From the discrete to a continuum shown on the example of an idealized skin

Ernst Binz
Universität Mannheim
Lehrstuhl Mathematik 1, Seminargebäude A5
68131 Mannheim

No. 2 0 0 / 1995

From the discrete to a continuum shown on the example of an idealized skin

0 Introduction

Here we treat an application of a very simple sort of Lie theory to mechanics of continua determined by finitely many particles.

The aim of this application is the description of a discrete medium as a continuum. 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 $h_P : P \to \mathbb{R}^n$ at a configuration j_P (cf. [He]). The configuration space is a collection O_P of injective maps from P to $\mathbb{R}^n$. O_P shall be open in the linear, finite dimensional space of all maps from P to $\mathbb{R}^n$. 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 the unity in the semidirect product $\mathbb{R}^+ \Diamond \mathbb{R}^n$ of the groups $\mathbb{R}^+$ and $\mathbb{R}^n$ of all dilatations and of all translations of $\mathbb{R}^n$, respectively. The last requirement implies in particular, that constant distortions cause no 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. [B1] to [B4] and [M,H]). 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 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. The invariance of A under $\mathbb{R}^+ \Diamond \mathbb{R}^n$ yields a constitutive map $\mathcal{H}$ characterizing the continuum.

The task 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 F_P on O respectively on O_P, relating them and identifying them as the free energies in respective Gibbs statistics. This relates our description of media to the one presented in [L,L]. The choice of F_P respectively F does not only determine Gibbs states, but also refines the description of the media via the virtual work.

We close this note by introducing the notion of a configuration of the skin fitting the discrete medium up to first order and present some descriptions of characteristics of A in terms those of A_P and vice versa at this kind of configuration. 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.

1 Characterization of an idealized skin

At first we treat the continuum since it is more common and -since it has more structure than a general discrete medium- it is more economic as far as the presentation is concerned.

1.1 An idealized skin

Here we describe an idealized skin, 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 will become apparent if we treat the virtual work caused by area deformations). For the geometric notions we refer to [G,H,V].

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

A mass density is a smooth positive map $\rho : O \longrightarrow C^\infty(M, \mathbb{R})$ for which the continuity equation

$$\mathbb{D}\, \rho(j)(h) = -\rho(j) \cdot tr\ B_h \qquad \forall\, h \in C^\infty(M, \mathbb{R}^n) \tag{1.1.1}$$

holds (cf. [Bi2]). Here $\mathbb{D}$ denotes the differentiation on function spaces (on O, here) in the sense of [Bi,Sn,Fi] or [Fr,Kr]. Moreover B_h is an element of $End\,TM$, the collection of all smooth bundle endopmorphism of TM over the identity, equipped with the C^∞-topology; it is defined as follows : Let $m(j) := j^* <,>$ be the pull back metric on M of $<,>$ by j. Given any other $j' \in E(M, \mathbb{R}^n)$, the metrics $m(j)$ and $m(j')$ are related by

$$m(j')(v, w) = m(j)\big(f^2(j')v, w\big) \qquad \forall\, v, w \in TqM \qquad \forall\, q \in M \tag{1.1.2}$$

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. Given a positive $\rho_0 \in C^\infty(M, \mathbb{R})$ the solution to (1.1.1) is obviously

$$\rho(j) = \rho_0 \cdot det\ f^{-1}(j) \qquad j \in O. \tag{1.1.3}$$

Denoting by $\mu(j)$ the volume element determined by $m(j)$ and the given orientation of M the total mass

$$m(j) := \int_M \rho(j)\ \mu(j) \tag{1.1.4}$$

is constant in $j \in O$, due to (1.1.1).

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

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

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. [He]), the one-form $A : O \times C^\infty(M, I\!R^n) \longrightarrow I\!R$ given by

$$A(j)(h) = \int_M < \Phi(j), h > \mu(j) \qquad \forall\, j \in O \qquad \forall\, h \in C^\infty(M, I\!R^n). \quad (1.1.5)$$

This virtual work is supposed to be invariant under the action of a neighbourhood of the neutral element of the semidirected product $I\!R^+ \Diamond I\!R$ on O. Here $I\!R^+$ and $I\!R^n$ are respectively the multiplicative group of all positive reals, called the group of dilations and the translation group $I\!R^n$ of the vector space $I\!R^n$. The action we have in mind is based on the splitting of any $j \in E^\infty(M, I\!R^n)$ into $j = j_\perp + z$ with $z \in I\!R^n$ where $j_\perp$ is orthogonal to $I\!R^n$ with respect to the L_2-metric $\mathcal{G}(j)$ given by

$$\mathcal{G}(j)(h,k) := \int_M < h, k > \mu(j) \qquad \forall\, h, k \in C^\infty(M, I\!R^n) \quad (1.1.6)$$

and is defined as follows: Given $j \in O$, and any $(\tau, z') \in I\!R^+ \Diamond I\!R^n$ near enough to the unity $(1,0) \in I\!R^+ \Diamond I\!R^n$ then

