Structural capillarity, equilibrium configurations and vibrational modes of an idealized skin made up by finitely many particle

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Abstract:

A skin made up by finitely many particles is a manifold passing through a finite system of interacting particles. The discrete medium as well as the continuum are characterized by the virtual work. We study equilibrium configurations of the discrete system as well as of the skin and compute the vibrational modes.

Non-trivial equilibrium configurations only exist if the virtual work is non-linear. Free energy, equilibrium configuration and the vibrational modes crucially depend on the structural capillarity. This sort of capillarity determines the work caused by distorting the area of the skin. The free energy of the skin is extracted from the virtual work by solving a boundary problem and is linked to a Gibbs statistics of the finite system. This yields various interplays between geometry, topology, analysis and statistics.

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0 Introduction

The aim of this application of analysis, mainly of a type of Hodge theory and of Neumann boundary problems, is the description of a discrete medium as a continuum. In doing so we will not pass to a limit by enlarging the particle number, we rather will investigate how to fit a continuum through the given particle system.

The discrete medium consists of a large but finite collection P of interacting material particles. The continuum is modeled on a compact nice manifold M (without boundary, for simplicity), equipped with a smooth mass density. M is called an idealized skin.

In characterizing the discrete deformable medium we use the virtual work $A_P(j_P)(h_P)$ resisting a distortion $h_P : P \to I\!R^n$ at a configuration j_P (cf. Hellinger [19]). The configuration space is a collection O_P of injective maps from P to $I\!R^n$. O_P shall be open in the linear, finite dimensional space of all maps from P to $I\!R^n$. The one-form A_P on O_P, is supposed to be smooth and to be invariant under the action on O_P of a neighbourhood of zero of the group of all translations of $I\!R^n$; in addition it is required that constant distortions cause no virtual work.

The continuum is characterized accordingly by a smooth one-form A on the configuration space O, a collection of smooth embeddings of M into $\mathbb{R}^n$ (cf. Binz [5] to [8] and Marsden & Hughes [23]). Again O is supposed to be open in the infinite dimensional Fréchet space of all smooth maps from M to $\mathbb{R}^n$. Let $P \subset M$. We construct the virtual work A out of A_P by slicing O into slices $\mathcal{W}$, each one diffeomorphic to O_P, via the restriction map r. Pulling back A_P to each slice $\mathcal{W}$ by r and setting it (in addition) equal to zero on the normal bundle of $\mathcal{W}$ yields A. This virtual work A inherits the invariance under the translation group $\mathbb{R}^n$ and the property that constant distortion cause no virtual work as well, at any configuration. The ladder fact yields a constitutive map $\mathcal{H}$ characterizing the continuum: The force density $\Phi(j)$ at j is of the form $\Phi(j) = \Delta(j)\mathcal{H}(j)$, where $\Delta(j)$ is the Laplacian of the pull back of $<,>$ by j.

The general goal is hence to deduce characteristics of A by those of A_P. We do so e.g. by using a Hodge type of splitting of A and A_P to exhibit the smooth maps $\bar{F}$ and $\bar{F}_P$ on O respectively on O_P, relating them and identifying them as the free energies in respective Gibbs statistics. The choice of densities F_P respectively F of $\bar{F}_P$ and $\bar{F}$ does not only determine Gibbs states, but also refines the description of the above mentioned media. It links, moreover, our description of a continuum to the one presented in Landau & Lifschitz [21].

We call $j_0 \subset O$ to be an equilibrium configuration if $A(j_0) = 0$ and $\mathbb{D}\bar{F}(j_0) = 0$ with $\mathbb{D}$ denoting the Fréchet derivative on function spaces. An equilibrium configuration of the discrete system is defined accordingly by using A_P and $\bar{F}_P$.

The main tasks we head for in this paper is two fold. One is to show that a non-trivial equlibrium configuration j_0 for a non-trivial medium ($A \neq 0$) of the skin only exists if A is non-linear near j_0 (If $\bar{F}$ is constant on an open set, the elements of this set are called trivial configurations). The other is to determine the spectrum of the medium forming the skin at an equlibrium.

Both rely on the notion of the structural capillarity: From the virtual work at j splits naturally off the amount proportional to the area deformation at j. This proportionality factor $a(j)$ is called the structural capillarity. The free energy $\bar{F}(j)$ at j contains in turn the amount $\frac{1}{2} \cdot a(j) \cdot \mathcal{A}(j)$ with $\mathcal{A}(j)$ being the area at j. This quantity is the free energy determined by the linearization of A at j.

In addition $a(j)$ contains a part which depends on the curvature and the topology in case of $\dim M = 2$; the Euler characteristics enters explicitly. Thus both the equilibrium configuration and the spectrum are topology dependent.

A rather large part of the paper is devoted to develop the formalism needed to obtain the results mentioned. It is needed to express the interplay between analysis, geometry and statistics. In particular we show that the first trace coefficient in the asymptotics of the partition function adapted to the Gibbs state in the discrete case, can replace the free energy in the variation determining the equlibrium configuration, provided the temperature is remained constant. The other coefficients contribute to the statistics.

We close this note by introducing the notion of a configuration of the skin fitting the discrete medium up to first order (a special sort of equilibrium configuration) and present, at this kind of configuration, some descriptions of characteristics of A in terms of those of A_P and vice versa. In particular we express the vibrational modes of the discrete medium in terms of the structural capillarity and the area function both defined on O. The finitely many Fourier coefficients of a first order fit, determined by the discrete system, are computed . However, the general verification of the existence of such a kind of fitting configuration will be done elsewhere.

1 Description of discrete media

In this section we are given a finite set P of points, thought of as mean locations of interacting material particles. We characterize the discrete medium in this generality via internal forces resisting distortion.

1.1 Discrete media

The configuration space of a discrete medium is O_P, some open set in the collection $E(P, \mathbb{R}^n)$ of all injective maps from P to $\mathbb{R}^n$.

By a distortion of the medium we mean a map $h_P : P \longrightarrow \mathbb{R}^n$. The collection of all distortions of P is denoted by $\mathcal{F}(P, \mathbb{R}^n)$, a finite dimensional linear space. A configuration j_P distorted by $h_P \in \mathcal{F}(P, \mathbb{R}^n)$ is $j_P + h_P$; this explains the term distortion. The mass distribution of the discrete medium is called

$$\rho_P : P \longrightarrow \mathbb{R};$$

its total mass is $m := \sum_{q \in P} \rho_P(q)$.

The center $z(j_P)$ of mass of any configuration j_P is determined by

$$m \cdot z(j_P) = \sum_{q \in P} \rho_P(q) \cdot j_P(q). \tag{1.1.1}$$

Thus any $h_P \in \mathcal{F}(P, \mathbb{R}^n)$ satisfies

$$m \cdot D\, z(j_P)(h_P) = \sum_{q \in P} \rho_P(q) \cdot h_P(q). \tag{1.1.2}$$

In the sequel we will assume that ρ_P is a constant map with value one. If hence $z(j_P) = 0$ then $\sum_q j_P(q) = 0$. Thus any distortion h_P leaving the center of mass fixed satisfies $\sum_q h_p(q) = 0$.

The physical quality of the medium at a configuration j_P is characterized by the internal force $\Phi_P(j_P)$ resisting any distortion; Φ_P is supposed to satisfies the following:

$$a) \quad \Phi_P(j_P + z) = \Phi_P(j_P) \qquad \forall\, j_P \in O_P \subset E(P, \mathbb{R}^n) \tag{1.1.3}$$

and for all z in a zero neighbourhood of $\mathbb{R}^n$, as well as

$$b) \quad \sum_{q \in P} < \Phi_P(j_P)(q), z >= 0 \qquad \forall j_P \in O_P \subset E(P, \mathbb{R}^n) \quad \text{and} \quad \forall z \in \mathbb{R}^n. \tag{1.1.4}$$

(a) expresses the invariance of the force Φ_P under the natural action of the translation group $\mathbb{R}^n$ of $\mathbb{R}^n$ on $E(P, \mathbb{R}^n)$ and (b) manifests that constant distortions cause no virtual work. This relates to (1.1.2) for $\mathbb{D}\, z(j_P)(h_P) = 0$. We refer to Binz [11] for a group theoretical explanation of (b).

The virtual work caused by an arbitrarily given distortion h_P at a configuration j_P is denoted by $A_P(j_P)(h_P)$ and is defined by

$$A_P(j_P)(h_P) = \sum_{q \in P} < \Phi_P(j_P), h_P(q) > \qquad \forall j_P \in O_P \quad \textit{and} \quad \forall h_P \in F(P, \mathbb{R}^n). \tag{1.1.5}$$

Introducing the metric $\mathcal{G}_P$ on $E(P, \mathbb{R}^n)$ by setting

$$\mathcal{G}_P(h_P, k_P) := \sum_{q \in P} < h_P(q), k_P(q) > \qquad \forall k_P, h_P \in \mathcal{F}(P, \mathbb{R}^n) \tag{1.1.6}$$

yields

$$A_P(j_P)(h_P) = \mathcal{G}_P(\Phi_P(j_P), h_P) \qquad \forall j_P \in O_P \quad \textit{and} \quad \forall h_P \in \mathcal{F}(P, \mathbb{R}^n).$$

If hence Φ_P is a $\mathcal{G}_P$-gradient of a smooth map $V_P : O_P \longrightarrow \mathbb{R}$ then

$$A_P(j_P)(h_P) = \mathbb{D}\, V_P(j_P)(h_P) \qquad \forall j \subset O_P.$$

Denoting by $u_q^z : P \longrightarrow \mathbb{R}^n$ the map given by

$$u_q^z(q') = \begin{cases} z & q = q' \\ 0 & q \neq q' \end{cases} \qquad z \in \mathbb{R}^n \text{ fixed,}$$

then $A_P(j_P)(u_q^z)$ is the work caused by distorting only one particle by z, namely the one at q.

1.2 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 zero- and one-simplices is denoted by P and $\boldsymbol{L}_1$, respectively. Two particles at q and q_i, 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 $nb(q)$ we mean the total number of n.n. of any $q \in P$. On the linear space $\mathcal{F}^1(\boldsymbol{L}, \mathbb{R}^n)$ of all one-cochains of $\boldsymbol{L}$ there is the natural scalar products $\mathcal{G}_{\boldsymbol{L}_1}$ given by

$$G_{\boldsymbol{L}_1}(c_1, c_2) := \sum_{\sigma \in \boldsymbol{L}_1} < c_1(\sigma), c_2(\sigma) > \tag{1.2.1}$$

for all $c_1, c_2 \in \mathcal{F}^1(\boldsymbol{L}, \mathbb{R}^n)$. The coboundary $\partial^1 : \mathcal{F}(P, \mathbb{R}^n) \longrightarrow \mathcal{F}^1(\boldsymbol{L}, \mathbb{R}^n)$ has an adjoint δ^1, the **divergence**, defined by

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

We therefore have the Hodge Laplacian $\Delta_T := \delta^1 \circ \partial^1$ on $\mathcal{F}(P, \mathbb{R}^n)$ (cf. Binz [4] and Eckmann [16]).

