Idealized skins constituted by finitely may material particles

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Introduction

In this article we present a link between the description of an idealized skin as a continuum on one hand and as a collection of finitely many interacting material particles on the other. In doing so, we restrict us, for simplicity, to the following set up: We take into account the quality of the medium in as far only, as it characterizes the internal force density responding an infinitesimal distortion. This is to say, we classify the medium by the virtual work only (cf.[He],[E,S]). (It is not hard to overcome this restriction).

Let P be a given finite collection of points and $j_P : P \rightarrow \mathbb{R}^n$ be an injective map. $j(P)$ visualizes the configuration of material points in $\mathbb{R}^n$. On the other hand let M with $\partial M = \emptyset$ be a given connected, smooth, compact manifold, the idealized skin, and $j : M \rightarrow \mathbb{R}^n$ be a smooth embedding. $j(M)$ visualizes the continuum in $\mathbb{R}^n$. We thus call j_P and j configurations of the discrete medium respectively of the continuum. The following observation provides the geometric grounds of the link mentioned above : Let $P \subset M$ and j_0 be a fixed configuration. To O_P, a small open collection of configurations of the discrete medium, there is a collection O of configurations of the continuum which constitutes of a collection of slices each diffeomorphic to O_P. The slicing is such that the tangent space $\mathcal{F}^\infty(M, \mathbb{R}^n)$ at each $j \in O$ is generated (independently of j) by a collection of eigenvectors in $C^\infty(M, \mathbb{R}^n)$ of $\Delta(j_0)$, where $\Delta(j_0)$ is the Laplacian of the pullback metric $m(j_0)$ determined by the fixed configuration j_0 ($\mathbb{R}^n$ is equipped with a fixed scalar product). The restriction map r_∞ from $\mathcal{F}^\infty(M, \mathbb{R}^n)$ to the collection $\mathcal{F}(P, \mathbb{R}^n)$ of all $\mathbb{R}^n$-valued maps of P is an isomorphism and determines a natural projection, called r_∞, too, from each slice to O_P. Here is the physical ground of the mentioned link: Any virtual work A_P on O_P , a one-form, is pulled back to each slice $W(j)$, passing through $j \in O$, say. The pull back $r^*_\infty A_P$ characterizes the the discrete medium on the continuum.
The slicing of O together with the pullback mechanism provides the above mentioned link between the two types of descriptions. The chosen slicing is based on the observation that the (smooth) internal force density $\hat{\Phi}(j)$ associated with a virtual work $A(j)$ of the continuum is of the form $\hat{\Phi}(j) = \Delta(j_0)\hat{\mathcal{H}}(j)$ for some $\hat{\mathcal{H}}(j) \in C^\infty(M, \mathbb{R}^n)$, at any configuration $j \in O$.

The natural L_2-structure on $\mathcal{F}(P, \mathbb{R}^n)$ and the one on $\mathcal{F}^\infty(M, \mathbb{R}^n)$ determined by $m(j_0)$ are related in a simple fashion. We use this relation to relate a Hodge-type of splitting of A_P on O_P with the slice wise formed analogon of its pullback $A := r^*_\infty A_P$ on O. The exact parts represent the differentials of the free energies $\bar{F}_P$ on O_P respectively $\bar{F}$ on O which are slice wise related by $\bar{F} = \bar{F}_P \circ r_\infty$.

The notion of free energy is associated with a particular observable derived from a chosen density of $\bar{F}_P$. We study various aspects of A_P, A, $\bar{F}_P$ and $\bar{F}$ together with their interplay. In particular we illustrate these notions in case of the nearest neighbour interaction (n.n.i.) scheme. Finally we introduce, preliminarily, the notion of a well fitting configuration j_0 expressing that $j_0(M)$ fits $j^0_P(P)$ well, here $j_0|P = j^0_P$. We work with $\mathbb{R}^n$ and a manifold M of this generality to make dimensional factors apparent. The formalism can easily be extended to the appropriate Sobolev spaces.
Finally let us point out that the concepts introduced can be generalized to fit into the theories presented by the professors Elzanowski, Epstein and de Leon.

A The general description of deformable media

We base our description of continua on the notion of the force and traction densities caused by a smooth infinitesimal distortion of a material body.

A1 Configuration space

Let M be a smooth, compact, connected and oriented manifold possibly with boundary of $dim\ M \geq 2$, embedable in $\mathbb{R}^n$. A configuration j is a smooth embedding of M into $\mathbb{R}^n$. The collection $E(M,\mathbb{R}^n)$ of all configurations is a Fréchet manifold if endowed with the C^∞-topology (cf. [Bi,Fi,Sn], [Hi], [Bi,Fi,1], [Fr,Kr]). The collection $C^\infty(M,\mathbb{R}^n)$ of all smooth $\mathbb{R}^n$-valued maps of M (a Fréchet space under the C^∞-topology) contains $E(M,\mathbb{R}^n)$ as an open set, is hence the tangent space at each embedding. An infinitesimal distortion is, therefore, a function in $C^\infty(M,\mathbb{R}^n)$.