$$j \cdot (\tau, z') := j_\perp + \tau \cdot z + z'. \quad (1.1.7)$$

The invariance of A under this action is thus expressed by

$$A(j_\perp + \tau \cdot z + z')(h + (\tau - 1) \cdot \bar{z}) = A(j_\perp + z)(h) \qquad \forall\, h \in C^\infty(M, I\!R^n) \quad (1.1.8)$$

with $\tau \in I\!R^+$ and $z', \bar{z} \in I\!R^n$. Hence $\tau = 1$ and $z' = -z$ for z near $0 \in I\!R$ yield

$$A(j_\perp)(h) = A(j)(h) \qquad \forall\, h \in C^\infty(M, I\!R^n), \quad (1.1.9)$$

saying that $A(j)$ depends on dj only. If $h = 0$, $\tau \neq 1$ and $z' := -(\tau - 1) \cdot z$ then (1.1.8) yields

$$A(j)(z'') = 0 \qquad \forall\, z'' \in I\!R^n, \quad (1.1.10)$$

saying that constant distortions cause no work, hence $A(j)(h)$ depends on dh only. Equation (1.1.9) and (1.1.10) specify the sorts of force densities and in turn of virtual work we will use in the sequel. This leads us to the following:

An idealized skin with underlying manifold M is given by a mass density ρ satisfying the continuity equation and a force density map $\Phi : O \longrightarrow I\!R^n$ obeying

$$\Phi(j + z) = \Phi(j) \qquad \forall\, j \in O \qquad \forall\, z \quad \text{near} \quad 0 \in I\!R^n \quad (1.1.11)$$

and

$$\int_M \Phi(j)\mu(j) = 0 \qquad \forall\, j \in O. \quad (1.1.12)$$

(1.1.12), however, is the integrability condition for the equation

$$\Delta(j)\mathcal{H}(j) = \Phi(j) \qquad \forall\, j \in O \quad (1.1.13)$$

with $\mathcal{H} \in C^\infty(O, C^\infty(M, I\!R^n))$ determined up to a map in $C^\infty(O, I\!R^n)$. Here $\Delta(j)$ is the Laplacian of $m(j)$ (cf. [Ma]). $\mathcal{H}$, resulting from the above mentioned invariance of A, 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 (1.1.1) and a smooth 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

$$\Delta(j_0)\hat{\mathcal{H}}(j) = det\ f(j) \cdot \Phi(j) \qquad j \in O \tag{1.1.14}$$

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

$$\hat{\Phi}(j) := det\ f(j) \cdot \Phi(j) \qquad \forall\, j \in O; \tag{1.1.15}$$

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

$$A(j)(h) = \mathcal{G}(j_0)(\hat{\Phi}(j), h) = \mathcal{G}(j_0)(\Delta(j_0)\hat{\mathcal{H}}(j), h) \qquad \forall\, h \in C^\infty(M, I\!R^n). \tag{1.1.16}$$

1.2 Structural capillarity

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

$$\mathcal{A}(j) := \int_M \mu(j) \qquad \forall\, j \in O. \tag{1.2.1}$$

The virtual work caused by distorting the area is

$$A(j)(h) := a(j) \cdot I\!D\,\mathcal{A}(j)(h) \qquad \forall\, j \in O \quad \text{and} \quad \forall\, h \in C^\infty(M, I\!R^n), \tag{1.2.2}$$

where $a \in C^\infty(O, I\!R)$ is called the **structural capillarity**. It is easily verified that any $\mathcal{H} \in C^\infty(O, C^\infty(M, I\!R^n))$ splits $\mathcal{G}(j)$-orthogonally into

$$\mathcal{H}(j) = a(j) \cdot j + \mathcal{H}_1(j) \qquad \forall\, j \in O \tag{1.2.3}$$

where $\mathcal{H}_1(j)$ is not sensitive to area deformations (cf. [Bi1] to [Bi3]), saying that $\Delta(j)j$ is $\mathcal{G}(j)$-orthogonal to $\mathcal{H}_1(j)$ for all $j \in O$. The map $\Delta(j)j$, pointwise normal to $TjTM$ with respect to $<,>$, is called the mean curvature tensor. Obviously (1.2.2) and (1.2.3) yield the following equation for a:

$$A(j)(j) = a(j) \cdot dim\, M \cdot \mathcal{A}(j) \qquad \forall\, j \in O \tag{1.2.4}$$

which in turn determines a directly out of A, a fact which will be used later. The notion of structural capillarity will be crucial in determining the vibrational modes of the continuum (cf. sec. 4 and 5). The sort of virtual work given by (1.2.2) justifies our non-local approach.

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 above sense is a rather naive approach from the continuum mechanics point of view (cf. [M,H]). We do so because it is on one hand appropriate for discrete media (cf. below) and keeps on the other the formalism simple. The relation of $\mathcal{H}$ to the first Piola-Kirchhoff stress tensor can be found in [Bi3].