Due to (1.1.4) any internal force $\Phi_P \in C^\infty(O, \mathcal{F}(P, \mathbb{R}^n))$ caused by distorting a n.n.i. admits a constitutive map $\mathcal{H}_P \in C^\infty(O_P, \mathcal{F}(P, \mathbb{R}^n))$, satisfying

$$\Delta_T \mathcal{H}_P(j_P) = \Phi_P(j_P) \qquad \forall\, j_P \in O_P. \tag{1.2.2}$$

We thus characterize this kind of a medium by the map $\mathcal{H}_P$, in the sequel. Since

$$\Delta_T \mathcal{H}_P(j_P)(q) = nb(q) \cdot \mathcal{H}_P(j_P)(q) - \sum_{i=1}^{nb(q)} \mathcal{H}_P(j_P)(q_i) \qquad \forall\, q \in P \tag{1.2.3}$$

(cf. Bien [4]) 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 particles at $j_P(q)$ and $j_P(q_i)$. It is alternatively described by

$$\mathcal{H}_P(j_P)(q) - \mathcal{H}_P(j_P)(q_i) = \pm\, \partial^1 \mathcal{H}_P(j_P)(\sigma_i) \qquad \forall\, i = 1, ..., nb(q), \tag{1.2.4}$$

with $\pm$ according as to whether $q = \sigma_i^+$ or $q = \sigma_i^-$, where $+$ and $-$ is given by the orientation. Since Φ_P satisfies (1.1.4) and $Ker\partial^1 = \mathbb{R}^n$ we conclude that Φ_P factors to $im\partial^1$. The quotient map is called Φ_P again. Similarly $\mathcal{H}_P$ depends only on $\partial^1 j_P$ for $j_P \in O_P$. Moreover $A_P(j_P) = A_P(\partial^1 j_P)$ for all $j_P \in O_P$. Forces of this kind may be determined by a smooth potential

$$V_{\boldsymbol{L}_1} : \partial^1 O_P \longrightarrow \mathbb{R}$$

such that for all $j_P \in O_P$

$$A_P(j_P)(h_P) = A_P(\partial^1 j_P)(\partial^1 h_P) = \mathbb{D} V_{\boldsymbol{L}_1}(\partial^1 j_P)(\partial^1 h_P) \quad \forall\, h_P \in O_P. \tag{1.2.5}$$

Hence the force is a $\mathcal{G}_{\boldsymbol{L}_1}$-gradient, i.e.

$$\Phi_P(\partial^1 j_P) = grad_{\mathcal{G}_{\boldsymbol{L}_1}} V_{\boldsymbol{L}_1}(\partial^1 j_P) \qquad \forall\, j_P \in O_P.$$

Setting $V_P(j_P) := V_{\boldsymbol{L}_1}(\partial^1 j_P)$, then the $\mathcal{G}_P$-gradient is

$$grad_{\mathcal{G}_P} V_P(j_P) = \delta^1 grad_{\mathcal{G}_{\boldsymbol{L}_1}} V_{\boldsymbol{L}_1}(\partial^1 j_P) \qquad \forall\, j_P \in O_P. \tag{1.2.6}$$

Taking the component of $grad_{\mathcal{G}_{\boldsymbol{L}_1}} V_{\boldsymbol{L}_1}(\partial^1 j_P)$ along $\partial^1 j_P$ yields the splitting

$$grad_{\mathcal{G}_{\boldsymbol{L}_1}} V_{\boldsymbol{L}_1}(\partial^1 j_P) = \psi(\partial^1 j_P) \cdot \partial^1 j_P + \theta_{\boldsymbol{L}_1}(\partial^1 j_P) \qquad \forall\, j_P \in O_P \tag{1.2.7}$$

where $\psi : \partial^1 O_P \longrightarrow I\!R$ is a smooth map and $\theta_{L_1}(\partial^1(j_P)$ is $\mathcal{G}_{L_1}$-orthogonal to $\partial^1 j_P$. Hence V_{L_1} splits into

$$V_{L_1}(\partial^1 j_P) = \frac{1}{2} \cdot \mathcal{G}_{L_1}(\psi(\partial^1 j_P) \cdot \partial^1 j_P, \partial^1 j_P) + V^1_{L_1}(\partial^1 j_P) \qquad \forall\, j_P \in O_P \quad (1.2.8)$$

where $V^1_{L_1}$ is defined by (1.2.8). In analogy to Hooke's law for a spring, we call $\psi(\partial^1 j_P)$ the **spring constant**, provided ψ is a constant map.

Clearly the above splitting (1.2.7) yields

$$A_P(j_P)(j_P) = \mathcal{G}_{L_1}(\psi(j_P) \cdot \partial^1 j_P, \partial^1 j_P) \qquad \forall\, j_P \in O_P, \qquad (1.2.9)$$

out of which the map ψ can be determined. We will use this fact later on.

2 The free energy

Given a discrete medium, we will split A_P on O_P 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 specific observables. To this end $\bar{O}_P$ will be the closure of the open set O_P and shall be further specified below.

2.1 The free energy of the discrete medium

Let $\mathcal{F}(P, I\!R^n)$ be oriented. $\bar{O}_P$ shall be a $\dim \mathcal{F}(P, I\!R^n)$-dimensional compact, smooth and connected manifold with boundary. Given A_P on $\bar{O}_P$ then

$$A_P = I\!D\, \bar{F}_P + \Psi_P \qquad (2.1.1)$$

with $\mathrm{div}_{O_P} A_P = \Delta_{O_P} \bar{F}_P$ and $A_P(n_{O_P}) = I\!D\, \bar{F}_P(n_{O_P})$ for some smooth positive map $\bar{F}_P : \bar{O}_P \longrightarrow I\!R$, determined up to a constant. Here div_{O_P} and Δ_{O_P} on $\mathcal{F}(P, I\!R^n)$ are respectively the divergence operator and the Laplacian of the scalar product $\mathcal{G}_P$. n_{O_P} denotes the positively oriented unit normal of the boundary of $\bar{O}_P$. $I\!D$ denotes the Fréchet derivativ on function spaces. Without loss of generality we may assume that $I\!D\, \bar{F}_P(j_P)$ vanishes on any constant map from P to $I\!R^n$. If Φ_P is caused by a nearest neighbour interaction, then

$$\bar{F}_P = V_P \circ \partial^1 + \text{ const.}. \qquad (2.1.2)$$

with V_P as in (1.2.6). Hence $\bar{F}_P$ admits a splitting according to (1.2.8).

Next we will establish $\bar{F}_P$ as a free energy. To this end let the Boltzmann constant be equals to 1. For each $j_P \in O_P$ the positive real $\bar{F}_P(j_P)$ is the free energy (cf. Bamberg & Sternberg [3]) associated with an inverse temperature map $\beta \in C^\infty(O_P, I\!R^+)$ and a state $\rho^P_{Gibbs}(j_P)$ as seen as follows:

Let $F_P \in C^\infty(O_P, \mathcal{F}(P, I\!R^+))$ be such that $\bar{F}_P(j_P) = \sum_{q \in P} F_P(j_P)(q)$ for all $j_P \in O_P$. Each such density F_P is of the form

$$F_P(j_P) = \frac{\bar{F}_P(j_P)}{\# P} + \xi_P(j_P) \qquad \text{with} \qquad \sum_{q \in P} \xi_P(j_P)(q) = 0 \qquad (2.1.3)$$

for a suitable $\xi_P \in C^\infty(O_P, \mathcal{F}(P, I\!R))$. Here $\#P$ denotes the number of points in P. The state $\rho^P_{Gibbs}(j_P)$ is defined by

$$\rho^P_{Gibbs}(j_P) := \frac{F_P(j_P)}{\bar{F}_P(j_P)} = \frac{\bar{F}_P(j_P)}{\#P} + \frac{\xi_P(j_P)}{\bar{F}_P(j_P)} \qquad \forall j_P \in O_P. \tag{2.1.4}$$

The observable $I_P \in C^\infty(O_P, \mathcal{F}(P, I\!R))$ associated with $\beta \in C^\infty(O_P, I\!R^+)$ and ρ^P_{Gibbs} is

$$I_P := \bar{F}_P - \frac{1}{\beta} \cdot ln\ \rho^P_{Gibbs} \tag{2.1.5}$$

and yields for each $j_P \in O_P$

$$\rho^P_{Gibbs}(j_P) = \frac{e^{-\beta(j_P)\cdot I_P(j_P)}}{\sum_{q\in P} e^{-\beta(j_P)\cdot I_P(j_P)(q)}}. \tag{2.1.6}$$

Hence $\rho^P_{Gibbs}(j_P)$ is a Gibbs state for each $j_P \in O_P$. This state implies

$$\bar{F}_P = \bar{I}_P - \beta^{-1} \cdot \bar{S}_P \tag{2.1.7}$$

with the usual notions

$$\bar{I}_P(j_P) := \sum_{q\in P} \rho^P_{Gibbs}(j_P)(q) \cdot I_P(j_P)(q)$$

and

$$\bar{S}_P(j_P) := \sum_{q\in P} \rho^P_{Gibbs}(j_P)(q) \cdot ln\ \rho^P_{Gibbs}(j_P)(q);$$

hence $\bar{F}$ is a **free energy**. $\Psi_P \neq S \cdot I\!D\,\beta$ 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.

Specifying β, ξ_P and F_P needed to interpret $\bar{F}_P$ as a free energy yields a finer characterisation of the discrete medium than the one determined by A_P only.

The partition function

$$Z_P(j_P) := \sum_{q\in P} e^{-\beta(j_P) I_P(j_P)(q)}$$

of the state ρ^P_{Gibbs}, defined for all $j_P \in O_P$, satisfies $Z_P(j_P) = e^{-\beta(j_P)\cdot \bar{F}(j_P)}$ and admits the following interpretation: Let $Q_P(j_P) \in End\ \mathcal{F}(P, I\!R)$ be the operator having the characteristic function $\mathbf{1}_q$ as eigen-vector with eigen-value $e^{-\beta(j_P)I_P(j_P)(q)}$ for any $q \in P$. Then the following is obvious:

Lemma 2.1.1 *Given $\rho^P_{Gibbs} := \frac{F_P}{\bar{F}_P}$ and a positive map $\beta \in C_\infty(O_P, \mathcal{F}(P, I\!R))$ then the partition function is of the form*

$$Z_P(j_P) = \#P + \beta(j_P) \cdot tr\ Q_P(j_P) + \frac{\beta(j_P)^2}{2} \cdot tr\ Q^2_P(j_P) - \ldots \tag{2.1.8}$$

Finally, let us introduce the concept of a (rather strong type of) **equilibrium configuration** $j_P \in O_P$: We require from j_P both to hold, namely $\Phi_P(j_P) = 0$ as well as $Grad_{\mathcal{G}_P} \bar{F}_P(j_P) = 0$, with $Grad_{\mathcal{G}_P}$ being the gradient formed with respect to $\mathcal{G}_P$. The following is rather obvious:

Lemma 2.1.2 *If $j_P \in O_P$ is an equilibrium configuration then the following are equivalent provided that β is kept constant*

$$(i)\ I\!D\, F_P(j_P) = 0,$$

$$(ii)\ I\!D\, I_P(j_P) = 0, \quad (iii)\ I\!D\, Q_P(j_P) = 0;$$

thus trQ_P serves as a Lagrangian density to determine the stationary configuration j_P of $\bar{F}_P$. The traces of $Q(j_P)$ and the higher order powers of $Q(j_P)$ in Z_P reflect the statistics chosen and hence the fluctuation about $trQ_P(j_P)$.

A first rather obvious remark, based on (1.2.5) and (1.2.7), on the existence of an equilibrium configuration is the following:

Proposition 2.1.3 *An equilibrium configuration j_P^0 in a n.n.i. medium with non-vanishing spring constant ψ exists only if $\theta_P(j_P^0) \neq 0$.*

3 Characterization of an idealized skin

Here we describe an idealized skin, a continuum, as a connected, smooth, compact and oriented manifold M, equipped with a mass density and a constitutive law, both configuration dependent. The constitutive law will be non-local in general. The reason for non-locality is two fold and will become apparent if we treat on one hand the virtual work caused by area deformations and on the other if we formulate conditions for equilibrium configurations. A relation to the discrete structure will follow in section four. For the geometric notions we refer to Greub et al [18].

3.1 An idealized skin

The **configuration space** is supposed to be an open subset O of the collection $E(M, I\!R^n)$ of all smooth embeddings of M into $I\!R^n$ endowed with the C^∞-topology, a principal Diff$M$-bundle (cf. Binz & Fischer [12]). The tangent space at each $j \in O$ is $C^\infty(M, I\!R^n)$, the collection of all smooth $I\!R^n$-valued maps of M into $I\!R^n$. On $I\!R^n$ a fixed scalar product $<,>$ is specified.