A2 The virtual work, deformable media and skins

Let $O \subset E(M,\mathbb{R}^n)$ be an open set. By the virtual work A, we mean a special sort (cf. (A2.2) below) of a smooth one-form

$$A : O \times C^\infty(M,\mathbb{R}^n) \longrightarrow \mathbb{R}$$

admitting a force density Φ and a traction density φ (cf. [M,H]) yielding the representation

$$A(j)(h) = \int_M < \Phi(j), h > \mu(j) + \int_{\partial M} < \varphi(j), h|_{\partial M} > \mu_{\partial M}(j) \qquad \text{(A2.1)}$$

for all $h \in C^\infty(M,\mathbb{R}^n)$. Here both $\Phi(j)$ and $\varphi(j)$ are smooth $\mathbb{R}^n$-valued maps of M and ∂M, respectively, depending smoothly on $j \in O$. The integrands are given by $< \Phi(j)(q), h(q) >$ and $< \varphi(j)(q), h(q) >$ for all $q \in M$ and $q \in \partial M$, respectively. $<,>$ is a fixed scalar product on $\mathbb{R}^n$ for which the natural basis is orthonormal (for simplicity). $\mu(j)$ and $\mu_{\partial M}(j)$ on M and ∂M respectively, are the volume forms of the pull back $m(j)$ of $<,>$ by j. We require from A to satisfy

$$\int_M \Phi(j)\mu(j) + \int_{\partial M} \varphi(j)\mu(j) = 0 \qquad \forall j \in O. \qquad \text{(A2.2)}$$

Thus there is a smooth map $\mathcal{H} : O \longrightarrow C^\infty(M,\mathbb{R}^n)$ obeying

$$\Delta(j)\mathcal{H}(j) = \Phi(j) \qquad \text{and} \qquad d\mathcal{H}(j)(\mathcal{N}_{\partial M}) = \varphi(j) \qquad \forall j \in O. \qquad \text{(A2.3)}$$

Here $\Delta(j)$ is the Laplacian of $m(j)$ (cf. [Ma]), and $\mathcal{N}_{\partial M}$ is the positive oriented unit normal of ∂M in M. Clearly $\mathcal{H}(j)$ is determined up to a constant only, for all $j \in O$. Hence (A2.1) turns into

$$A(j)(h) = \int_M < \Delta(j)\mathcal{H}(j), h > \mu(j) + \int_{\partial M} < d\mathcal{H}(\mathcal{N}_{\partial M}), h > \mu_{\partial M}(j). \qquad \text{(A2.4)}$$

Specifying the virtual work via $\Phi(j)$ and $\varphi(j)$ for any $j \in O$ is thus equivalent to specify $\mathcal{H} : O \longrightarrow C^\infty(M,\mathbb{R}^n)$. In these notes we characterize the deformable medium only in as far as Φ and φ are determined (a rather simplified point of view, in deed). Consequently we specify here the deformable medium by the map $\mathcal{H}$, which hence is called a constitutive map (cf. [Bi1] to [Bi6] and [Bi,Fi2]).

If a medium would be specified by a first Piola-Kirchhoff stress tensor (cf. [M,H],[L,L])

$$\alpha : TM \longrightarrow \mathbb{R}^n$$

then $\mathcal{H}$ is given by the Neumann boundary problem

$$\Delta(j)\mathcal{H}(j) = div_j\alpha \qquad \text{and} \qquad \alpha(\mathcal{N}_{\partial M}) = d\mathcal{H}(j)(\mathcal{N}_{\partial M}) \tag{A2.5}$$

where div_j is the divergence operator determined by the Riemannian metric $m(j)$. Hence

$$\alpha = d\mathcal{H}(j) + \gamma(j) \qquad \forall j \in O \tag{A2.6}$$

where $\gamma(j) : TM \longrightarrow \mathbb{R}^n$ is a smooth one-form depending smoothly on $j \in O$, regardless as to whether α depends on j or not (cf. [Bi1,2,3]). Thus $\gamma(j)$ encodes qualities of the material which neither influence the internal force density $div_j\alpha$ nor the traction density $\alpha(\mathcal{N}_{\partial M})$. Finally let us remark that (A2.3) does not imply, in general, that A has to be exact on O, as we will see by an example in section D2.
An idealized skin is meant to be a manifold M as in A1 with $\partial M = \emptyset$. On a skin (A2.4) hence reduces to

$$A(j)(h) = \int_M < \Phi(j), h > \mu(j) = \int_M < \Delta(j)\mathcal{H}(j), h > \mu(j) \tag{A2.7}$$

for all $j \in O$ and any $h \in C^\infty(M, \mathbb{R}^n)$. Clearly

$$A(j)(h) = \int_M d\mathcal{H}(j) \bullet dh \; \mu(j) \tag{A2.8}$$

where the right hand side is the Dirichlet integral (cf. [Bi2],[Bi,Fi2]). For a later purpose, we will rewrite (A2.7) with respect to a fixed configuration $j_0 \in O$ by solving

$$det\ f(j) \cdot \Delta(j)\mathcal{H}(j) = \Delta(j_0)\hat{\mathcal{H}}(j)$$

for $\hat{\mathcal{H}}$ with $\hat{\mathcal{H}}(j_0) = 0$. Here f is a smooth strong bundle endomorphisms of TM given by

$$< djv, djw >= m(j)(v, w) = m(j_0)(f^2(j)(q)v, w) \tag{A2.9}$$

for all $v, w \in T_qM$ and all $q \in M$. We thus have for all $j \in O$ and any $h \in C^\infty(M, \mathbb{R}^n)$ the equation

$$A(j)(h) = \int_M < \Delta(j_0)\hat{\mathcal{H}}(j), h > \mu(j_0). \tag{A2.10}$$

By using [A] and [W] these notions can be extended to the scenario presented by the Professors Elzanowski, Epstein and de Leon.