2 Description of discrete media

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

2.1 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 in the finite dimensional space $\mathcal{F}(P, \mathbb{R}^n)$ of all maps from P to $\mathbb{R}^n$. The discrete medium is determined by a positive smooth mass distribution

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

with total mass $m = \sum_{q\in P} \rho_P(q)$ and by a smooth internal force map $\Phi_P \in C^\infty(O_P, \mathcal{F}(P, \mathbb{R}^n))$, causing the virtual work A_P defined by

$$A_P(j_P)(h_P) = \sum_{q\in P} < \Phi_P(j_P)(q), h_P(q) > \quad \forall\, j_P \in O_P \quad \forall\, h_P \in \mathcal{F}(P, \mathbb{R}^n)$$

which is supposed to be invariant under the action on O_P of a neighbourhood of the neutral element in $\mathbb{R}^+ \Diamond \mathbb{R}^n$. Hence

$$\sum_{q\in P} \Phi_P(j_P) = 0 \tag{2.1.1}$$

as well as

$$\Phi_P(j_P + z) = 0 \qquad \text{and} \qquad \forall\, z \qquad \text{near} \qquad 0 \in \mathbb{R}^n, \tag{2.1.2}$$

the analoga of (1.1.12) and (1.1.11), respectively. Let $\rho_P = 1$ from now on.

2.2 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_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 $nb(q)$ 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 respectively one-cochains of $\boldsymbol{L}$ there are the natural scalar products $\mathcal{G}_P$ and $\mathcal{G}_{\boldsymbol{L}_1}$ given respectively by

$$\mathcal{G}_P(h_P, k_P) = \sum_{q \in P} < h_P(q), k_P(q) > \quad \text{and} \quad \mathcal{G}_{\boldsymbol{L}_1}(c_1, c_2) = \sum_{\sigma \in \boldsymbol{L}_1} < c_1(\sigma), c_2(\sigma) > \tag{2.2.1}$$

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

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

We therefore have the Hodge Laplacian $\Delta_T := \delta^1 \circ \partial^1$ on $\mathcal{F}(P, I\!R^n)$ (cf. [B],[E]). Due to (2.1.1) any internal force $\Phi_P \in C^\infty(O, \mathcal{F}(P, I\!R^n))$ caused by n.n.i. admits a constitutive map $\mathcal{H}_P \in C^\infty(O_P, \mathcal{F}(P, I\!R^n))$, satisfying

$$\Delta_T \mathcal{H}_P(j_P) = \Phi_P(j_P) \qquad \forall\, j_P \in O_P. \tag{2.2.2}$$

We characterize this kind of a medium by ρ_P and the map $\mathcal{H}_P$. Since

$$\Delta_T \mathcal{H}_P(j_P)(q) = nb(q) \cdot \mathcal{H}_P(j_P)(q) - \sum_{i=1}^{nb(q)} \mathcal{H}_P(j_P)(q_i) \qquad \forall\, q \in P \tag{2.2.3}$$

(cf. [B]) 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

$$\mathcal{H}_P(j_P)(q) - \mathcal{H}_P(j_P)(q_i) = \pm \partial^1 \mathcal{H}_P(j_P)(\sigma_i) \qquad \forall\, i = 1, ..., nb(q), \tag{2.2.4}$$

with $\pm$ accordingly as to whether $q = \sigma_i^+$ or $q = \sigma_i^-$. Here $+$ and $-$ is given by the orientation. Forces of this kind may be determined by a potential which is proportional to the square of the length of $\partial j_P(\sigma)$.

Thus n.n.i. resemble the type of structure met in the case of the continuum. In fact the first Piola-Kirchhoff stress tensor can be introduced here as well; it is just a one-cochain (which depends on the configuration in the non-local-case).

3 The discrete medium modeled as a continuum

To describe the discrete medium as an idealized skin 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 $O \subset E(M, I\!R^n)$. 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. Since $r^{-1}O_P \subset E(M, I\!R^n)$ for $O_P \subset E(P, I\!R^n)$ small enough, we intend to set $A := r^* A_P$. However, the requirement of the existence of a force density $\hat{\Phi}$ (cf. (1.1.15) and (1.1.16)) implies the existence of a $\mathcal{G}(j_0)$-orthogonal complement to $ker\, r \subset C^\infty(M, I\!R^n)$. This however does not exist in general, otherwise the δ-function would admit a density. 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.

3.1 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 (1.1.15) and (1.1.14) 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 eigenvectors of $\Delta(j_0)$. But there is still a choice involved. Here is how we proceed: Let $z_1, ..., z_n \in \mathbb{R}^n$ be a $<,>$-orthonormal basis. We choose $\mathcal{G}(j_0)$-orthonormed eigenvectors $e_{i_1}, ..., e_{i_b}$ in $C^\infty(M, \mathbb{R}^n)$ of $\Delta(j_0)$ with respective eigenvalues $0 < \lambda_{i_1} \leq ... \leq \lambda_{i_b}$ such that $z_1, ..., z_n, r(e_{i_1}), ..., r(e_{i_b})$ forms a basis of $\mathcal{F}(P, \mathbb{R}^n)$ and that $\sum_{s=1}^b \lambda_{i_s}$ is as small as possible. The last condition expresses our choice. The complement $\mathcal{F}^\infty(M, \mathbb{R}^n) \subset C^\infty(M, \mathbb{R}^n)$ 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 $s = 1, ..., b$. Clearly

$$C^\infty(M, \mathbb{R}^n) = \ker r \oplus \mathcal{F}^\infty(M, \mathbb{R}^n). \tag{3.1.1}$$