A mass density is a smooth map $\rho : O \longrightarrow C^\infty(M, I\!R)$ with positive values for which the equation

$$\int_M \rho(j)\mu(j) = \text{const.} \qquad \forall\, j \in O$$

holds. $\mu(j)$ denotes the volume element of the metric $m(j)$. The above equation implies (cf. Binz [6])

$$\int_M (I\!D\, \rho(j)(h) + \rho(j) \cdot tr\ B_h)\mu(j) = 0 \qquad \forall\, h \in C^\infty(M, I\!R^n). \tag{3.1.9}$$

$I\!\!D$ denotes the differentiation on function spaces (on O, here) in the sense of Binz et al [15] or Frölicher & Kriegel [17]. Moreover B_h is an element of $End\, TM$, the collection of all smooth bundle endomorphism of TM over the identity, equipped with the C^∞-topology; it is defined as follows : Let $m(j) := j^* <,>$ be the pull back metric of $<,>$ by j on the manifold M. Given any other $j' \in E(M, I\!\!R^n)$, the metrics $m(j)$ and $m(j')$ are related by

$$m(j')(v,w) = m(j)(f^2(j')v, w) \qquad \forall\, v, w \in T_qM \qquad \forall\, q \in M \tag{3.1.10}$$

with $f(j') \in End\, TM$ being smooth and pointwise positive definite with respect to $m(j)$. The derivative of f at j in the direction of h is denoted by B_h. Equation (3.1.9) implies the following:

$$I\!\!D\,\rho(j)(h) + \rho(j) \cdot trB_h = \Delta(j)y(j,h) \qquad \forall\, j \in O \text{ and } \forall\, h \in C^\infty(M, I\!\!R^n)$$

where $\Delta(j)$ is the Laplacian of $m(j)$, for which we refer to Matsushima [24] and $y(j,h) : M \longrightarrow I\!\!R$ is a smooth function, uniquely determined up to a constant (cf. Hörmander [20]). However, we choose ρ such that the continuity equation

$$I\!\!D\,\rho(j)(h) + \rho(j) \cdot trB_h = 0 \qquad \forall\, j \in O \tag{3.1.11}$$

holds true. Densities of this type are determined as follows. Given a positive $\rho_0 \in C^\infty(M, I\!\!R)$, the solution to (3.1.9) is obviously

$$\rho(j) = \rho_0 \cdot det\ f^{-1}(j) \qquad j \in O \tag{3.1.12}$$

with f as above (cf. A1.5 in appendix one).

The constitutive entity which describes the quality of the medium phenomenologically, will be a special sort of a smooth force density map

$$\Phi : O \longrightarrow C^\infty(M, I\!\!R^n)$$

which will prescribe at each $j \in O$ the force density $\Phi(j) \in C^\infty(M, I\!\!R^n)$ resisting an infinitesimal distortion $h \in C^\infty(M, I\!\!R^n)$ of $j(M) \subset I\!\!R^n$. The special quality we will impose on Φ is inherited from its virtual work (cf. Hellinger [19]), the one-form $A : O \times C^\infty(M, I\!\!R^n) \longrightarrow I\!\!R$ given for all $j \in O$ by

$$A(j)(h) = \int_M < \Phi(j), h > \mu(j) \qquad \forall\, h \in C^\infty(M, I\!\!R^n). \tag{3.1.13}$$

The force density map $\Phi : O \longrightarrow I\!\!R^n$ is such that

$$\Phi(j+z) = \Phi(j) \qquad \forall\, j \in O \text{ and } \forall\, z \quad \text{near} \quad 0 \in I\!\!R^n \tag{3.1.14}$$

and

$$\int_M \Phi(j)\mu(j) = 0 \qquad \forall\, j \in O \tag{3.1.15}$$

are satisfied. (3.1.15), however, is the integrability condition for the equation

$$\Delta(j)\mathcal{H}(j) = \Phi(j) \qquad \forall\, j \in O \tag{3.1.16}$$

with $\mathcal{H} \in C^\infty(O, C^\infty(M, I\!R^n))$ determined up to a map in $C^\infty(O, I\!R^n)$. The map $\mathcal{H}$, resulting from (3.1.15), is referred to as a **constitutive map** in these notes. Given $\mathcal{H}$, the force density map Φ is determined and vice versa. We thus reformulate:

An idealized skin with underlying manifold M is given by a mass density $\rho \in C^\infty(O, C^\infty(M, I\!R))$ satisfying the continuity equation (3.1.11) and a smooth constitutive map $\mathcal{H} \in C^\infty(O, C^\infty(M, I\!R^n))$.

In later sections we will base the description of an idealized skin on a reference configuration $j_0 \in O$. To this end we solve the following equation

$$\Delta(j_0)\hat{\mathcal{H}}(j) = det\ f(j) \cdot \Phi(j) \qquad j \in O \tag{3.1.17}$$

for a constitutive map $\hat{\mathcal{H}}$ (now adapted to the reference configuration) and set

$$\hat{\Phi}(j) := det\ f(j) \cdot \Phi(j) \qquad \forall j \in O; \tag{3.1.18}$$

$\hat{\Phi}$ reproduces the virtual work A for all $j \in O$, as seen by

$$A(j)(h) = \mathcal{G}(j_0)(\hat{\Phi}(j), h) = \mathcal{G}(j_0)(\Delta(j_0)\hat{\mathcal{H}}(j), h) \qquad \forall h \in C^\infty(M, I\!R^n). \tag{3.1.19}$$

Here

$$\mathcal{G}(j)(h,k) := \int < h, k > \mu(j) \qquad \forall j \in O \quad \text{and} \quad \forall h, k \in C^\infty(M, I\!R^n).$$

The map $\hat{\mathcal{H}}(j)$ has a Fourier expansion

$$\hat{\mathcal{H}}(j) = \sum \kappa^i(j) \cdot e_i \qquad \forall j \in O \tag{3.1.20}$$

where $e_1, e_2, \cdots \in C^\infty(M, I\!R^n)$ form a complete system of eigen-vectors of $\Delta(j_0)$ with respective non-vanishing eigen-values $\lambda_1 \leq \lambda_2 \leq \cdots$

In appendix one the Dirichlet integral associated with $\Delta(j)$ and the L_2-metric $\mathcal{G}(j)$ is presented and studied in a fashion suitable for the purpose in view.

Remarks:

a) (3.1.15) allows to write

$$\Phi(j) = \delta_j \alpha(j)$$

where $\alpha(j) : TM \longrightarrow I\!R^n$ is a smooth one-form smoothly dependent on j and δ_j denotes the divergence operator associated with the metric $m(j)$. The Hodge decomposition of $\alpha(j)$ yields (cf. Binz [5] and Wenzelburger [25])

$$\alpha(j) = d\mathcal{H}(j) + \alpha_1(j) + \alpha_2(j) \qquad \forall j \in O \tag{3.1.21}$$

where $\alpha_1(j)$ and $\alpha_2(j)$ are some $I\!R^n$-valued one-forms; $\alpha_1(j)$ is coexact, i.e. $\delta_j \alpha_1(j) = 0$ and $\alpha_2(j)$ is harmonic. Hence α and $d\mathcal{H}$ yield the same Φ. However, specifying α to be the constitutive part yields obviously a finer classification of media then the one produced by specifying $\mathcal{H}$ only.

b) The geometric foundation of media with micro structures are studied in Ackermann [1] where configurations are embeddings of a principal bundle into another one. The mechanisms used here are generalized accordingly (cf. Binz & Ackermann [2]).

A word to the type of constitutive laws we use for the continuum here: To base the constitutive properties of a continuum on the notion of virtual work in the sense (3.1.13) is a rather naive approach from the continuum mechanics point of view (cf. Marsden & Hughes [23] and the remarks above). We do so, however, because it is on one hand convenient for discrete media and keeps on the other the formalism simple.

The relation of $\mathcal{H}$ with the first Piola-Kirchhoff stress tensor α is evident by (3.1.21). We refer to Binz [11] for a group theoretic justification for (3.1.15).

3.2 Structural capillarity

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

$$\mathcal{A}(j) := \int_M \mu(j) \qquad \forall j \in O. \tag{3.2.1}$$

The virtual work $A_{\mathcal{A}}$ caused by distorting the area is

$$A_{\mathcal{A}}(j)(h) := a(j) \cdot I\!D\,\mathcal{A}(j)(h) \qquad \forall j \in O \quad \text{and} \quad \forall h \in C^\infty(M, I\!R^n) \tag{3.2.2}$$

where $a \in C^\infty(O, I\!R)$ is called the **structural capillarity.** The force density of any $j \in O$ caused by distorting the area is $a(j) \cdot \Delta(j)j$. The map $\Delta(j)j$, pointwise normal to $TjTM$ with respect to $<,>$, is called the **mean curvature** tensor (cf. Lawson [22]). It is the $\mathcal{G}(j)$−gradient of $\mathcal{A}$ at j.

It is easily verified that any $\mathcal{H} \in C^\infty(O, C^\infty(M, I\!R^n))$ splits into

$$\mathcal{H}(j) = a(j) \cdot j + \mathcal{H}_1(j) \qquad \forall j \in O \tag{3.2.3}$$

where $\mathcal{H}_1(j)$ is not sensitive to area deformations (cf. Binz [5] to [7]), saying that $\Delta(j)j$ is $\mathcal{G}(j)$-orthogonal to $\mathcal{H}_1(j)$ for all $j \in O$. The virtual work A caused by $\mathcal{H}(j)$ in (3.2.3) yields the following equation for a:

$$A(j)(j) = a(j) \cdot dim\,M \cdot \mathcal{A}(j) \qquad \forall j \in O \tag{3.2.4}$$

which in turn determines a directly out of A, a fact which will be used later. Clearly (3.2.4) shows that $a \in C^\infty(O, I\!R)$.

The notion of structural capillarity will be crucial in determining the free energy and the vibrational modes of the continuum (cf. sec. 5 and 6) describing a finite collection of interacting particles. The sort of virtual work given by (3.2.2) justifies partly our non-local approach.

Let us study and illustrate the structural capillarity somewhat closer in case of $dimM = 2$ and $I\!R^n = I\!R^3$. As we will see it is influenced by the Gaussian curvature. To establish this, we consider the **Ricci tensor** $Ric(j)$ of $m(j)$.

Denoting by $W(j)$ the Weingarten map of the smooth embedding j, then the equation of Gauss (cf. Binz et al [15]) yields for any $j \in E(M, \mathbb{R}^3)$ immediately

$$Ric(j)(X,Y) = m(j)\Big((H(j)\cdot W(j) - W^2(j))X, Y\Big) \tag{3.2.5}$$

for all smooth vector field X, Y on M. Here $H(j) := trW(j)$. Let $R(j)$ denote the symmetric operator such that

$$Ric(j)(X,Y) = m(j)\big(R(j), X, Y\big). \tag{3.2.6}$$

$R(j)$, being an intrinsic object of $m(j)$, is expressed by the extrinsic object $W(j)$ as

$$R(j) = H(j)\cdot W(j) - W^2(j). \tag{3.2.7}$$

In particular the **scalar curvature** $\lambda(j)$, being the trace of $R(j)$, is

$$\lambda(j) = H(j)^2 - trW^2(j). \tag{3.2.8}$$

Using the Cayley Hamilton theorem for $W(j)$ we easily derive from (3.2.7)

$$\kappa(j) = \frac{\lambda(j)}{2} \tag{3.2.9}$$

where $\kappa(j) := det\ W(j)$ is the **Gaussian curvature.** (3.2.7) yields thus

$$R(j) = \frac{\lambda(j)}{2}\cdot id,$$

a well known fact.