A3 Structural capillarity

Let $\mathcal{A} : O \subset E(M, \mathbb{R}^n) \longrightarrow \mathbb{R}$ be the area functional of a skin given by

$$\mathcal{A}(j) = \int_M \mu(j) \qquad \forall j \in O. \tag{A3.1}$$

A particular sort of virtual work A, the virtual work caused by distorting the area, is

$$A(j)(h) := a(j) \cdot \mathbb{D}\mathcal{A}(j)(h) \qquad \forall j \in O \quad \text{and} \quad \forall h \in C^\infty(M, \mathbb{R}^n). \tag{A3.2}$$

Here $a : O \longrightarrow I\!R$ is a smooth map, called the structural capillarity (cf. [Bi3]); $I\!D$ denotes the Fréchet derivative on O (cf. [Bi,Sn,Fi]). It is not hard to see, that any $\mathcal{H} : O \longrightarrow C^\infty(M, I\!R^n)$ splits into

$$\mathcal{H}(j) = a(j) \cdot j + \mathcal{H}_1(j) \qquad \forall j \in O \tag{A3.3}$$

for some map a, where $\mathcal{H}_1(j)$ is not sensitive to area deformation (cf. [Bi2] to [Bi3]); i.e $\Delta(j)j$ is $\boldsymbol{L}_2$-orthogonal to $\mathcal{H}_1(j)$ for all $j \in O$. Let us point out that $\Delta(j)j$ is the mean curvature tensor (cf. [L,M],[Bi3]).

B General description of discrete media

In this section we are given a finite set P of points, thought of as material points. We characterize the discrete medium via internal forces. The analogy to the previous section is apparent in the case of nearest neighbour interaction (n.n.i.).

B1 Configuration space, discrete media

The discrete configuration space is $E(P, I\!R^n)$, the collection of all injective maps from P to $I\!R^n$. Again we restrict us to some open set $O_P \subset E(P, I\!R^n)$. Clearly O_P is open in the finite dimensional space $\mathcal{F}(P, I\!R^n)$ of all maps from P to $I\!R^n$.

An internal force $\Phi_P(j_P)$ at a configuration $j_P \in O_P$, resisting distortions in $\mathcal{F}(P, I\!R^n)$, is supposed to be a smooth map $\Phi_P : O_P \longrightarrow \mathcal{F}(P, I\!R^n)$ satisfying

$$\sum_{q \in P} \Phi_P(j_P) = 0 \qquad \forall j_P \in O_P, \tag{B1.1}$$

the analogon of (A2.2). The virtual work A_P at j_P caused by any distortion $h_P \in \mathcal{F}(P, I\!R^n)$ is given by

$$A_P(j_P)(h_P) = \sum_{q \in M} < \Phi_P(j_P)(q), h_P(q) > .$$

An equilibrium configuration $j_P^0 \in O_P$ has to satisfy $\Phi_P(j_P^0) = 0$.

B2 Nearest neighbour interaction (n.n.i.)

We think of P as the collection of all null-simplices of a finite, one-dimensional and oriented simplicial complex $\boldsymbol{L}$. The collection of all one-simplices is denoted by $\boldsymbol{L}_1$. Two particles at q and q_1, say, interact, iff they bound the same one-simplex $\sigma \in \boldsymbol{L}_1$. Any $q_i \in P$ interacting with q is called a nearest neighbour (n.n.) of q. By $k(q)$ we mean the total number of n.n. of any $q \in P$.
On the linear spaces $\mathcal{F}(P, I\!R^n)$ and $\mathcal{F}^1(\boldsymbol{L}, I\!R^n)$ of all zero and one-cochains of $\boldsymbol{L}$ there are the natural scalar products $\mathcal{G}_P$ and $\mathcal{G}_{\boldsymbol{L}_1}$ given respectively by

$$\mathcal{G}_P(h_P, k_P) = \sum_{q \in P} < h_P(q), k_P(q) > \qquad \forall h_P, k_P \in \mathcal{F}(P, I\!R^n) \tag{B2.1}$$

and

$$\mathcal{G}_{\boldsymbol{L}_1}(c_1, c_2) = \sum_{\sigma \in \boldsymbol{L}_1} < c_1(\sigma), c_2(\sigma) > \qquad \forall c_1, c_2 \in \mathcal{F}^1(\boldsymbol{L}, I\!R^n). \tag{B2.2}$$

The coboundary operator $\partial^1 : \mathcal{F}(P, I\!R^n) \longrightarrow \mathcal{F}^1(\boldsymbol{L}, I\!R^n)$ has an adjoint $\delta^1 : \mathcal{F}^1(\boldsymbol{L}, I\!R^n) \longrightarrow \mathcal{F}(P, I\!R^n)$ defined by

$$\mathcal{G}_{\boldsymbol{L}_1}(\partial^1 h_P, c) = \mathcal{G}_P(h_P, \delta^1 c) \qquad \forall\, h_P \in \mathcal{F}(P, I\!R^n) \quad \forall\, c \in \mathcal{F}^1(\boldsymbol{L}, I\!R^n).$$

We therefore have the Hodge Laplacian

$$\Delta_T := \delta^1 \circ \partial^1$$

on $\mathcal{F}(P, I\!R^n)$, a Laplacian of topological nature (cf. [B],[E],[Ch,St]).

B3 Internal forces in n.n.i.