Obviously the $\mathcal{G}(j_0)$-orthogonal complement $\mathcal{F}^\infty(M, \mathbb{R}^n)^\perp \subset C^\infty(M, \mathbb{R}^n)$ to $\mathcal{F}^\infty(M, \mathbb{R}^n)$ is not identical with $ker\, r$ but

$$C^\infty(M, \mathbb{R}^n) = \mathcal{F}^\infty(M, \mathbb{R}^n) \oplus \mathcal{F}^\infty(M, \mathbb{R}^n)^\perp \tag{3.1.2}$$

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

$$C^\infty(M, \mathbb{R}) = \mathcal{F}^\infty(M, \mathbb{R}) \oplus \mathbb{R}. \tag{3.1.3}$$

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

$$O - j_0 = O_{ker} \oplus \mathcal{W}' \tag{3.1.4}$$

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

$$O = \bigcup_{j \in E_o} \mathcal{W}(j) \qquad \text{with} \qquad E_0 := r^{-1}(j_P^0) \cap O \tag{3.1.5}$$

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 (3.1.5).

3.2 The construction of ρ and A

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

$$\int_M \rho_0 \; \mu(j_0) = \sum_q \rho_P(q) = m$$

where m is the total mass. Letting $f(j)$ as in (1.1.2) with $f(j_0) = id$ then

$$\rho(j) := \rho_0 \cdot det\; f^{-1}(j) \qquad \forall\, j \in O \tag{3.2.1}$$

determines a mass density on M in the sense of sec. 1.1. Clearly $\rho(j_0) = \rho_0$ and $\rho(j) \notin \mathcal{F}^\infty(M, \mathbb{R})$, in general except for j_0.

The virtual work A is constructed 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

$$A := r_\infty^* A_P \qquad \text{on each slice } \mathcal{W}(j) \qquad \text{and} \qquad A \mid O \times \mathcal{F}^\infty(M, I\!R^n)^\perp = 0 \tag{3.2.2}$$

Hence A is constant along $r^{-1}(j_P^0) \cap O$. Given $j \in O$ and $k \in ker\, r$ 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 $j \in r^{-1}(j_P^0) \cap O$.

4 The free energy

Given a discrete medium described as an idealized skin M, we will split A_P on O_P (to be further 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 specific observables.

4.1 The free energy of the discrete medium

Let $\mathcal{F}(P, I\!R^n)$ be oriented and O_P shall be a compact, smooth and connected manifold with boundary ∂O_P, sliced as in (3.1.5). Moreover, O_P shall be a neighbourhood of $j_P^0 := j_0|P$. Here j_0 is fixed again. Given A_P on O_P then

$$A_P = I\!D\, \bar{F}_P + \Psi_P \tag{4.1.1}$$

with $\mathrm{div}_{O_P} A_P = \Delta_{O_P} \bar{F}_{P_{\bar{F}}}$ 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 (cf. [Hö]). Here div_{O_P} and Δ_{O_P} on $\mathcal{F}(P, I\!R^n)$ are the divergence operator and the Laplacian of $\mathcal{G}_P$, respectively. $\boldsymbol{n}_{O_P}$ denotes the positively oriented unit normal of ∂O_P in O_P. Let the Boltzmann constant be equal to 1. For each $j_P \in O$ the positive real $\bar{F}(j_P)$ is the free energy (cf. [B,St]) associated with a temperature map $\beta \in C^\infty(O_P, I\!R^+)$ and a Gibbs state $\rho_{Gibbs}^P(j_P)$ as seen as follows: Let $F_P \in C^\infty(O_P, \mathcal{F}(P, I\!R^+))$ be such that $\bar{F}(j_P) = \sum_{q \in P} F_P(j_P)(q)$ for all $j_P \in O_P$. Each such density F_P is of the form

$$F_P(j_P) = \frac{\bar{F}_P(j_P)}{\#P} + \xi_P(j_P) \qquad \text{with} \qquad \sum_{q \in P} \xi_P(j_P)(q) = 0 \tag{4.1.2}$$

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 $\rho_{Gibbs}^P(j_P)$ is defined by

$$\rho_{Gibbs}^P(j_P) := \frac{F_P(j_P)}{\bar{F}_P(j_P)} = \frac{\bar{F}_P(j_P)}{\#P} + \frac{\xi_P(j_P)}{\bar{F}_P(j_P)} \qquad \forall\, j_P \in O_P. \tag{4.1.3}$$

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

$$I_P := \bar{F}_P - \frac{1}{\beta} \cdot ln\, \rho_{Gibbs}^P, \tag{4.1.4}$$

and yields for each $j_P \in O_P$

$$\rho^P_{Gibbs}(j_P) = \frac{e^{-\beta(j_P)\cdot I_P}}{\sum_{q\in P} e^{-\beta(j_P)\cdot I_P(j_P)(q)}}. \tag{4.1.5}$$

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

$$\bar{F}_P = \bar{I}_P - \beta^{-1} \cdot \bar{S}_P \tag{4.1.6}$$

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 $\bar{F}$ as a free energy yields a finer characterisation of the discrete medium than the one determined by A_P.