Clearly $\frac{\lambda(j)}{2}\cdot dj$ is in general not a differential. It is easy to see (cf. Binz [7]) that $\frac{\lambda(j)}{2}\cdot dj$ is a differential iff $\lambda(j)$ is a constant map on M. Let us call the **exact part** of $djR(j)$ by $dr(j)$; it is obviously determined by

$$\Delta(j)r = \delta_j(\frac{\lambda}{2}\cdot dj) = -grad_{m(j)}\frac{\lambda}{2} + \frac{\lambda}{2}\cdot\Delta(j)j.$$

To establish the influence of the curvature to the structural capillarity, we have to determine the component of $djR(j)$ along dj formed with respect to L_2-metric $\mathcal{G}(j)$ on the Fréchet space of all $\mathbb{R}^3$-valued one-forms of M (cf. appendix one for $\mathcal{G}(j)$). This is to say we split $\frac{\lambda}{2}\cdot dj$ into

$$\frac{\lambda(j)}{2}\cdot dj = K(j)\cdot dj + \gamma_r(j) \qquad \forall j \in O \tag{3.2.10}$$

with $K(j) \in \mathbb{R}$ and $\gamma_r(j)$ a smooth $\mathbb{R}^3$-valued one-form satisfying $\mathcal{G}(j)(\gamma_r(j), dj) = 0$ or reformulated, for which $\mathcal{G}(j)(\delta_j\gamma_r(j), j) = 0$. Hence

$$\mathcal{G}(j)(\frac{\lambda(j)}{2}dj, dj) = \int_M \frac{\lambda(j)}{2}\cdot dj \bullet_j dj\mu(j) = K(j)\cdot\int_M dj \bullet_j dj\ \mu(j) \tag{3.2.11}$$

has to hold for each $j \in E(M, \mathbb{R}^3)$. We refer to appendix one for $\bullet_j$. Obviously we have $\int_M \frac{\lambda(j)}{2} \cdot 2\mu(j) = 2 \cdot K(j) \cdot \mathcal{A}(j)$ with $\mathcal{A}(j)$ being the area of $j(M)$. By the theorem of Gauss-Bonnet we conclude

$$\frac{1}{4\pi} \cdot \boldsymbol{X} = 2 \cdot K(j) \cdot \mathcal{A}(j) \quad \forall j \in E(M, \mathbb{R}^3) \tag{3.2.12}$$

with $\boldsymbol{X}$ the **Euler-characteristic** of M. (3.2.12) determines the map $K : E(M, \mathbb{R}^3) \longrightarrow \mathbb{R}$ and hence yields the following:

Lemma 3.2.1 $K(j) = \frac{1}{8\pi \cdot \mathcal{A}(j)} \cdot \boldsymbol{X}$ *or* $\mathcal{A}(j) = \frac{\boldsymbol{X}}{8\pi \cdot K(j)}$ $\forall j \in E(M, \mathbb{R}^3)$. *Thus K is not constant, in general. The density of $K(j)$ on M is $\frac{\lambda(j)}{2 \cdot \mathcal{A}(j)}$.*

Using (3.2.1) the following is immediate as well:

Lemma 3.2.2 *The one-form $K \cdot \mathbb{D}\mathcal{A}$ is exact on all of $E(M, \mathbb{R}^3)$, in fact*

$$K \cdot \mathbb{D}\mathcal{A} = \frac{\boldsymbol{X}}{8\pi} \cdot \mathbb{D}\ln\mathcal{A}. \tag{3.2.13}$$

Hence $K(j) = 0$ if $\boldsymbol{X} = 0$, since $\mathbb{D}\mathcal{A}(j) \neq 0$ for all $j \in E(M, \mathbb{R}^3)$.

Given a constitutive map $\mathcal{H}$, we split $d\mathcal{H}$ at $j \in E(M, \mathbb{R}^3)$ with respect to $\mathcal{g}(j)$ into a component along $d\boldsymbol{r}$ and a component dH_2 which is $\mathcal{g}(j)$-perpendicular to it, yielding

$$d\mathcal{H}(j) = a_{\boldsymbol{r}}(j) \cdot d\boldsymbol{r} + d\mathcal{H}_2(j) \tag{3.2.14}$$

with

$$a_{\boldsymbol{r}} : E(M, \mathbb{R}^3) \longrightarrow \mathbb{R}$$

being smooth. $d\boldsymbol{r}(j)$ depends on dj rather than j itself and so do a, $a_{\boldsymbol{r}}$ and $\mathcal{H}_2$. The map $a_{\boldsymbol{r}} \cdot d\boldsymbol{r}$ is the **curvature sensitive** part of $d\mathcal{H}$.

The influence of the curvature to the structural capillarity (cf. 3.2.4) relies on equation (3.2.14) and (3.2.10). It reads as

$$a(j) = a_{\boldsymbol{r}}(j) \cdot K(j) + a_1(j) \qquad \forall j \in O \tag{3.2.15}$$

for some smooth map $a_1 : E(M, \mathbb{R}^3) \longrightarrow \mathbb{R}^3$. Here $a_1(j) \cdot dj$ is the $\mathcal{g}(j)$-component of $d\mathcal{H}_2(j)$ along dj. The part of the structural capillarity affected by the curvature is thus $a_{\boldsymbol{r}} \cdot K$. The equation above reformulates hence as

$$a(j) = a_{\boldsymbol{r}}(j) \cdot \frac{\boldsymbol{X}(j)}{8\pi \cdot \mathcal{A}(j)} + a_1(j) \qquad \forall j \in O. \tag{3.2.16}$$

The structural capillarity is not affected by the curvature for any medium under consideration if M is a torus, since $K = 0$ for this kind of a surface.

The following is a direct consequence of (3.2.16) and (3.2.3):

Proposition 3.2.3 *If $\Phi(j) = 0$ then $a(j) = 0$ and hence*

$$a_{\boldsymbol{r}}(j) \cdot K(j) = -a_1(j).$$

4 The discrete medium modeled as a continuum

To describe the discrete medium as an idealized skin, consisting of a large number of interacting material particles, we have to assume that $P \subset M$ and need to construct out of the given data ρ_P and Φ_P a mass density ρ and a constitutive map $\mathcal{H}$ on an open set $O \subset E(M, I\!R^n)$, respectively. To do so, we fix $j_o \in O$. Let $r : C^\infty(M, I\!R^n) \longrightarrow \mathcal{F}(P, I\!R^n)$ denote the restriction map. Clearly $r^{-1}O_P \subset E(M, I\!R^n)$ for $O_P \subset E(P, I\!R^n)$ small enough. The following lemma shows that the most obvious to do to construct A out of A_P, namely to set $A := r^* A_P$, is useless for our purpose:

Lemma 4.0.4 *$r^* A_P$ admits no force density with respect to the metric $\mathcal{G}$ nor $\mathcal{G}(j_0)$, in general.*

Proof:
Let us assume that for any A_P the following holds:

$$r^* A_P(j)(h) = \int_M < \Phi(j), h > \mu(j) \qquad \forall\, j \in O \text{ and } \forall\, h \in C^\infty(M, I\!R^n)$$

for some Φ. Since $A_P(j_P)(h_P) = \sum_{q \in P} < \Phi_P(j_P(q)), h_P(q) >$ for any $j_P \in O_P$ and $h_P \in \mathcal{F}(P, I\!R^n)$ we conclude that

$$\Phi_P(j_P) = \sum_{i, q \in P} \xi^i_P(j_P) \cdot \Phi^q_i$$

Here Φ^q_i is defined by

$$\Phi^q_i(q') := \begin{cases} z_i & q = q' \\ 0 & q \neq q' \end{cases}$$

for any fixed $q \in P$ and a given basis $z_i, \cdots, z_n$ of $I\!R^n$. Setting

$$A^q_P(j_P)(h_P) :=< \Phi^q_i, h_P > \qquad \forall\, j_P \in O_P \text{ and } \forall\, h \in \mathcal{F}(P, I\!R^n)$$

yields

$$A^q_P\big(r(j)\big)\big(r(h)\big) =< \Phi^q_i, r(h) >$$

for any $j \in O$ and any $h \in C^\infty(M, I\!R^n)$ and therefore

$$r^* A^q_P(j)(h) = \int_M < \Phi(j), h > \mu(j) \quad j \in O.$$

However, this means that the point evaluation $r^* A^q_P$ admits a density which is not true. The result of course holds accordingly if $\mathcal{G}$ is replaced by $\mathcal{G}(j_0)$.

The constitutive laws we have chosen to characterize idealized skins are based on force densities, however. In these notes we prefer the following way out of this dilemma:

The requirement of the existence of a force density $\hat{\Phi}$ (cf.(3.1.18) and (3.1.19)) implies the existence of a $\mathcal{G}(j_0)$-orthogonal complement to $ker\ r \subset C^\infty(M, I\!R^n)$. This , as we saw, does not exist, in general. We therefore look for a complement to $ker\,r$ not $\mathcal{G}(j_0)$-orthogonal but isomorphic to $\mathcal{F}(P, I\!R^n)$ via the restriction map r. This means that we will choose a flat connection on the trivial vector bundle $O_P \times ker\,r$ of O_P. This will imply, however, that distortions in $ker\,r$ may cause non-vanishing virtual work, or expressed in an other fashion: The choice of *a* connection is in effect a choice of an approximation of $r^* A_P$.

4.1 The construction of a complement to *ker r*

Let $O \subset r^{-1}O_P$ with $j_0 \in O$. We require for each $j \in O$ that the maps $\hat{\Phi}(j)$ and $\hat{\mathcal{H}}(j)$ in (3.1.18) and (3.1.17) are in the complement to construct. Hence the finite dimensional complement has to be invariant under $\Delta(j_0)$, and thus has to be generated by eigen-vectors of $\Delta(j_0)$. But there is still a choice involved. Here is how we proceed: Let $z_1, ..., z_n \in I\!R^n$ be a $<,>$-orthonormal basis. We choose $\mathcal{G}(j_0)$-orthonormed eigen-vectors $e_{i_1}, ..., e_{i_b}$ in $C^\infty(M, I\!R^n)$ of $\Delta(j_0)$ (cf. sec. 3.1) with respective eigen-values $0 < \lambda_{i_1} \leq ... \leq \lambda_{i_b}$ such that $z_1, ..., z_n, r(e_{i_1}), ..., r(e_{i_b})$ forms a basis of $\mathcal{F}(P, I\!R^n)$ and that $\sum_{s=1}^{b} \lambda_{i_s}$ is as small as possible. The complement $\mathcal{F}^\infty(M, I\!R^n) \subset C^\infty(M, I\!R^n)$ to ker r^*, we look for, is the span of $z_1, ..., z_n, e_{i_1}, ..., e_{i_b}$. For simplicity we write just e_s instead of e_{i_s} for $s = 1, ..., b$. Hence we conclude

$$C^\infty(M, I\!R^n) = \ker r \oplus \mathcal{F}^\infty(M, I\!R^n) \cong ker\,r \oplus \mathcal{F}(P, I\!R^n). \tag{4.1.1}$$

The flat connection, mentioned in the previous section, is given by $\mathcal{F}^\infty(M, I\!R^n)$ as horizontal subspace everywhere. Obviously the $\mathcal{G}(j_0)$-orthogonal complement $\mathcal{F}^\infty(M, I\!R^n)^\perp \subset C^\infty(M, I\!R^n)$ to $\mathcal{F}^\infty(M, I\!R^n)$ is not identical with $ker\,r$, but

$$C^\infty(M, I\!R^n) = \mathcal{F}^\infty(M, I\!R^n) \oplus \mathcal{F}^\infty(M, I\!R^n)^\perp \tag{4.1.2}$$

holds certainly true as well. Constructing $\mathcal{F}^\infty(M, I\!R)$ just accordingly, yields the $\mathcal{G}(j_0)$-orthogonal splitting

$$C^\infty(M, I\!R) = \mathcal{F}^\infty(M, I\!R) \oplus \mathcal{F}^\infty(M, I\!R)^\perp. \tag{4.1.3}$$

Let $j_P^0 := r(j_0)$. We require $O \subset r^{-1}O_P$ to be of the form

$$O - j_0 = O_{kerr} \oplus \mathcal{W}' \tag{4.1.4}$$

with $O_{ker} \subset ker\,r$ and $\mathcal{W}' \subset \mathcal{F}^\infty(M, I\!R^n)$ being neighbourhoods of zero, respectively. Hence O slices into

$$O = \bigcup_{j \in E_o} \mathcal{W}(j) \qquad \text{with} \qquad E_0 := r^{-1}(j_P^0) \cap O \tag{4.1.5}$$

where $\mathcal{W}(j) = j + \mathcal{W}'$ for all $j \in r^{-1}(j_P^0) \cap O$. From now on O is as in (4.1.5).