Any internal force $\Phi_P : O_P \longrightarrow \mathcal{F}(P, I\!R^n)$ caused by n.n.i. admits a map $\mathcal{H}_P : O_P \longrightarrow \mathcal{F}(P, I\!R^n)$, called a constitutive map too, satisfying

$$\Delta_T \mathcal{H}_P(j_P) = \Phi_P(j_P) \qquad \forall\, j_P \in O_P. \tag{B3.1}$$

We thus characterize this kind of a medium by $\mathcal{H}_P$. Since

$$\Delta_T \mathcal{H}_P(j_P)(q) = k(q) \cdot \mathcal{H}_P(j_P)(q) - \sum_{i=1}^{k(q)} \mathcal{H}_P(j_P)(q_i) \qquad \forall\, q \in P \tag{B3.2}$$

we immediately observe that $\mathcal{H}_P(j_P)(q) - \mathcal{H}_P(j_P)(q_i)$ is the interaction force off equilibrium between the material points q and q_i, which is alternatively described by

$$\mathcal{H}_P(j_P)(q) - \mathcal{H}_P(j_P)(q_i) = \pm \partial^1 \mathcal{H}_P(j_P)(\sigma_i) \qquad \forall\, i = 1, ..., k(q) \tag{B3.3}$$

with $\pm$ accordingly as to whether $q = \sigma_i^+$ or $q = \sigma_i^-$.

These forces may be determined by a potential which is proportional to the square of the length of $\partial j_P(\sigma)$. Hence $\Phi_P(j_P)$ is determined by the potential

$$V_P(j_P) := \frac{1}{2} \cdot \mathcal{G}_{\boldsymbol{L}_1}(\psi \cdot \partial^1 j_P, \partial^1 j_P) \qquad \forall\, j_P \in O_P; \tag{B3.4}$$

$\psi(\sigma) \in I\!R$ is called the spring constant along $\partial j_P(\sigma)$ for all $\sigma \in \boldsymbol{L}_1$. In this case $A_P = I\!D\, V_P$ where $I\!D$ denotes the Fréchet derivative on O_P.

C The relation between the two descriptions

In order to link the descriptions of media presented in the sections A and B, we assume here that $P \subset M$ and in case of n.n.i. that also $\boldsymbol{L} \subset M$. Again $\partial M = \emptyset$. We fix $j_0 \in O$.

C1 The geometric setting

Given some internal force Φ_P we consider the virtual work A_P associated with it. What would seem to be the simplest way to link the descriptions in section B1 with the ones in A2 is to consider $r^* A_P$ where $r : C^\infty(M, I\!R^n) \longrightarrow \mathcal{F}(P, I\!R^n)$ denotes the restriction map (sending any h into $h|P$) and to look for a $\mathcal{G}(j_0)$-orthogonal complement K to $ker\ r^*$. The $\boldsymbol{L}_2$-metric $\mathcal{G}(j_0)$ on $E(M, I\!R^n)$ is given by

$$\mathcal{G}(j_0)(h, k) = \int_M < h, k > \mu(j_0) \qquad \forall\, h, k \in C^\infty(M, I\!R^n). \tag{C1.1}$$

However, this kind of a complement does not exist (since otherwise the point-evaluation (δ-functions) would admit a density (cf. [Bi5])). What we have to drop is the orthogonality condition.

Our choice of a complement is based on the observation (A2.10) involving $\Delta(j_0)$. In principal $\hat{\mathcal{H}}(j)$ can be replaced by just an eigenvector of $\Delta(j_0)$. Therefore we proceed as follows (cf. [Bi5],[Bi6]): We use the fixed (reference) configuration j_0. (It will be an equilibrium configuration later). We order the eigenvectors $\bar{e}_i \in C^\infty(M, \mathbb{R}^n)$ of $\Delta(j_0)$ with non-vanishing eigenvalues λ_i for $i = 1, \ldots$ such that $\lambda_1 \leq \lambda_2 \ldots$ (we use the natural basis in $\mathbb{R}^n$). Out of $\{r(\bar{e}_i) | i = 1, \ldots\} \subset \mathcal{F}(P, \mathbb{R}^n)$ we pick a maximal system of linearity independent vectors $r(\bar{e}_{i_1}), \ldots, r(\bar{e}_{i_b})$, say, such that $\sum_{s=1}^{b} \lambda_{i_s}$ is the smallest value for all possible choices. The b-dimensional span of this system is called $\mathcal{F}_0^\infty(M, \mathbb{R}^n)$. Set $e_s := \bar{e}_{i_s}$ for all $s = 1, \ldots, b$ and let $\mathcal{F}^\infty(M, \mathbb{R}^n) := \mathcal{F}_0^\infty(M, \mathbb{R}^n) \oplus \mathbb{R}^n$. Clearly $r | \mathcal{F}^\infty(M, \mathbb{R}^n)$ is an isomorphism onto $\mathcal{F}(P, \mathbb{R}^n)$. This isomorphism is denoted by r_∞.

The collection of the eigenvectors of $\Delta(j_0)$ not in $\mathcal{F}^\infty(M, \mathbb{R}^n)$ generates a complement to $\mathcal{F}^\infty(M, \mathbb{R}^n)$ in $C^\infty(M, \mathbb{R}^n)$, not identical to *ker r*. The complement to *ker r* we looked for is $\mathcal{F}^\infty(M, \mathbb{R}^n)$. Let $j_P^0 := r(j_0)$ be fixed. We let $O := r^{-1} O_P \subset E(M, \mathbb{R}^n)$ for O_P small enough. Any $j + h \in O$ with $j \in r^{-1}(j_P^0)$ and $h \in \mathcal{F}^\infty(M, \mathbb{R}^n)$ is projected to $j_P^0 + r_\infty(h)$. This projection is called r_∞ too.