Instead of dealing with ξ_P from above, we may choose $\zeta_P \in C^\infty(O_P, \mathcal{F}(\{1,...,b\}, I\!R))$ for which $\sum_{i=1}^b \zeta_P(j_P)(i) = 0$ for all $j_P \in O_P$ and proceed accordingly. In this case the density f of $\bar{F}_P$ is defined by

$$\mathrm{f}(j_P)(i) := \frac{\bar{F}_P(j_P)}{b} + \frac{\zeta(j_P)(i)}{\bar{F}(j_P)} \qquad \forall\, i = 1,...,b \qquad \forall\, j_P \in O_P.$$

The observable associated with β is thus

$$\varphi(j_P)(i) := \bar{F}_P(j_P) - \frac{1}{\beta(j_P)} \cdot ln\ \frac{\mathrm{f}(j_P)(i)}{\bar{F}_P(j_P)} \quad \forall\, i \in \{1,...,b\} \quad \text{and} \quad \forall\, j_P \in O_P. \tag{4.1.7}$$

Choosing $Q(j_P) \in End\ \mathcal{F}^\infty(M, I\!R^n)$ for each $j_P \in O$ such that it vanishes on $I\!R^n$ and has $\varphi(j_P)(1), ..., \varphi(j_P)(b)$ as its eigenvalues for any $j_P \in O$ then

$$\bar{F}_P = -\frac{1}{\beta} \cdot ln\ tr\ e^{-\beta\cdot Q} \qquad \text{on} \qquad O_P \tag{4.1.8}$$

and the state $\tilde{\rho}^P_{Gibbs} := \frac{\mathrm{f}}{\bar{F}_P}$ is determined by the partition function

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

Moreover $\frac{1}{b} \cdot tr\ Q^m = \lim_{\beta \longrightarrow 0} \mu_m$, where μ_m is the m-th order momentum of the Gibbs state $\tilde{\rho}^P_{Gibbs} = \frac{e^{-\beta\varphi}}{Z_P}$ on $\{1,...,b\}$. Clearly

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

Finally, let us introduce the concept of an **equilibrium configuration** $j_P \in O_P$: We require from j_P both to hold, namely $\Phi_P(j_P) = 0$ and $Grad_{\mathcal{G}_P} \bar{F}_P(j_P) = 0$, with $Grad_{\mathcal{G}_P}$ being the gradient formed with respect to $\mathcal{G}_P$.

4.2 The concept of free energy of the continuum

Let $\bar{F}_P$ on O_P be the free energy of A_P and $j_P^0 \in O_P$ be an equilibrium configuration. We regard $I\!D\,\bar{F}_P$ as a virtual work by itself and hence lift $I\!D\,\bar{F}_P$ by (3.2.2), 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

$$\bar{F}(j) = \bar{F}_P(r(j)) + const. \qquad \forall j \qquad \text{near any fixed} \qquad j' \in r^{-1}(j_P^0) \cap O.$$

Setting $const. = 0$ yields

$$\bar{F} = r^* \bar{F}_P. \tag{4.2.1}$$

The gradient $Grad_{\mathcal{G}(j_0)} \bar{F}$ formed with respect to $\mathcal{G}(j_0)$ satisfies

$$r_\infty(Grad_{\mathcal{G}(j_0)} \bar{F}(j')) = \varphi^P(j_P^0) \cdot Grad_{\mathcal{G}_P} \bar{F}_P(j_P^0) \qquad \forall j' \in r^{-1}(j_P^0) \cap O \tag{4.2.2}$$

for some $\varphi^P(j_P^0) \in \mathcal{F}(P, I\!R^+)$ as seen by lemma A2.1. Clearly A splits into

$$A = I\!D\,\bar{F} + \Psi \qquad \text{near any} \quad j' \in r^{-1}(j_P^0) \cap O \tag{4.2.3}$$

with $\Psi := A - I\!D\,\bar{F}$ and is the Neumann splitting formed slicewise with respect to $r_\infty^* \mathcal{G}_P$. In determining the divergence $\operatorname{div}_{\mathcal{W}(j')} A$ on each slice $\mathcal{W}(j')$, formed with respect to $r_\infty^* \mathcal{G}_P$, the structural capillarity a of A as defined in sec. one plays a crucial role. To see this we let $K_{\boldsymbol{r}} \subset \mathcal{W}(j')$ be a closed ball of radius $\boldsymbol{r}$ centered about $j \in \mathcal{W}(j')$. Due to (1.2.4), (4.2.3) and (A3.3)

$$\Delta_{\mathcal{W}(j')} \bar{F}(j) = \operatorname{div}_{\mathcal{W}(j')} A(j) = -dim M \cdot \lim_{\boldsymbol{r} \to 0} \frac{1}{\boldsymbol{r} \cdot vol\ K_{\boldsymbol{r}}} \cdot \int_{\partial K_{\boldsymbol{r}}} (a - a(j)) \cdot \mathcal{A}\ \mu_{\partial K_{\boldsymbol{r}}}. \tag{4.2.4}$$