4.2 The constructions of ρ and A

Let $j_0 \in O$ and $j_P^0 = r(j_0)$ again. The discrete mass density ρ_P (cf. sec. two) yields by lemma A2.1 some positive map $\rho_0 \in \mathcal{F}^\infty(M, I\!R)$ satisfying

$$\int_M \rho_0 \, \mu(j_0) = \sum_q \rho_P(q) = m \tag{4.2.1}$$

where m is the total mass. Let $f(j)$ as in (3.1.10) with $f(j_0) = id$. Then

$$\rho(j) := \rho_0 \cdot det\ f^{-1}(j) \qquad \forall j \in O$$

determines a mass density on M in the sense of (3.1.12). Clearly $\rho(j_0) = \rho_0$ and $\rho(j) \notin \mathcal{F}^\infty(M, I\!R)$, in general.

The virtual work A on O is constructed out of A_P as follows : Let $r_\infty := r|\mathcal{F}^\infty(M, I\!R^n)$ and accordingly $r_\infty := r|\mathcal{W}(j)$ for all $j \in r^{-1}(j_P^0) \cap O$. We set on each slice $\mathcal{W}(j)$

$$A := r_\infty^* A_P \qquad \text{and} \qquad A \mid O \times \mathcal{F}^\infty(M, I\!R^n)^\perp = 0. \tag{4.2.2}$$

Clearly A admits a force density on each slice and A is constant along $r^{-1}(j_P^0) \cap O$. Given $j \in O$ and $k \in kerr$ then in general $A(j)(k) \neq 0$. However,if $A_P(r(j_0)) = 0$ then indeed $A(j)(h) = 0$ for all $h \in C^\infty(M, I\!R^n)$ and for all $j \in r^{-1}(j_P^0) \cap O$, as it is easy to see.

A word to the structural capillarity: Due to (3.2.4) the structural capillarity exists for $r^* A_P$ but is of course not identical to the one determined by A in (4.2.2). To describe the difference we split $j \in O$ into $j = j_\infty + j_\perp$ with $j_\infty \in \mathcal{F}^\infty(M, I\!R^n)$ and $j_\perp \in \mathcal{F}^\infty(M, I\!R^n)^\perp$. Since $A(j)(j) = A(j)(j_\infty)$ it is clear that the structural capillarities mentioned above may differ.

The constitutive map $\hat{\mathcal{H}}$ of the virtual work A is given for each $j \in O$ by $\hat{\mathcal{H}}(j) = \sum_{i=1}^b \kappa^i(j) \cdot e_i$ where $\kappa^i(j) = \lambda_i^{-1} \cdot A_P\big(r(j)\big)\big(r(e_i)\big)$ for any $i = 1, \cdots, b$.

Due to (3.2.4), the structural capillarity a of the medium at hand is obviously determined by

$$a(j) = \sum_{i=1}^b \kappa^i(j) \cdot j^i \cdot \lambda^i \qquad \forall j \in O$$

where $j = \sum_{i=1}^b j^i \cdot e_i$ and λ^i is the i^{th} eigen-value of $\Delta(j_0)$ in the enumeration chosen above.

4.3 The concept of free energy of the continuum

Let $\bar{F}_P$ on $\bar{O}_P$ be the free energy of A_P and $j_P^0 \in O_P$ be an equilibrium configuration. Here $\bar{O}_P$ is as in sec. 2.1. We regard $I\!D\,\bar{F}_P$ as a virtual work by itself and hence lift $I\!D\,\bar{F}_P$ by (4.2.2), to a one-form $A_{\bar{F}_P}$ on O. i.e. we set slicewise $A_{\bar{F}_P} := r_\infty^* I\!D\,\bar{F}_P$ and $A_{\bar{F}_P}|O \times \mathcal{F}^\infty(M, I\!R^n)^\perp = 0$. Hence $A_{\bar{F}_P}|r^{-1}(j_P^0) \cap O = 0$.

Clearly there is some $\bar{F} \in C^\infty(O, I\!R^+)$ such that $I\!D\bar{F} = A_{\bar{F}_P}$ near any $j \in O$. Moreover

$$\bar{F}(j) = \bar{F}_P(r(j)) + \text{const.} \quad \forall j \in \mathcal{W}(j') \quad \text{with} \quad j' \in r^{-1}(j_P^0) \cap O;$$

setting const.=0 yields

$$\bar{F} = r_\infty^* \bar{F}_P \quad \text{on} \quad \mathcal{W}(j'). \tag{4.3.1}$$

The gradient $Grad_{\mathcal{G}(j')}\bar{F}$ formed with respect to $\mathcal{G}(j')$ satisfies

$$r_\infty(Grad_{\mathcal{G}(j')}\bar{F}(j')) = \varphi^P(j') \cdot Grad_{\mathcal{G}_P}\bar{F}_P(j') \qquad \forall j' \in r^{-1}(j_P^0) \cap O \tag{4.3.2}$$

for some $\varphi^P(j') \in \mathcal{F}(P, I\!R^+)$ as seen by lemma A2.1 in the second appendix. Clearly A splits into

$$A = I\!D\bar{F} + \Psi \qquad \text{near any} \quad j' \in r^{-1}(j') \cap O \tag{4.3.3}$$

with $\Psi := A - I\!D\bar{F}$ and is the Neumann splitting formed slicewise with respect to the scalar product $r_\infty^*\mathcal{G}_P$. In determining the divergence $\mathbf{div}_{\mathcal{W}(j')}A$ on each slice $\mathcal{W}(j')$, formed with respect to $r_\infty^*\mathcal{G}_P$, the structural capillarity a of A in (3.2.4) plays a crucial role. To see this we let $K_s \subset \mathcal{W}(j')$ be a closed ball of radius s centered about $j \in \mathcal{W}(j')$. Then the following holds true:

Theorem 4.3.1 *For $j \in \mathcal{W}(j')$*

$$\begin{aligned} \Delta_{\mathcal{W}(j')}\bar{F}(j) = & \quad \mathbf{div}_{\mathcal{W}(j')}A(j) = \\ - & \quad dim M \cdot \lim_{s\to 0} \frac{1}{s \cdot vol\, K_s} \cdot \int_{\partial K_s} (a \cdot \mathcal{A} - a \cdot A(j))\mu_{\partial K_s} \\ + & \quad tr_{r^*\mathcal{G}_P} I\!D^2 A(j)(\cdots,\cdots)(j) \end{aligned} \tag{4.3.4}$$

with $tr_{r^*\mathcal{G}_P}$ being the trace formed with respect to $r_\infty^*\mathcal{G}_P$. The equation (4.3.4) is reformulated as

$$\Delta_{\mathcal{W}(j')}\bar{F}(j) = \frac{1}{2} \cdot \Delta_{\mathcal{W}(j')}(a \cdot \mathcal{A}(j)) + \frac{1}{2} \cdot tr_{r_\infty^*\mathcal{G}_P} I\!D^2 A(j)(\cdots,\cdots)(j); \tag{4.3.5}$$

if $I\!D^2A(j) = 0$, in particular, then

$$\mathbf{div}_{\mathcal{W}(j')} I\!D A(j)(h) = \frac{1}{2} \cdot \Delta_{\mathcal{W}(j')}(a \cdot \mathcal{A})(j + h)$$

for any $h \in \mathcal{F}^\infty(M, I\!R^n)$ with $j_0 + h \in \mathcal{W}(j')$. Therefore,

$$\bar{F} = \frac{1}{2} \cdot a \cdot \mathcal{A} - \bar{F}_2 + \text{const.} \quad \text{on } W(j') \tag{4.3.6}$$

where $\Delta_{\mathcal{W}(j')}\bar{F}_2(j) = -\frac{1}{2} \cdot tr_{r_\infty^*\mathcal{G}_P} I\!D^2 A(j)$. If $A(j+h)$ is linear in h then obviously

$$\bar{F} = \frac{1}{2} \cdot a \cdot \mathcal{A} + \text{const.} \qquad \text{on } \mathcal{W}^\infty(j'). \tag{4.3.7}$$

Proof:
Let $j \in \mathcal{W}(j')$ for $j' \in r_\infty^{-1}(j_p^0) \cap O$ be fixed. Moreover let K_s be a closed ball in $\mathcal{W}(j)$ centered about j. Its radius is denoted by s. Then

$$\operatorname{div} A(j) = - \lim_{s \longrightarrow 0} \frac{1}{vol\ K_s} \cdot \int_{\partial K_s} A(...)(n(...)) \mu_{\partial K_s}. \tag{4.3.8}$$

Here $\Delta_{\mathcal{W}(j')}$ is the Laplacian on $\mathcal{W}(j')$. The integrand takes the value $A(j_\partial)(n(j_\partial))$ for any $j_\partial \in \partial K_s$. Any $j_\partial \in \partial K_s$ has the form

$$j_\partial = j + h \qquad \text{for some} \qquad h \in \mathcal{F}^\infty(P, I\!R^n). \tag{4.3.9}$$

Hence

$$A(j_\partial)(n(j_\partial)) = \frac{1}{s} \cdot A(j_\partial)(h) \tag{4.3.10}$$

and therefore for any $j_\partial \in K_s$

$$\begin{aligned} A(j_\partial)(j) = A(j+h)(j) = & \quad A(j)(j) + I\!D\, A(j)(h)(j) \\ + & \quad \tfrac{1}{2} \cdot I\!D^2 A(j)(h,h)(j) + \text{higher order terms.} \end{aligned} \tag{4.3.11}$$

Due to (3.2.4) and (4.3.10) equation (4.3.11) implies

$$\begin{aligned} A(j_\partial)(n(j_\partial)) = & \ \tfrac{1}{s} \cdot \big(A(j_\partial)(j_\partial) - A(j_\partial)(j)\big) = dim M \cdot \tfrac{1}{s} \cdot \big((a \cdot \mathcal{A})(j_\partial) - (a \cdot \mathcal{A})(j)\big) \\ - & \quad \tfrac{1}{s} \cdot I\!D\, A(j)(h)(j) - \tfrac{1}{2 \cdot s} \cdot I\!D^2 A(j)(h,h)(j) \\ - & \quad \text{higher ord terms in h.} \end{aligned} \tag{4.3.12}$$

We reformulate the terms on the right hand side in several steps.
Step 1: To treat

$$lim_{s \to \infty} \frac{1}{vol K_s} \int_{\partial K_s} I\!D\, A(j)(n(\cdots))(j) \mu_{\partial K_s}$$

we consider the linear map $I\!D\, A(j)(\cdots)(j) : \mathcal{F}^\infty(M, I\!R^n) \longrightarrow I\!R$. Since

$$\operatorname{div}\big(I\!D\, A(j)(\cdots)\big)(j) = - \lim_{s \to \infty} \frac{1}{vol K_s} \int_{\partial K_s} I\!D\, A(j)(n(\cdots))(j) \mu_{\partial K_s}$$

and $\operatorname{div}\big(I\!D\, A(j)(\cdots)\big)(j) = 0$ (since $I\!D\, A(j)(\cdots)(j)$ does not vary on O). Thus the linear term $\frac{1}{s} \cdot I\!D\, A(j)(\cdots)(j)$ does not contribute to $\operatorname{div} A(j)$.
Step 2: To study the influence of the term involving the second derivative of A at j in (4.3.11) we set

$$I\!D^2 A(j)(h,h)(j) = r_\infty^* \mathcal{G}_P(Sh, h)$$

with $S \in End\mathcal{F}^\infty(M, I\!R^n)$ and consider the one-form

$$\gamma : TO \longrightarrow I\!R$$

given by

$$\gamma(j'')(k) := r^*_\infty \mathcal{G}_P(S(j)j'', k) \qquad \forall j'' \in O \text{ and } \forall k \in \mathcal{F}^\infty(M, I\!R^n)$$

which is linear in j''. Setting $h(j_\partial) = j_\partial - j$ we find

$$\gamma(j_\partial)(n(j_\partial)) = \gamma(j)(n(j_\partial)) + I\!D^2 A(j)(h(j_\partial), n(j_\partial)).$$

By the result of step one, we therefore observe that the quadratic term in (4.3.12) contributes to (4.3.8) by the amount

$$\begin{aligned} lim_{s\to 0} \frac{1}{volK_s} \cdot \int_{\partial K_s} I\!D^2 A(j)(h(\cdots), n(\cdots))\mu_{\partial K_s} \\ = \quad lim_{r\to 0} \tfrac{1}{volK_s} \int_{\partial K_s} \cdot\gamma(\cdots)(n(\cdots))\mu_{\partial K_s} \\ = \quad -\mathrm{div}\gamma(j) = trS(j). \end{aligned} \tag{4.3.13}$$

The higher order terms on the right hand side of (4.3.12) do not contribute to $\mathrm{div}A$. Hence (4.3.4) is established. To verify (4.3.5) we observe that

$$\begin{aligned} \frac{1}{s}((a\cdot\mathcal{A})(j_\partial) - (a\cdot\mathcal{A})(j)) = \quad & \tfrac{1}{s}\cdot I\!D(a\cdot\mathcal{A})(j)(h) + \tfrac{1}{2\cdot s}\cdot I\!D^2(a\cdot\mathcal{A})(j)(h,h) \\ + \quad & \text{terms of higher order.} \end{aligned} \tag{4.3.14}$$

Using step one we hence verify that

$$\frac{1}{s}\cdot\int_{\partial K_s}(a\cdot\mathcal{A})(\cdots) - (a\cdot\mathcal{A})(j)\mu_{\partial K_s} = \frac{1}{2}\cdot\int_{\partial K_s} I\!D^2(a\cdot\mathcal{A})(j)(h(\cdots), n(\cdots))\mu_{\partial K_s}.$$

Applying the method in step two hence yields (4.3.5). This completes the proof.