Hence

$$\mathcal{W}^\infty(j) := O \cap (\{j\} + \mathcal{F}^\infty(M, \mathbb{R}^n)) \qquad \forall j \in r^{-1}(j_P^0) \tag{C1.2}$$

satisfies $r_\infty(\mathcal{W}^\infty(j)) = O_P$. By construction

$$O = \bigcup_{j \in r^{-1}(j_P^0)} \mathcal{W}^\infty(j). \tag{C1.3}$$

This is the slicing of O needed in the sequel, i.e. O is as in (C1.3) from now on. (C1.2) defines a flat connection on the vector bundle $O \times C^\infty(M, \mathbb{R}^n)$.

C2 The link

Now, suppose there is a virtual work A_P given on O_P. Let $O \subset E(M, \mathbb{R}^n)$ be as in (C1.3). We form the pull back

$$A := r_\infty^* A_P \tag{C2.1}$$

of A_P to O. The one-form A on O characterizes the discrete medium (given by A_P) on the continuum M. Since the force Φ_P of A_P satisfies (B1.1) the one-form A admits a force density $\hat{\Phi}$ satisfying (A2.2) with respect to $\mathcal{G}(j_0)$. Therefore A_P defines a constitutive map $\hat{\mathcal{H}} : O \longrightarrow \mathcal{F}^\infty(M, \mathbb{R}^n)$ for A, yielding

$$\hat{\Phi}(j) = \Delta(j_0) \hat{\mathcal{H}}(j) \qquad \forall j \in O$$

(cf. (A2.10) where $j_0 \in O$ is fixed). Thus $\hat{\mathcal{H}}$ exists on O even if we have no n.n.i. If, however, the discrete medium is one of n.n.i. then $\mathcal{H}_P$ exists on O_P. As shown in F1(c), $r_\infty(\hat{\mathcal{H}}(j)) \neq \mathcal{H}_P(r_\infty(j))$ for all $j \in O$, in general. For each $j \in O$ the coefficients in $\hat{\mathcal{H}}(j) = \sum_{i=1}^{b} \kappa^i(j) \cdot e_i$ are called the characteristic coefficients of the medium.

D The free energy

Here we split A_P on O_P of a skin M (to be specified below) via a Neumann boundary problem into exact and non-exact parts and show that the exact part can be identified as the differential of the free energy associated with a specific observable. As far as the continuum description is concerned we only work on $\mathcal{W}^\infty(j_0)$, where $j_0 \in O$ is fixed.

D1 Geometric preliminaries

As it is easily seen the two metrics $\mathcal{G}_P$ (B2.1) and $\mathcal{G}(j_0)$ in (C1.1) are related by

$$\mathcal{G}_P(\rho_P \cdot r_\infty(h), r_\infty(k)) = \mathcal{G}(j_0)(h,k) \qquad \forall\, h,k \in \mathcal{F}^\infty(M, I\!R^n) \tag{D1.1}$$

where ρ_P is an area density. On the other hand there is a $\rho_M : M \longrightarrow I\!R$ such that

$$r_\infty^* \mathcal{G}_P(h,k) = \mathcal{G}_P(r_\infty(h), r_\infty(k)) = \int_M \rho_M \cdot < h,k > \mu(j_0) = \mathcal{G}(j_0)(\rho_M \cdot h, k) \tag{D1.2}$$

for all $h,k \in \mathcal{F}^\infty(M, I\!R^n)$. In general $\rho_M^{\frac{1}{2}} \cdot h$ and $\rho_M^{\frac{1}{2}} \cdot k$ are not in $\mathcal{F}^\infty(M, I\!R^n)$. (D1.2) shows that there is a Riemannian metric, g, namely $\rho_M^{\frac{1}{dim\ M}} \cdot m(j)$ for which its L_2-metric $\mathcal{G}(g)$ on $\mathcal{F}^\infty(M, I\!R^n)$ agrees with $r_\infty^*\mathcal{G}_P$ on $\mathcal{W}^\infty(j_0)$. However, there is no $j \in E(M, I\!R^n)$ in general such that $g = m(j)$ unless the codimension of M in $I\!R^n$ is high enough (cf. [Gr,Ro]).

D2 The free energy

Let $\mathcal{F}(P, I\!R^n)$ be oriented and O_P be a compact neighbourhood of $j_P^0 := j_0|P$ with smooth boundary ∂O_P. Given A_P on O_P we use the Neumann decomposition to write

$$A_P = I\!D\, \bar{F}_P + \Psi_P \tag{D2.1}$$

with div $A_P = \Delta \bar{F}_{P_{\bar{F}}}$ and $A_P(\boldsymbol{n}_{O_P}) = I\!D\, \bar{F}_P(\boldsymbol{n}_{O_P})$ for some smooth positive map $\bar{F}_P : O_P \longrightarrow I\!R$, determined up to a constant. Here Δ is the Laplacian of $\mathcal{G}_P$ on $\mathcal{F}(P, I\!R^n)$ and $\boldsymbol{n}_{O_P}$ the positively oriented unit normal of ∂O_P in O_P.
Choosing a density F_P of $\bar{F}_P$, i.e. $\sum_{q\in P} F_P(j_P)(q) = \bar{F}(j_P)$ for all $j_P \in O_P$, each $\beta \in C^\infty(O_P, I\!R^+)$ defines

$$I_P := \bar{F}_P - \frac{1}{\beta} \cdot ln\, \frac{F_P}{\bar{F}_P} \qquad \text{on} \qquad O_P \qquad (\beta \neq 0). \tag{D2.2}$$