Here $\Delta_{\mathcal{W}(j')}$ is the Laplacian on $\mathcal{W}(j')$. The structural capillarity a can be deduced by discrete data and $dim\, M$ only: a as given by (1.2.4) can be determined by the differential of the free energy $\bar{F}$ of A as seen from the observation

$$I\!D\,\bar{F}(j)(j) = I\!D\,\bar{F}(j)(j^\infty) = a(j) \cdot dim\, M \cdot \mathcal{A}(j) \qquad \forall j \in \mathcal{W}(j'). \tag{4.2.5}$$

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 j^∞ is the $r_\infty^* \mathcal{G}_P$-gradient at j. Here j^∞ is the component of j in $\mathcal{F}^\infty(M, I\!R^n)$. We thus find due to (A3.5), (1.2.3) and (A2.1) the following:

Proposition 4.2.1 *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*

$$a(j) \cdot dim\, M \cdot \sum_{q \in P} \varphi^P(j)(q) = I\!D\,\bar{F}_P(r(j))(r_\infty(j^\infty)). \tag{4.2.6}$$

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

Defining an **equilibrium configuration** $j' \in O$ by $A(j') = 0$ and $I\!\!D\,\bar{F}(j') = 0$ we immediately deduce that any $j' \in r^{-1}(j) \cap O$ is an equilibrium configuration if $r(j') \in O_P$ is one. Differentiating both sides of (4.2.6) and representing $I\!\!D^2 \bar{F}_P(j_0)$ by $\mathcal{G}_P$ via $I\!\!F_P \in End\ \mathcal{F}(P, I\!\!R^n)$, say, then by (4.2.2), proposition 4.2.1 and lemma A2.1 the following holds true:

Corollary 4.2.2

$$r_\infty(Grad_{\mathcal{G}(j_0)} a)(j_P^0) = \frac{1}{dim\, M \cdot \sum_{q \in P} \varphi^P(j_0)(q)} \cdot \bar{I\!\!F}_P j_P^0 \tag{4.2.7}$$

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

4.3 Linearized free energy, vibrational modes

Let $j_0 \in O$ be an equilibrium configuration. The force density map $\hat{\Phi}$ on $\mathcal{W}(j_0)$ of A (cf. (1.1.15) and (3.2.2)) is dominated near j_0 by the linear part, i.e

$$\hat{\Phi}(j_0 + l) = I\!\!D\,\hat{\Phi}(j_0)(l) \qquad + \text{higher order terms}$$

for all l near zero. Accordingly

$$\bar{F}(j_0 + l) = \bar{F}(j_0) + \frac{1}{2} I\!\!D^2 \bar{F}(j_0)(l, l) + \text{higher order terms.} \tag{4.3.1}$$

To define and compute the vibrational modes at j_0 let $I\!\!F \in End \mathcal{F}^\infty(M, I\!\!R^n)$ be such that $I\!\!D^2 \bar{F}(j_0) = \mathcal{G}(j_0)(I\!\!F ..., ...)$ and let $a_{\bar{F}}$ be the structural capillarity of the linearized $I\!\!D\,\bar{F}$. Due to (A3.4), the analogon of (4.2.4) on $\mathcal{W}(j_0)$ formed at j_0 reads here

$$tr\ I\!\!F = dim\, M \cdot \frac{1}{r \cdot vol\ K_r} \cdot \int_{K_r} (a_{\bar{F}} \cdot \mathcal{A})\ \mu_{\partial k_r}. \tag{4.3.2}$$

The i-th eigenvalue ν_i is called the i-th **vibrational mode** (cf. [Ch,St]), $i = 1, ..., b$. Let $\bar{F}$ be as in (4.3.1) and $a^i_{\bar{F}}$ be the structural capillarity of the linearized $I\!\!D\,(\bar{F} \circ \pi_i)$ where π_i is the $\mathcal{G}(j_0)$-orthogonal projection on $I\!\!R \cdot u_i$ and u_i is the i-th eigenvector of $I\!\!F$. Since $I\!\!D\,\bar{F} = \sum_i I\!\!D\,(\bar{F} \circ \pi_i)$ obviously $a_{\bar{F}} = \sum_{i=1}^b a^i_{\bar{F}}$ holds true and we thus find due to (4.3.2) the following:

Theorem 4.3.1 *For each $i = 1, ..., b$ the vibrational mode ν_i at j_0 is determined by*

$$\nu_i = dim\, M \cdot \frac{1}{r \cdot vol\ K_r} \cdot \int_{K_r} (a^i_{\bar{F}} - a^i_{\bar{F}}(j_0)) \cdot \mathcal{A}\ \mu_{\partial K_r} \tag{4.3.3}$$

5 A concept of a fitting surface

Let A_P, A and $\bar{F}$ be as in sec. 4.2. Moreover $j_P \in O_P$ and $j_0 \in O$ with $r(j_0) = j_P$ are supposed to be equilibrium configurations. The latter implies that $\bar{F}$ is constant along $r^{-1}(j_P)$ near j_0. We may work on $\mathcal{W}^\infty(j_0)$ only.