Comparing (4.3.6) with (3.2.12) and (3.2.15) we observe the following:

Theorem 4.3.2 *$\bar{F}$ splits in case of* $\dim M = 2$ *into*

$$\bar{F} = \frac{X}{16\pi}\cdot a_r + \frac{a_1}{2}\cdot\mathcal{A} - \bar{F}_2 + \text{ const.} \tag{4.3.15}$$

with a_r and a_1 as in (3.2.15). The influence of the topology of M on $\bar{F}(j)$ is given by the map $\bar{F}_{top} : \mathcal{W}(j)' \longrightarrow I\!R$ defined by

$$\bar{F}_{top} := \frac{X}{16\pi}\cdot a_r + \text{ const..}$$

From (3.2.4) we immediately deduce that the structural capillarity a is determined by discrete data and $dim\, M$ only: a, as given by (3.2.4), can be determined by the differential of the free energy $\bar{F}$ of A as seen from the observation

$$I\!D\, \bar{F}(j)(j) = I\!D\, \bar{F}(j)(j^\infty) = a(j) \cdot dim\, M \cdot \mathcal{A}(j) \qquad \forall\, j \in \mathcal{W}(j'). \qquad (4.3.16)$$

To verify this we assign to each $j \in \mathcal{W}(j')$ the value $\frac{1}{2} \cdot r_\infty^* \mathcal{G}_P(r(j), r(j))$ and observe that for this map the $r_\infty^* \mathcal{G}_P$-gradient at j is j^∞, therefore (4.3.3) implies (4.3.16). Here j^∞ is the component of j in $\mathcal{F}^\infty(M, I\!R^n)$. We thus find due to (4.3.16), (4.3.1), (4.3.2) and (A2.1) the following:

Proposition 4.3.3 *For any $j' \in r^{-1}(j_P^0) \cap O$, each $j \in \mathcal{W}(j')$ and some $\varphi^P(j) \in C^\infty(O, \mathcal{F}(P, I\!R))$ the structural capillarity a of A is given by*

$$a(j) \cdot dim\, M \cdot \sum_{q \in P} \varphi^P(j)(q) = I\!D\, \bar{F}_P(r(j))(r_\infty(j^\infty)). \qquad (4.3.17)$$

If $r(j)$ is an equilibrium configuration then $a(j) = 0$.

In case of an (n.n.i.)-medium equations (1.2.9) and (4.3.16) together with (4.3.17) yield on the other hand:

Proposition 4.3.4 *In case of an (n.n.i.)-interaction scheme the structural capillarity is given by*

$$a(j) = dim\, M \cdot \sum_{q \in P} \varphi^P(j)(q) = \mathcal{G}_{L_1}\left(\psi(j_P) \cdot \partial^1 j_P, \partial^1 j_P\right) \quad .$$

for any $j \in \mathcal{W}(j')$.

5 On the notion of equilibrium configuration

Defining a (strong) equilibrium configuration $j' \in O$ by $A(j') = 0$ and $I\!D\, \bar{F}(j') = 0$ we immediately deduce that $j' \in O$ is an equilibrium configuration provided $r(j') \in O_P$ is one. An equilibrium configuration j' is trivial if $\bar{F}$ is constant in a neighbourhood of $j' \in \mathcal{W}(j')$. Let $j_0 \in r^{-1}(j_P^0) \cap O$ for $j_P^0 \in O_P$.

5.1 On the existence of an equilibrium configuration for a skin

At first we derive a necessary condition for the existence of a non-trivial equilibrium configuration. Differentiating both sides of (4.3.17) and representing $I\!D^2 \bar{F}_P(j')$ by $\mathcal{G}_P$ via $I\!F_P(j') \in End\, \mathcal{F}(P, I\!R^n)$, say, then by (4.3.2), proposition 4.3.3 and lemma A2.1 the following holds true:

Proposition 5.1.1 *Let $j_0 \in O$ be an equilibrium configuration*

$$r_\infty(Grad_{\mathcal{G}(j_0)} a)(j_P^0) = \frac{\varphi^P(j_0)}{dim\, M \cdot \sum_{q \in P} \varphi^P(j_0)(q)} \cdot I\!F_P(j_P^0) j_P^0 \qquad (5.1.1)$$

where $Grad_{\mathcal{G}(j_0)} a$ is formed with respect to $\mathcal{G}(j_0)$.

To illustrate the notion of an equilibrium configuration in a simple example we assume that j_0 is an equilibrium configuration for which

$$\bar{F}(j_0 + h) = \bar{F}(j_0) + \frac{1}{2} I\!D^2 \bar{F}(j_0)(h,h) \qquad \forall\, h \in \mathcal{F}^\infty(M, I\!R^n)$$

holds. Then $I\!D\,\bar{F}(j_0 + h)$ is linear in h and by theorem (4.3.1) the free energy $\bar{F}$ is of the form

$$\bar{F} = \frac{1}{2} \cdot a \cdot \mathcal{A} + \text{const. on } \mathcal{W}(j_0).$$

Since $a(j_0) = 0$ we deduce immediately $I\!D\,a(j_0)|\mathcal{F}^\infty(M, I\!R^n) = 0$. Hence proposition 5.1.1 shows $I\!D^2\bar{F}(j_0) = 0$, implying that $\bar{F}$ is constant. We thus have that A has to be non-linear to admit a non-trivial equilibrium configuration :

Theorem 5.1.2 *A linear constitutive law only admits an equilibrium configuration j_0 if $\mathbf{div}_{\mathcal{W}(j_0)} A = 0$ meaning that $\bar{F}$ is constant on $\mathcal{W}(j_0)$. If hence j_0 is an equilibrium configuration with $\bar{F}$ not constant on $\mathcal{W}(j_0)$, the virtual work A has be non-linear at j_0, implying $I\!D\,a(j_0)|\mathcal{F}^\infty(M, I\!R^n) \neq 0$.*

5.2 Statistics and geometry

To link $\bar{F}$ of the previous section with a statistical set up let us choose a smooth map $F : O \longrightarrow I\!R$ such that

$$\bar{F}(j) = \int_M F(j)\mu(j). \tag{5.2.1}$$

Since by assumption $\bar{F}(j) \neq 0$ (cf. sec. 4.3) we have

$$1 = \int_M \frac{F(j)}{\bar{F}(j)} \cdot det f(j)\mu(j_0). \tag{5.2.2}$$

The solution to the associated continuity equation (cf. 3.1.12) is

$$F = \bar{F} \cdot \frac{F(j_0)}{\bar{F}(j_0)} \cdot det f^{-1} \qquad \text{on O} \tag{5.2.3}$$

where f is determined by $m(j)(\cdots,\cdots) = m(j_0)(f^2(j)\cdots,\cdots)$ as in (3.1.10) or appendix one. The above equation has no discrete analogon. It relates the free energy $\bar{F}$ via a density with the Riemannian metric. (5.2.3) shows moreover

$$\frac{F}{\bar{F}}(j_0 + h) = \frac{F(j_0)}{\bar{F}(j_0)} \cdot det f^{-1}(j + h) \qquad \forall\, h \in \mathcal{F}^\infty(M, I\!R^n). \tag{5.2.4}$$

The influence of the geometry to F is therefore obtained by A1.24:

Proposition 5.2.1 *If (5.2.3) holds, then the density F on $\mathcal{W}(j_0)$ of $\bar{F}$ is given by*

$$F(j_0+h) = \frac{F(j_0)}{\bar{F}(j_0)} \cdot \bar{F}(j_0+h) \cdot e^{-\int_0^1 trB_h(j_0+\tau\cdot h)d\tau} \quad \forall\, h \in \mathcal{W}(j_0) - j_0 \quad (5.2.5)$$

with $dh = c_h(j)\cdot dj + dj\big(C_h(j) + B_h(j)\big)$ for $j \in O$ (cf. appendix one).

An immediate consequence of (5.2.1) is the following: Due to the fact that $trB_h \neq 0$ for $h \in \mathcal{F}^\infty(M, \mathbb{R}^n)$ in general, we deduce:

Lemma 5.2.2 *Let (5.2.3) hold true. If $I\!D\,\bar{F}(j_0) = 0$ and $trB_h \neq 0$ then*

$$I\!D\,F(j_0)(h) = -F(j_0)\cdot trB_h(j_0) \qquad \forall h \in \mathcal{F}^\infty(M, \mathbb{R}^n); \qquad (5.2.6)$$

if hence both $I\!D\,\bar{F}(j_0) = 0$ and $I\!D\,F(j_0) = 0$ then $F(j_0) = 0$.

In contrast to the discrete case expressed in lemma 2.1.2, we therefore can not require that an equilibrium configuration $j_0 \in O \cap r_\infty^{-1}(j_P^0)$ has to satisfy both $I\!D\,\bar{F}(j_0) = 0$ and $I\!D\,F(j_0) = 0$. Hence, $F(j_0) \neq 0$ for a non-trivial equilibrium configuration j_0, if 5.2.3 should hold true (compare with F_P in sec. 2.1).

5.3 A Gibbs state associated with F

Let $F > 0$. Setting for each $j \in O$

$$\rho_{Gibbs}(j) := \frac{F(j)}{\bar{F}(j)}$$

yields

$$I(j) := \bar{F} - \beta^{-1}(j)\cdot ln\rho(j)$$

as an observable and hence

$$\rho_{Gibbs}(j) = \frac{e^{-\beta(j)\cdot I(j)}}{e^{-\beta\bar{F}(j)}} = \frac{e^{-\beta(j)\cdot I(j)}}{\int_M e^{-\beta(j)\cdot I(j)\mu(j)}}.$$

Using (5.2.6) immediately yields the following:

Lemma 5.3.1 *Let $j_0 + h \in O$ with $h \in \mathcal{F}^\infty(M, \mathbb{R}^n)$. Then (5.2.4) yields*

$$\rho_{Gibbs}(j_0+h) = \frac{F(j_0)}{\bar{F}(j_0)}\cdot e^{-\int_0^1 trB_h(j_0+\tau\cdot h)d\tau}.$$

6 The modes of the skin

6.1 The modes of a constitutive law

Let $\hat{\Phi} : O \longrightarrow \mathcal{F}^{\infty}(M, I\!R^n)$ be the force density characterizing the skin as considered in sec. four. $j_0 \in O$ shall be an equilibrium configuration. Then

$$\hat{\Phi}(j_0 + k) = I\!D\,\hat{\Phi}(j_0)(k) + \text{ higher order terms.} \tag{6.1.1}$$

For k with small room $\|k\| := \mathcal{G}(j_0)(k,k)^{\frac{1}{2}}$ we may omit the higher order terms and set

$$\hat{\Phi}(j_0 + k) = I\!D\,\hat{\Phi}(j_0)(k) \qquad k \in \mathcal{F}^{\infty}(M, I\!R^n) \text{ and } \|k\| \text{ small.}$$

The virtual work caused by $\hat{\Phi}$ is hence linear in k and the free energy $\bar{F}$ satisfies by (4.3.7) for all $h \in \mathcal{F}^{\infty}(M, I\!R^n)$ the following:

$$I\!D^2 \bar{F}(j_0)(h,h) = \frac{1}{2} \cdot I\!D^2(a \cdot \mathcal{A})(j_0)(h,h). \tag{6.1.2}$$

The eigen-values of $I\!D^2 \bar{F}(j_0)$ are called the **modes** of the skin. Thus the modes are entirely determined by the structural capillarity a of the medium and the geometrical map $\mathcal{A}$ both defined near j_0.

Expanding the term of the right hand side of (6.1.2) we observe for all $h \in \mathcal{F}^{\infty}(M, I\!R^n)$ the following equation:

$$I\!D^2 \bar{F}(j_0)(h,h) = \frac{1}{2} \cdot \mathcal{A}(j_0) \cdot I\!D^2 a(j_0)(h,h) + I\!D\, a(j_0)(h) \cdot I\!D\,\mathcal{A}(j_0)(h). \tag{6.1.3}$$

If hence $\bar{u}_i$ is the i^{th} eigen-vector of $I\!D^2 \bar{F}(j_0)$ with eigen-value ν_i, then for all $i = 1, \cdots, b$, we easily deduce by (6.1.2) the following:

Proposition 6.1.1 *The modes of the medium are determined by the structural capillarity via the following formula*

$$\nu_i = \frac{1}{2} \cdot \mathcal{A}(j_0) \cdot I\!D^2 a(j_0)(\bar{u}_i, \bar{u}_i) + I\!D\, a(j_0)(\bar{u}_i) \cdot I\!D\,\mathcal{A}(j_0)(\bar{u}_i) \quad i = 1, \cdots, b.$$

In case of $dim M = 2$ the i^{th} eigen-value is affected by the curvature due to (3.2.16), namely by the Euler characteristic in the following manner

Proposition 6.1.2 *For all $i = 1, \cdots, b$ the value of ν_i is*

$$\begin{aligned} \nu_i = &\quad \tfrac{\boldsymbol{X}}{16\pi} \cdot I\!D^2 a_r(j_0)(\bar{u}_i, \bar{u}_i) + \tfrac{1}{2} \cdot \mathcal{A}(j_0) \cdot I\!D^2 a_1(j_0)(\bar{u}_i, \bar{u}_i) \\ + &\quad \left(\tfrac{\boldsymbol{X}}{8\pi} \cdot I\!D\, a_r(j_0)(u_i) + I\!D\, a_1(j_0)(\bar{u}_i)\right) \cdot I\!D\,\mathcal{A}(j_0)(\bar{u}_i) \end{aligned} \tag{6.1.4}$$

6.2 Fit of first orders and their modes

Let us call an equilibrium configuration j_0 to be a **fit of first order**, if φ^P in (5.1.1) is identically one. A first order fit j_0 satisfies

$$\mathcal{A}(j_0) = \#P$$

by corollary A2.2 in appendix two. If in addition $j_0 = \sum \iota_0^i \cdot \bar{u}_i$, then by (5.1.1)

$$I\!D\, a(j_0)(\bar{u}_i) = \frac{\iota_0^i \cdot \nu_i}{\dim M \cdot \#P} \quad ,$$

saying that ν_i is determined by $I\!D\, a(j_0)(\bar{u}_i)$, if $\iota_0^i \neq 0$. The general formula for ν_i is derived from (6.1.3) and reads for each $i = 1, \cdots, b$

$$\nu_i \cdot \left(1 - \frac{\iota_P^i}{\dim M \cdot \#P} \cdot I\!D\, \mathcal{A}(j_0)(\bar{u}_i)\right) = \frac{\#P}{2} \cdot I\!D^{\,2} a(j_0)(\bar{u}_i, \bar{u}_i).$$

If $\nu_i = 0$ then

$$\iota_0^i = \frac{\dim M \cdot \#P}{I\!D\, \mathcal{A}(j_0)(\bar{u}_i)} = \frac{\dim M}{I\!D\, ln\mathcal{A}(j_0)(\bar{u}_i)}.$$

If $\nu_i \neq 0$ then

$$\iota_0^i = \frac{\dim M \cdot \#P}{\nu_i} \cdot I\!D\, a(j_0)(\bar{u}_i).$$

Since $\bar{F} = r_\infty^* \bar{F}_P$ we conclude by equation (2.1.8)

$$-ln\beta\bar{F} = \#P + \sum_{n=1}^{b} (-1)^n \beta^n \cdot trQ^n.$$

The moments μ_m of ρ_{Gibbs} are related with the partition function Z by

$$\lim_{\beta\to 0} \mu_m = \frac{1}{\#P} \cdot trQ^m = \frac{1}{\#P} \cdot \lim_{\beta\to 0} \frac{\partial^m Z}{\partial \beta^m}.$$

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APPENDIX 1

Here we will present what is called the **Dirichlet-integral** in fashions different from the usual one (cf. Binz & Schwarz [14]) but adapted to the treatment of deformable media as presented above (cf. Binz [10]). Let $<,>$ be a fixed scalar product on $\mathbb{R}^n$. At first we consider $h \in C^\infty(M, \mathbb{R}^n)$ and a fixed embedding $j \in E(M, \mathbb{R}^n)$. The differential $dh : TM \longrightarrow \mathbb{R}^n$ can be represented via dj as

$$dh = c_h(j) \cdot dj + dj \cdot (C_h(j) + B_h(j)) \tag{A1.1}$$

which applied to any tangent vector $v_q \in T_qM$ for any $q \in M$ reads as

$$dh\ v_q = c_h(j)(q)\left((dj\ v_q)\right) + dj\left((C_h(j) + B_h(j))v_q\right).$$

Here $c_h : M \longrightarrow so(n)$ is a smooth map sending vectors in djT_qM into vectors in the orthogonal complement $(djT_qM)^\perp$ and vice versa for any $q \in M$; thus c_h is an infinitesimal Gauss map. The maps C_h and B_h are both smooth (strong) bundle endomorphisms of TM, skew - respectively selfadjoint with respect to the pull back metric $j^*<,>$ denoted by $m(j)$. For this representation we refer to Binz [6] or Binz & Fischer [13]. For any $q \in M$ the linear map $c_h^2(q)$ on $\mathbb{R}^n$ is a selfadjoint endomorphism of djT_qM respectively of $(djT_qM)^\perp$. The part of c_h^2 mapping (djT_qM) into itself is called $\left(c_h^2(q)\right)^\top$. For simplicity we will omit the variable j in the coefficients of (A1.1) if no confusion arises. For any two $h, k \in C^\infty(M, \mathbb{R}^n)$ we define

$$dh \bullet_j dk := -tr(c_h \circ c_k)^\top - tr\ C_h \circ C_k + tr\ B_h \circ B_k \tag{A1.2}$$

and observe that

$$\mathcal{g}(j)(dh, dk) := \int_M dh \bullet_j dk\ \mu(j) = \int_M < \Delta(j)h, k > \mu(j) \tag{A1.3}$$

where $\mu(j)$ is the Riemannian volume element of $m(j)$. The operator $\Delta(j)$ is the Laplacian associated with $m(j)$. Thus the dot $\bullet_j$ in (A1.2) is j-dependent. For (A.1.2) and (A.1.3) we refer to Binz [5]. Clearly the metric $\mathcal{G}$, given by

$$\mathcal{G}(j)(h,k) = \int_M < h,k > \mu(j) \quad \forall E(M, \mathbb{R}^n),$$

is a weak Riemannian metric on $E(M, \mathbb{R}^n)$. The left hand side of (A1.3) is called the Dirichlet integral usually formulated via the Hodge star operator. Clearly $\mathcal{G}$ is a weak Riemannian metric on $\{dj | j \in E(M, \mathbb{R}^n)\}$.

Next we will represent the integral (A1.3) in a complete different way, based on the second derivative of $m(j)$ formed with respect to j. To this end let $j_0 \in E(M, \mathbb{R}^n)$ be fixed and let $h \in C^\infty(M, \mathbb{R}^n)$ be such that $j := j_0 + h \in E(M, \mathbb{R}^n)$. Then for any $v, w \in T_qM$ and any $q \in M$

$$\begin{aligned} m(j_0+h)(v,w) = &\; m(j_0)(v,w) + < dj_0\, v, dh\, w > + < dh\, v, dj_0\, w > \\ + &\; < dh\, v, dh\, w > \\ = &\; m(j_0) + \mathbb{D} m(j_0)(h) + \tfrac{1}{2} \cdot \mathbb{D}^2 m(j_0)(h,h). \end{aligned} \qquad \text{(A1.4)}$$

According to (3.1.10) we write

$$m(j_0+h)(v,w) = m(j_0)(f^2(j_0+h)v, w) \qquad \text{(A1.5)}$$

for a well defined smooth strong bundle endomorphism $f(j_0+h)$ of TM, fibre-wise positive definite with respect to $m(j_0)$ and observe by (A1.4) that

$$\begin{aligned} &m(j_0+h)(v,w) = m(j_0)\big(f^2(j_0+h)v, w\big) \qquad \text{(A1.6)} \\ = \;& m(j_0)(v,w) + m(j_0)\big(\mathbb{D} f^2(j_0)(h)v, w\big) + \tfrac{1}{2} \cdot m(j_0)\big(\mathbb{D}^2 f^2(j_0)(h,h)v, w\big) \end{aligned}$$

for all $v, w \in T_qM$ and for all $q \in M$. Using (A1.3) we conclude

$$< dh\, v, dh\, w > = < (c_h + \bar{B}_h + \bar{C}_h) \circ (c_h + \bar{B}_h + \bar{C}_h)^* \cdot dj_0\, v, dj_0\, w >$$

where $\bar{C}_h \cdot dj_0$ and $\bar{B}_h \cdot dj_0$ are respectively defined by

$$\bar{C}_h \cdot dj_0 = dj_0 \circ C_h \quad \text{and} \quad \bar{B}_h \cdot dj_0 = dj_0 \circ B_h$$

and the requirement that both $\bar{C}_h$ and $\bar{B}_h$ vanish on the normal bundle of Tj_0TM. By * we mean the adjoint. Therefore the following equations hold

$$\begin{aligned} < dh\, v, dh\, w > = &\; < -c_h^2 \cdot dj_0\, v, dj_0\, w > + < dj_0 \circ (B_h + C_h) \circ (B_h + C_h)^* v, dj_0\, w > \\ = &\; \tfrac{1}{2} \cdot m(j_0)\big(\mathbb{D}^2 f^2(j_0)(h,h)v, w\big). \end{aligned}$$

Since $c_h^2 \cdot dj_0 = (c_h^2)^\top \cdot dj_0$ we find for all $h \in C^\infty(M, \mathbb{R}^n)$

$$\frac{1}{2} \cdot \mathbb{D}^2 f^2(j_0)(h,h) = -dj_0^{-1} \circ c_h^2 \cdot dj_0 - C_h^2 + B_h^2 + C_h \circ B_h - B_h \circ C_h \qquad \text{(A1.7)}$$

and $f^2(j_0+h)$ computes by (A1.4) and (A1.7) to

$$f^2(j_0+h) = id + 2\cdot B_h - dj_0^{-1}\circ c_h^2 \cdot dj_0 - C_h^2 + B_h^2 + C_h \circ B_h - B_h \circ C_h.$$

Using (A1.2) and (A1.7) yields immediately

$$dh \bullet_{j_0} dh = \frac{1}{2}\cdot tr\ I\!D^2 f^2(j_0)(h,h) = \frac{1}{2}\cdot I\!D^2 (tr\ f^2(j_0))(h,h)$$

linking the above integrand of the Dirichlet integral with the Taylor expansion of the metric. By polarization we obtain the following:

Proposition A1.1

$$dh \bullet_{j_0} dk = \frac{1}{2}\cdot tr\ I\!D^2 f^2(j_0)(h,k) = \frac{1}{2}\cdot I\!D^2 (tr\ f^2(j_0))(h,k)$$

for any $j_0 \in E(M, I\!R^n)$ *and any two* $h, k \in C^\infty(M, I\!R^n)$.

Corollary A1.2 *The Dirichlet integral allows therefore the following interpretation:*

$$\mathcal{G}(j_0)(dh, dk) = \frac{1}{2}\cdot \int_M I\!D^2 tr\ f^2(j_0)(h,k)\mu(j_0) = \int_M < \Delta(j_0)h, k > \mu(j_0)$$

for any $j_0 \in E(M, I\!R^n)$ *and for all* $h, k \in C^\infty(M, I\!R^n)$. *Hence (A1.6) yields*

$$\int_M tr\ f^2(j_0+h)\mu(j_0) = \dim S \cdot \mathcal{A}(j_0) + \int_M tr\ I\!D f^2(j_0)(h)\mu(j_0) + \int_M < \Delta(j_0)h, h > \mu(j_0). \quad \text{(A1.8)}$$

Our next aim is to express f in terms of the map B_h via the exponential map. We first will do so for $f^2(j)$ in terms of $B_h(j)$. Comparing

$$I\!D\, m(j)(h) = m(j_0)(I\!D f^2(j)(h)\cdots,\cdots) \quad \text{(A1.9)}$$

where $I\!D f^2(j)(h)$ is $m(j_0)$-selfadjoint, with

$$I\!D\, m(j)(h) = 2\cdot m(j_0)(f^2(j)\cdot B_h(j)\cdots,\cdots) \quad \text{(A1.10)}$$

yields immediately

$$f^{-2}(j)\cdot I\!D f^2(j)(h) = 2\cdot B_h(j). \quad \text{(A1.11)}$$

In particular (A1.6) yields for $j := j_0 + t\cdot h$

$$f^2(j_0 + t\cdot h) = id + 2\cdot t\cdot B_h(j_0) + \frac{t^2}{2}\cdot I\!D^2 f^2(j_0)(h,h). \quad \text{(A1.12)}$$

To prepare commutativity relations in order to solve (A1.11), we compare for $j = j_0 + t\cdot h$ the equation

$$m(j) = m(j_0) + t\cdot I\!D\, m(j_0)(h) + \frac{t^2}{2}\cdot I\!D^2 m(j_0)(h,h) \quad \text{(A1.13)}$$

with

$$m(j_0) = m(j) - t \cdot I\!D\, m(j)(h) + \frac{t^2}{2} \cdot I\!D^2 m(j_0)(h,h) \qquad \text{(A1.14)}$$

and conclude for $j = j_0 + t \cdot h$

$$I\!D\, m(j)(h) = I\!D\, m(j_0)(h) + t \cdot I\!D^2 m(j_0)(h,h). \qquad \text{(A1.15)}$$

In turn we derive by (A1.10), (A1.11) and (A1.12)

$$2 \cdot f^2(j) \cdot B_h(j) = 2 \cdot B_h(j_0) + t \cdot I\!D^2 f^2(j_0)(h,h) = I\!D\, f^2(j)(h). \qquad \text{(A1.16)}$$

Here all terms are $m(j_0)$-selfadjoint and $B_h(j)$ is $m(j)$-selfadjoint.

Differentiating (A1.16) with respect to j at j in the direction of h and using (A1.11) as well as (A1.13) yields therefore

$$2 \cdot f^2(j) \cdot B_h^2(j) + f^2(j) \cdot I\!D\, B_h(j)(h) = \frac{1}{2} \cdot I\!D^2 f^2(j_0)(h,h) \qquad \text{(A1.17)}$$

showing that $I\!D\, B_h(j)$ is $m(j)$-selfadjoint. Differentiating once more yields

$$\begin{aligned} 4 \cdot f^2(j) \cdot B_h^3(j) + {} & 2 \cdot f^2(j) B_h(j) \cdot I\!D\, B_h(j)(h) + 2 \cdot f^2(j) \cdot I\!D\, B_h^2(j)(h) \\ + {} & f^2(j) \cdot I\!D^2 B_h(j)(h,h) = 0 \end{aligned} \qquad \text{(A1.18)}$$

showing

$$4 \cdot B_h^3(j) + 2 \cdot B_h(j) \cdot I\!D\, B_h(j)(h) + I\!D\, B_h^2(j)(h) + 2 \cdot I\!D^2 B_h(j)(h,h) = 0. \quad \text{(A1.19)}$$

Since $B_h(j)$ as well as $I\!D\, B_h^2(j)(h)$ and $I\!D^2 B_h(j)(h,h)$ are $m(j)$-selfadjoint we find immediately the following

$$B_h(j) \cdot I\!D\, B_h(j)(h) = I\!D\, B_h(j)(h) \cdot B_h(j). \qquad \text{(A1.20)}$$

Setting $j = j_0$ in (A1.17) we observe that

$$I\!D^2 f^2(j_0)(h,h) = 2 \cdot I\!D\, B_h(j_0)(h) + 4 \cdot B_h^2(j) \qquad \text{(A1.21)}$$

where the operators at the right hand side commute, due to (A1.20). (Accordingly the operator $B_h(j_0)$ commutes with $I\!D^2 f^2(j_0)(h,h)$). Thus (A1.11) reformulates as

$$f^2(j_0 + t \cdot h) = id + 2 \cdot t B_h(j_0) + t^2 \cdot \left(I\!D\, B_h(j_0)(h) + 2 \cdot B_h^2(j_0)\right). \qquad \text{(A1.22)}$$

Due to (A1.22) $f^{-2}(j)$ can be expanded in terms of powers of $B_h(j_0)$, $I\!D\, B_h(j_0)(h)$ and t. Due to (A1.16) $I\!D\, f^2(j)(h)$ and by (A1.11) the bundle endomorphism $B_h(j)$ both expand in terms of these powers, too. Therefore, $\int_0^t B_h(j_0 + \tau \cdot h) d\tau$ commutes with $B_h(j + t \cdot h)$. Thus the following theorem is true:

Theorem A1.3

$$f(j_0 + h) = e^{\int_0^1 B_h(j_0 + \tau \cdot h) d\tau} \qquad \text{(A1.23)}$$

for any $h \in C^\infty(M, I\!R^n)$ for which $j_0 + h \in E(M, I\!R^n)$.

The following is an immediate consequence (or use directly A1.11):

Corollary A1.4

$$det f(j_0 + t \cdot h) = e^{\int_0^t tr B_h(j_0+\tau\cdot h)d\tau}. \tag{A1.24}$$

APPENDIX 2

Here we will link $\mathcal{G}_P$ with $\mathcal{G}(j_0)$.

Let $P \subset M$. On $\mathcal{F}(P, \mathbb{R})$ the discrete L_2-scalar product is given by

$$\mathcal{G}_P(r(h), r(k)) := \sum_{q\in P} r(h)(q) \cdot r(k)(q) \qquad \forall\, r(h), r(k) \in \mathcal{F}(P, \mathbb{R}).$$

On the the other hand, given a Riemannian metric g on M with volume element $\mu(g)$ the associated L_2-metric is defined by

$$\mathcal{G}(g)(h,k) = \int_M h \cdot k \; \mu(g) \qquad \forall\, h, k \in C^\infty(M, \mathbb{R}).$$

where the product $h \cdot k$ is taken pointwise. The relation between $r^*\mathcal{G}_P$ and $\mathcal{G}(g)$ on a complement $L \subset C^\infty(M, \mathbb{R})$ of $ker\, r$ is as follows:

Lemma A2.1 *Given a positive map $\varphi^P \in \mathcal{F}(P, \mathbb{R})$ there is a unique positive map $\varphi(g) \in L$ smoothly depending on g such that*

$$\mathcal{G}(g)(\varphi(g) \odot h, k) = \mathcal{G}_P(\varphi^P \cdot r(h), r(k)) \qquad \forall\, h, k \in L \tag{A2.1}$$

and vice versa any $\varphi(g)$ yields some φ^P in a unique manner. The multiplication $h \odot k$ for $h, k \in L$ is given by $h \odot k := s\big(r(h) \cdot r(k)\big)$ where $s : \mathcal{F}(P, \mathbb{R}) \to L$ is such that $r \circ s = id$. Given φ^P then

$$\mathbb{D}\varphi(g)(S) = -\frac{1}{2} \cdot pr_L(\varphi(g) \cdot tr_g S) \tag{A2.2}$$

for any smooth symmetric two-tensor S on M; moreover $pr_L := s \circ r$.

Proof: Obviously

$$\mathcal{G}(g)(Qh, k) = \mathcal{G}_P(\varphi^P \cdot r(h), r(k)) \qquad \forall\, h, k \in L$$

for some well defined selfadjoint $Q \in End\, L$. Let $h_q := s(\mathbf{1}_q)$ for all $q \in P$ where $\mathbf{1}_q$ is the characteristic function of q. Since for any two $q, q' \in P$

$$\mathcal{G}(g)(Qh_q, h_{q'}) = \mathcal{G}_P(\varphi^P \cdot \mathbf{1}_q \mathbf{1}_{q'}) = \varphi^P(q) \cdot \delta_{q,q'}$$

we conclude $Qh_q = \xi(q) \cdot h_q$ for some $\xi(q) \in \mathbb{R}^+$. This shows

$$\mathcal{G}(g)(h,k) = \mathcal{G}_P(\xi^{-1} \cdot \varphi^P \cdot r(h), r(k)) \qquad \forall\, h, k \in L.$$

Setting $\varphi(g) := s(\xi)$ yields

$$\mathcal{G}(g)(\varphi(g) \odot h, k) = \mathcal{G}_P(\xi^{-1} \cdot \varphi^P \cdot \xi \cdot r(h), r(k)) = \mathcal{G}_P(\varphi^P \cdot r(h), r(k)) \qquad \forall\, h, k \in L.$$

Thus $Qh = \varphi(g) \odot h$ for all $h \in L$; hence $\varphi(g)$ is uniquely determined. On the other hand given $\varphi(g)$ then φ^P obviously exists and is unique as well. To show the continuity equation (A2.2) we choose some Riemannian metric g' in the Fréchet manifold $\mathcal{M}$ of all Riemannian metrics on M and observe that

$$g'(v,w) = g(f(g')^2 \cdot v, w) \qquad \forall\, v, w \in TqM \qquad \forall\, q \in M$$

for some well defined g-selfadjoint strong bundle isomorphism $f(g')$ of TM. Hence

$$pr_L(\varphi(g') \cdot det\ f^{-1}(g')) = \varphi(q).$$

Differentiating this in the Fréchet space of all smooth Riemannian metrics with respect to g' in the direction of S at g yields A2.2.

Since $\mathcal{F}^\infty(M, \mathbb{R}^n) \cong \mathcal{F}^\infty(M, \mathbb{R}) \otimes \mathbb{R}^n$ the restriction $n = 1$ in lemma A2.1 can be dropped.

Choosing $h = k = 1 \in \mathbb{R}$ in (A2.1) yields

$$\int_M \varphi(q)\ \mu(q) = \mathcal{G}(g)(\varphi(g) \cdot \mathbf{1}, \mathbf{1}) = \mathcal{G}_P(\varphi^P \cdot \mathbf{1}, \mathbf{1}) = \sum_{q \in P} \varphi^P(q)$$

implying the following:

Corollary A2.2 *Given a positive function $\varphi^P \in \mathcal{F}(P, \mathbb{R})$ then $\varphi(g)$ in A2.1 satisfies*

$$\int_M \varphi(g)\ \mu(g) = \sum_{q \in M} \varphi^P(q) \qquad \forall\, g \in \mathcal{M}.$$

Hence $g' := \varphi(g)^{\frac{2}{dim\ M}} \cdot g$ yields

$$\mathcal{A}(g') = \#P,$$

provided $\varphi^P = 1$. Here $\#P$ denotes the number of points in P and $\mathcal{A}(g') := \int_M \mu(g')$ is the area of M defined by g' and the given orientation.