Defining the Gibbs state $\rho_P(j_P) := \frac{F_P(j_P)}{\bar{F}_P(j_P)}$ we let $\bar{S}_P(j_P) := \sum_{q\in P} \rho_P(j_P)(q) ln\ \rho_P(j_P)(q)$ and observe that

$$\bar{F}_P = \bar{I}_P - \beta^{-1} \cdot \bar{S}_P \qquad \text{and} \qquad \sum_{q\in P} e^{-\beta I_P(q)} = e^{-\beta \bar{F}_P} \qquad \text{on} \qquad O_P \tag{D2.3}$$

where $\bar{I}_P(j_P) := \sum_{q\in P} \rho_P(j_P)(q) \cdot I_P(j_P)(q)$. Thus $\bar{F}_P$ is the free energy associated with the observable I_P (cf. [B,St.]). Here $\Psi_P \neq S \cdot I\!D\, \beta$ unless Ψ_P admits an integrating factor in which case F_P can be chosen such that $\Psi_P = S \cdot I\!D\, \beta$ holds indeed. Clearly we can use $r_\infty^* \mathcal{G}_P$ in (D1.2) to determine $\bar{F}$ on $\mathcal{W}^\infty(j_0)$ yielding $\bar{F} = \bar{F}_P \circ r_\infty$.

Next assume a n.n.i. to be given. For the eigenvector e_P^i of Δ_T with non-vanishing eigenvalue λ_P^i we set $A_P^i := A_P | I\!R \cdot e_P^i$ for $i = 1, ..., b$ (where, however, $e_P^i \neq r_\infty(e_i)$ with e_i as in C1). Due to (B3.1) this implies $A_P^i = \lambda_P^i \cdot \kappa_P^i \cdot \mathcal{G}_P(e_P^i, ...)$ with $\kappa_P^i \in C^\infty(O_P, I\!R)$, called the i-th characteristic coefficient of the discrete n.n.i. medium. Clearly A_P^i is not exact in general! However, it is, provided that $I\!D\, \kappa_P^i(j)(e_P^s) = 0$ for all $s \neq i$. Setting

$$\varphi_i(j_P) := \bar{F}_P(j_P) - \frac{1}{\beta(j_P)} \cdot ln\, \frac{f_i(j_P)}{\bar{F}_P(j_P)} \qquad \forall\, i \in \{1, ..., b\} \quad \text{and} \quad \forall\, j_P \in O_P \tag{D2.4}$$

with f_i being the free energy of A^i_P, then

$$\bar{F}_P = -\frac{1}{\beta} \cdot ln\ tr\ e^{-\beta Q} \qquad \text{on} \qquad O_P \tag{D2.5}$$

with $Q(e^i_P) := \varphi^i_P \cdot e^i_P$ for $i = 1, ..., b$. The heat kernel of Q given by

$$\xi_P(j_P)(\beta(j_P), q, q') = \sum_{q,q' \in P} e^{-\beta(j_P)\cdot\varphi_i(j_P)} < e^i_P(q), e^i_P(q_i) > \qquad \forall\, j_P \in O_P \quad \forall\, q, q' \in P$$

for $\beta(j_P) \neq 0$ (cf. C1) contains all the information on the statistics introduced. Moreover

$$Z_P(j_P) := \sum_{i=1}^{b} e^{-\beta(j_P)\cdot\varphi_i(j_P)} = b - \beta(j_P) \cdot tr\ Q + \frac{\beta^2(j_P)}{2} \cdot tr\ Q^2(j_P) - ...$$

showing that $\frac{1}{b} \cdot tr\ Q^m = \lim_{\beta \longrightarrow 0} \mu_m$, where μ_m is the m-th order momentum of the Gibbs state $\frac{e^{-\beta\varphi}}{Z_P}$ on $\{1, ..., b\}$ with parameters in O_P. Clearly

$$tr\ Q = b \cdot \bar{F} - \frac{1}{\beta} \cdot \sum_{i=1}^{b} ln \frac{f_i}{\bar{F}_P} \qquad \text{on} \qquad O_P.$$

Finally, let us restrict the concept of an equilibrium configuration j_P: We require both to hold $\Phi_P(j_P) = 0$ and $Grad_{\mathcal{G}_P} \bar{F}_P(j_P) = 0$, with $Grad_{\mathcal{G}_P}$ being the gradient formed with respect to $\mathcal{G}_P$. An equilibrium configuration $j \in O$ is defined accordingly by yusing $\mathcal{G}(j_0)$.

E Linearization

In this section we deal with skins as previously. In addition we assume that O is as in D2 and that $j_0 \in O$ as well as $j^0_P := j_0|P$ are equilibrium configurations. The purpose is here to link the modes of the Hessian at j^0_P of the free energy $\bar{F}_P$ with the characteristic coefficients in the setting of n.n.i..