5.1 The motivation of the concept of first order fitting

The vibrational modes of the discrete medium and the continuum are the eigenvalues ν_P^i of $\mathbb{F}_P$ respectively ν_i of $\mathbb{F}$ for $i = 1, ..., b$ (cf. sec. 4.2 and 4.3). To link the two endomorphisms $\mathbb{F}_P$ and $\mathbb{F}$ we use lemma A2.1: There is a map $\varphi \in \mathcal{F}^\infty(M, \mathbb{R}^n)$ such that

$$\varphi \bullet r_\infty^{-1} \circ \mathbb{F}_P \circ r_\infty = \mathbb{F}.$$

Since the continuum is supposed to describe the discrete medium we require from j_0 that

$$r_\infty \circ \mathbb{F} = \mathbb{F}_P \circ r_\infty. \tag{5.1.1}$$

This implies in particular that $\nu_P^i = \nu_i$ and $r_\infty(u_i) = u_P^i$ for $i = 1, ..., b$, where u_i and u_P^i are the respective eigenvectors of $\mathbb{F}$ and $\mathbb{F}_P$. We thus call the equilibrium configuration a **first order fitting configuration** if $\varphi = 1$.

5.2 Simple conclusions for a first order fitting configuration

We present equations associated with a first order fitting configuration j_0 involving the structural capillarity. At first let us remark that j_0 is not uniquely determined, if it exists at all. Since the first order fitting configuration is defined via the linearization $\mathbb{D}^2\bar{F}(j_0)$ of $\mathbb{D}\bar{F}$ at j_0, the equations for j_0 have to emanate from this linearization. Due to (4.3.3) and (5.1.1)

$$v_P^i = v_i = dim\, M \cdot \frac{1}{\boldsymbol{r} \cdot vol\ K_{\boldsymbol{r}}} \cdot \int_{K_{\boldsymbol{r}}} (a_{\bar{F}}^i - a_{\bar{F}}^i(j_0)) \cdot \mathcal{A}\ \mu_{\partial K_{\boldsymbol{r}}} \qquad i = 1, ..., b$$

has to hold. Setting $j^\infty = \sum_{i=1}^b \iota_i \cdot u_i$ with u_i as in sec. 5.1, equation (4.2.7) together with corollary A2.2 yields

$$r_\infty\big(Grad_{\mathcal{G}(j_0)} a\big)(j_P^0) = \frac{1}{dim\, M \cdot \#P} \cdot \bar{\mathbb{F}}_P(j_P^0) \tag{5.2.1}$$

and hence ι_i satisfies

$$\mathbb{D}\, a(j_0)(u_i) = \nu_i \cdot \frac{\iota_i}{dim\, M \cdot \#P} \qquad \forall i = 1, ..., b$$

where $\#P$ denotes the number of points in P.

Appendices

A1 Complement in $C^\infty(M, I\!R^n)$ to $ker\, r$

Given a finite set $P \subset M$ the restriction map r, sending any $h \in C^\infty(M, I\!R)$ into its restriction $r(h)$ on P is a surjective $I\!R$-algebra homomorphism to $\mathcal{F}(P, I\!R)$, the $I\!R$-algebra of all $I\!R$-valued maps of P (the operations are defined pointwise). Constant maps in both $C^\infty(M, I\!R)$ and $\mathcal{F}(P, I\!R)$ are identified with their values in $I\!R$. Given a linear map $s : \mathcal{F}(P, I\!R) \longrightarrow C^\infty(M, I\!R)$ with $r \circ s = id$, we let $L := s(\mathcal{F}(P, I\!R))$. Setting $h \bullet k := s(r(h) \cdot r(k))$ for any two $h, k \in L$ turns L into an $I\!R$-algebra with unity, however, not into a subalgebra of $C^\infty(M, I\!R^n)$, in general. The projection $pr_L : C^\infty(M, I\!R) \longrightarrow L$ assigning to any $h \in C^\infty(M, I\!R)$ the function $sr(h) \in L$ is linear and satisfies $pr_L(h \cdot k) = pr_L\, h \bullet pr_L\, k$ for any $h, k \in C^\infty(M, I\!R)$, as seen by

$$pr_L(h \cdot k) = s\big(r(h \cdot k)\big) = s(r(h) \cdot r(k)) = (s(r(h)) \bullet (s(r(k))) = pr_L h \bullet pr_L k.$$

Thus $L \cong C^\infty(M, I\!R^n)/_{ker\, r}$ as $I\!R$-algebras with units. Moreover

$$C^\infty(M, I\!R) = ker\, r \oplus L \tag{A1.1}$$

as linear spaces. Due to $C^\infty(M, I\!R^n) = C^\infty(M, I\!R^n) \otimes I\!R^n$ we set $L(M, I\!R^n) := L \otimes I\!R^n$ and obtain

$$C^\infty(M, I\!R^n) = ker\, r \oplus L(M, I\!R^n). \tag{A1.2}$$

A2 L_2-scalar products on the discrete and the continuum

Let $P \subset M$ be as in A1. On $\mathcal{F}(P, I\!R)$ the discrete L_2-scalar product is given by

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

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

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

The relation between $r^*\mathcal{G}_P$ and $\mathcal{G}(g)$ on a complement $L \subset C^\infty(M, I\!R)$ of $ker\, r$ is as follows:

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

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

and vice versa any $\varphi(g)$ yields some φ^P in a unique manner. Given φ^P then

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

for any smooth symmetric two-tensor S on M.

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 $q, q' \in P$

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

we conclude $Qh_q = \xi(q) \cdot h_q$ for some $\xi(q) \in \mathbb{R}^+$. Thus $\mathcal{G}(q)(h,k) = \mathcal{G}_P(\xi^{-1} \cdot \varphi^P \cdot r(h), r(k))$ for all $h,k \in L$. Setting $\varphi(g) := s(\xi)$ yields

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

Thus $Qh = \varphi(g) \bullet h$ 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 on $\mathcal{M}$ 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 $h = k = \mathbf{1} \in \mathbb{R}$ in (A2.1) yields

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

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.

A3 On the Neumann problem

Let N be a smooth, compact, connected and oriented Riemannian manifold with boundary ∂N and metric g. The metrical divergence and the Laplacian are denoted by div and Δ respectively. Given $k \in C^\infty(N, \mathbb{R}^n)$ and $\varphi \in C^\infty(\partial N, \mathbb{R}^n)$ the Neumann boundary problem (cf. [Hö])

$$k = \Delta H \qquad \text{with} \qquad dH(\boldsymbol{n}) = \varphi \tag{A3.1}$$

has a solution H unique up to a constant iff the integrability condition

$$\int_N k\ \mu_N + \int_{\partial N} \varphi\ \mu_{\partial N} = 0 \tag{A3.2}$$

holds. Here $\boldsymbol{n}$ is the positively oriented unit normal of ∂N in N and μ_N as well as $\mu_{\partial N}$ denote the Riemannian volume forms on N respectively ∂N. Given any smooth $\mathbb{R}^n$-valued one-form α the integrability condition (A3.2) holds for $k = div\ \alpha$ and $\varphi = \alpha(\boldsymbol{n})$. Hence (A3.2) yields for any $q \in N$

$$k(q) = -\frac{1}{vol\ N} \cdot \int_{\partial N} \varphi\ \mu_{\partial N} + \qquad \text{higher order terms.} \tag{A3.3}$$

Here $vol\ N := \int_N\ \mu_N$. If $N = \mathbb{R}^m$ and $n = 1$ with g being a scalar product, (A3.3) yields for any $B \in End\ \mathbb{R}^m$ in particular

$$tr\ B = \frac{1}{vol\ N} \cdot \int_{\partial N} g(B..., \boldsymbol{n}(...))\ \mu_{\partial N}. \tag{A3.4}$$

For any $x \in \partial N$ the integrand takes the value $g(B(x), \boldsymbol{n}(x))$. Let X_α be such that $\alpha = g(X_\alpha, ...)$ then

$$\int_N g(X_\alpha, grad\ h)\mu_N = \int_N div\ \alpha \cdot h\ \mu_N + \int_{\partial N} \alpha(\boldsymbol{n}) \cdot h\ \mu_{\partial N}$$

yielding for $div\ \alpha = 0$ and $\alpha(\boldsymbol{n}) = 0$ the orthogonality relation

$$\int_N g(x_\alpha, grad\ h)\mu_N = 0. \tag{A3.5}$$

References:

[B,St] P.Bamberg, S.Sternberg : *A Course in Mathematics for Students of Physics 2*, Cambridge University Press, Cambridge, New York (1988)

[B] F. Bien : *Construction of Telephone Networks by Group Representation*, Notices of AMS, Vol.36, No.1 (1989)

[Bi1] E.Binz :*Symmetry, Constitutive Laws of Bounded Smoothly Deformable Media and Neumann Problems*, Symmetries in Science V, Ed. B.Gruber, L.C. Biedenharn and H.D. Doebner, Plenum Press, New York, London (1991)

[Bi2] E.Binz : *Global Differential Geometric Methods in Elasticity and Hydrodynamics, Differential Geometry, Group Representations, and Quantization*, Ed. J.B. Hennig, W. Lücke and J. Tolar, Lecture Notes in Physics, 379, Springer-Verlag, Berlin, