincides with $\mathbb{R}^3$ (see [34,40]).

7. Ground states of thermodynamically stable quasicrystals

A special class of quasi-periodic alloys is the one of quasicrystals in which atomic clusters display symmetries incompatible with periodic tilings in space, symmetries such as the icosahedral one in three-dimensions and the pentagonal one in the plane (see, *e.g.*, [34]). Atomic rearrangements assure quasiperiodicity in space by creating and annihilating (randomly) the so-called worms, that are clusters of atoms with symmetry different from the prevailing one. The local degrees of freedom associated with these atomic changes are described by a vector $\nu \in \mathbb{R}^3$ in the three-dimensional case. ν belongs to $\mathbb{R}^3$ for two-dimensional quasicrystals. Experiments show that the elastic energy of quasicrystals does not depend on ν while it depends only on its spatial gradient N besides the gradient of macroscopic deformation. Moreover, quasicrystals are characterized by a self-action of dissipative nature, that is by dissipation inside each material element, a dissipation strictly associated with substructural events (see [40]). Although this type of tendence to material metastability, it has been shown experimentally that quasicrystals may admit in some cases ground states (see [54] and references therein). Moreover, the occurrence of ground states have been also analyzed in the generic material element by looking directly to the lattice behavior (see [15,43]). Additionally, it has been shown also that frustration between neighboring ground states may occur in special conditions [14].

Here, the framework presented above is applied to analyze the existence of ground states in quasicrystalline bodies from a macroscopic point of view. The energy to be accounted for is then

$$\int_{\mathcal{B}_0} e\left(Du, D\nu\right)\ \mathrm{d}x$$

and one tries to find minimizers for it in some functional space. The appropriate constitutive choice of the functional environment seem to be the space

$$\mathcal{W}_{r,2} := \left\{(u,\nu)\,|u \in \mathrm{dif}^{r,1}(\mathcal{B}_0, \hat{\mathbb{R}}^3),\ \nu \in W^{1,2}\left(\mathcal{B}_0, \mathbb{R}^3\right)\right\}.$$

In this case the growth condition for the energy becomes

$$e\left(F,N\right) \geq C_1\left(\left|M\left(F\right)\right|^r + \left|N\right|^2\right) + \vartheta\left(\det F\right).$$

It means that the energy grows faster than the one of an ideal quasicrystal behaving isotropically and having an unlocked phase. Precisely, one says that the atomic rearrangements occurring in quasicrystals are in a unlocked phase when the energy has a quadratic dependence on N. Such a phase is the only one existing in two-dimensional setting (see [35]) so that the growth condition above has physical meaning in one, two and three-dimensional ambient space.

As a consequence, once $e\left(F,N\right)$ is substituted by its polyconvex extension, existence of minimizers in $\mathcal{W}_{r,2}$ follows as a consequence of Theorem 2.

Analogous analyses can be developed for other prominent cases of complex bodies.

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