E1 Linearized forces

Given A_P on O_P the force Φ_P splits into

$$\Phi_P(j^0_P + h_P) = I\!D\, \Phi_P(j^0_P)(h_P) + \quad \text{higher order terms} \quad \forall\, h_P \in O_P - j^0_P. \tag{E1.1}$$

The respective force $\Phi_{\bar{F}_P}$ of $I\!D\, \bar{F}_P$ (a gradient with respect to $\mathcal{G}_P$) and the force Φ_{Ψ_P} of Ψ_P split accordingly (cf. [Bi5]). In case of n.n.i., the constitutive map $\mathcal{H}_{\bar{F}_P}$ associated with $\Phi_{\bar{F}_P}$ writes as

$$\mathcal{H}_{\bar{F}_P}(j^0_P + h_P) = I\!D\, \mathcal{H}_{\bar{F}_P}(j^0_P)(h_P) + \quad \text{higher order terms} \quad \forall\, h_P \in O_P - j^0_P. \tag{E1.2}$$

with the choice of $\mathcal{H}_{\bar{F}_P}(j^0_P) = 0$. The linearization of $\Phi_{\bar{F}_P}$ yields

$$\bar{F}_P(j^0_P + h_P) = \bar{F}_P(j^0_P) + \frac{1}{2} \cdot I\!D^2 \bar{F}_P(j^0_P)(h_P, h_P) \tag{E1.3}$$

up to higher order terms. Let the modes of $I\!D^2 \bar{F}_P$ and their eigenvectors be denoted by ν_i and u^i_P respectively, $i = 1, ..., b$.

E2 The modes of $I\!D^2\bar{F}_P(j_0)$:

Here we assume a n.n.i. to be given. Since $\mathcal{H}_{\bar{F}_P}(j_P) = \sum_{i=1}^{b} \kappa^i_{\bar{F}_P}(j_P) \cdot e^i_P$ for all $j_P \in O$

$$I\!D^2\bar{F}_P(j^0_P)(h_P, h_P) = \sum_{i=1}^{b} \lambda^i_P \cdot I\!D\,\kappa^i_{\bar{F}_P}(j^0_P)(h_P) \cdot \mathcal{G}_P(e^i_P, h_P) \qquad \text{(E2.1)}$$

for all $h_P \in \mathcal{F}(P, I\!R^n)$ implying

$$\nu_r = \sum_{i=1}^{b} \lambda^i_P \cdot I\!D\,\kappa^i_{\bar{F}_P}(j^0_P)(u^r_P) \cdot \mathcal{G}_P(e^i_P, u^r_P). \qquad \text{(E2.2)}$$

Thus

$$\nu_i = \lambda^i_P \cdot I\!D\,\kappa^i_{\bar{F}_P}(j^0_P)(e^i_P), \qquad \text{(E2.3)}$$

provided all $\kappa^i_{\bar{F}_P}$ decouple near j^0_P, i.e. $I\!D\,\kappa^i_{\bar{F}_P}(j^0_P)(e^s_P) = \delta_{i,s}$.Therefore (E2.3) yields

$$I\!D\,\mathcal{H}_{\bar{F}_P}(j^0_P)(h_P) = \sum_{i=1}^{P} \frac{\nu_i}{\lambda^i_P} \cdot e^i_P \cdot \mathcal{G}_P(e^i_P, h_P) + \quad \text{higher order terms.} \qquad \text{(E2.4)}$$

By (E2.2) the linear maps $I\!D\,\kappa^i_{\bar{F}_P}(j^0_P)$ can be expressed in terms of ν_r, λ^i_P and $\mathcal{G}_P(e^i_P, u^r_P)$ with $i, r = 1, ..., b$, i.e. the modes determine $\mathcal{H}_{\bar{F}_P}$ on O_P up to higher order terms.

Instead of working on O_P we can work on $\mathcal{W}^\infty(j_0)$ using $r^*_\infty \mathcal{G}_P$ in (D1.2) and get the same type of formulas, since $\bar{F}_P \circ r_\infty = \bar{F}$. In particular $\mathcal{H}_{\bar{F}} = \sum_{i=1}^{b} \kappa_{\bar{F}} \cdot e_i$ implies

$$\nu_r = \sum_{i=1}^{b} \lambda^i \cdot I\!D\,\kappa^i_{\bar{F}}(j_0)(u_r) \cdot \mathcal{G}(j_0)(\rho_M \cdot e_i, u_r) \qquad \text{(E2.5)}$$

with ν_r and $u_r := r^{-1}_\infty(u^r_P)$ for $r = 1, ..., b$ being the eigenvalues and eigenvectors of $I\!D^2\bar{F}(j_0)$ and ρ_M is the map introduced in (D1.2). If hence all $\kappa^i_{\bar{F}}$ decouple near j_0 then

$$\nu_r = \lambda^r \cdot I\!D\,\kappa^r_{\bar{F}}(j_0)(e_r) \cdot \mathcal{G}(j_0)(\rho_M \cdot e_r, e_r) \qquad r = 1, ..., b \qquad \text{(E2.6)}$$

saying that the modes are proportional to the eigenvalues of $\Delta(j_0)$ provided $\rho_M = 1$; the proportionality factors are the first order characteristic coefficients in $\mathcal{H}_{\bar{F}_P}$.

Let A_P be linear, i.e. $\Phi_P(j_P + h_P) = I\!D\,\Phi_P(j^0_P)(h_P)$ for all $h_P \in O_P - j^0_P$. The free energy $\bar{F}$ on $\mathcal{W}^\infty(j_0)$ satisfies then

$$A(j)(j) = I\!D\,\bar{F}(j)(j) = a(j) \cdot I\!D\,\mathcal{A}(j)(j) \quad \forall j \in O \qquad \text{(E2.7)}$$

with a as in (A3.2). Since $a(j_0) = 0$ and $I\!D\,\bar{F}(j_0) = 0$ (j_0 is an equilibrium configuration!)

$$I\!D^2\bar{F}(j_0)(h, j_0) = I\!D\,a(j_0)(h) \cdot \mathcal{A}(j_0)(j_0) \qquad \text{(E2.8)}$$

showing

$$\nu_i \cdot \iota^0_i = dim\ M \cdot \mathcal{A}(j_0) \cdot I\!D\,a(j_0)(u_i) \qquad \forall i = 1, ..., b \qquad \text{(E2.9)}$$

where $j_0 = \sum \iota^0_i \cdot u_i$. Hence a on $\mathcal{W}^\infty(j_0)$ is determined up to first order by the modes ν_i; The reader may link (D2.5) and (E2.9).

F Preliminary definition of a well fitting configuration

Given a skin M, let $A := r_\infty^* A_P$ on $\mathcal{W}^\infty(j_0)$ for a given A_P on O_P with $A_P(j_P^0) = 0$ and $I\!D\,\bar{F}_P(j_P^0) = 0$. Here $j_0|P = j_P^0$ again. We call, preliminary, j_0 to be a well fitting configuration (expressing that $j_0(M)$ fits $j_P^0(P)$ well) if

$$\rho_P = 1$$

(cf. (D1.1). If $\rho_P = 1$ then the Neumann decompositions of A_P and $A = r_\infty^* A_P$ formed with respect to $\mathcal{G}_P$ and $\mathcal{G}(j_0)$ yield $\bar{F} = \bar{F}_P \circ r_\infty$ (cf. sec. D2), the reason of the above definition of well fitting.

F1 Some consequences for well fitting configurations in case of n.n.i.

Let j_0 be a well fitting configuration for $A = r_\infty^* A_P$ on $\mathcal{W}^\infty(j_0)$. We assume that A_P is caused by n.n.i.. At first we remark that due to (C2.1)

$$\Delta(j_0)\hat{\mathcal{H}}(j) = \Delta_T \mathcal{H}_P(r_\infty(j)) \quad \forall j \in \mathcal{W}^\infty(j_0). \tag{F1.1}$$

The simple consequences we have in mind here are the following ones:
a) By (E2.7) the structural capillarity a on $\mathcal{W}^\infty(j_0)$ of $A = r_\infty^* I\!D\,V_P$ satisfies for all $j \in O$

$$a(j) = \frac{1}{dim\ M \cdot \mathcal{A}(j)} \cdot \mathcal{G}_{\boldsymbol{L}_1}(\psi \cdot \partial^1 j_P, \partial^1 j_P)$$

(cf. (B3.4)) with $j_P := j|P$.

b) The derivative of the characteristic coefficient of $\hat{\mathcal{H}}_{\bar{F}}$ and $\mathcal{H}_{\bar{F}_P}$ at j_0 respectively j_P^0 (cf. E2) are linked by (D2.1) and its analogon on $\mathcal{W}^\infty(j_0)$. Hence (E2.6) and (E2.2) yield

$$\nu_r = \lambda_r \cdot I\!D\,\kappa_{\bar{F}}^r(j_0)(e_r) = \sum_{i=1}^{b} \lambda_P^i \cdot I\!D\,\kappa_{\bar{F}_P}^i(j_P^0)(r_\infty(e_r)) \cdot \mathcal{G}_P(e_P^i, r_\infty(e_P^r)). \tag{F1.2}$$

There is an analogous equation if all $\kappa_{\bar{F}_P}^i$ decouple near j_P^0.

c) Finally let us compare $\Delta(j_0)h$ and $\Delta_T h_P$ with $h_P = h|P$ for $h \in \mathcal{F}^\infty(M, I\!R^3)$ for $dim\ M = 2$ in order to understand (F1.1). One easily verifies from Gausse's theorem

$$\Delta(j_0)h(q) = -\lim_{|B_q| \longrightarrow 0} \frac{1}{|B_q|} \int_{\partial B_q} dh(\mathcal{N}_{B_q}) \mu_{B_q} \tag{F1.3}$$

where $|B_q|$ is the volume of a geodesic ball B_q centered about $q \in M$ and $\mathcal{N}_{B_q}$ is the oriented unit normal of ∂B_q. Since

$$-dh(q_i)(\mathcal{N}_{B_q}) \cdot |\sigma_i| = h(q) - h(q_i) + \quad \text{higher order terms}$$

(cf. B2) for each nearest neighbour q_i (assumed to be on ∂B_q) of q, equation (F1.3) yields

$$\Delta(j_0)h(q) = \frac{2}{k(q) \cdot r^2} \cdot \Delta_T h_P(q)$$

as an approximation for symmetrically distributed n.n.. Here $r = |\sigma_i|$ for $i = 1, ..., k(q)$. Hence $\hat{\mathcal{H}}(j)(q) = \frac{2}{k(q) \cdot r^2} \cdot \mathcal{H}_P(r_\infty(j)(q))$ for all $j \in \mathcal{W}^\infty(j_0)$ holds approximately.

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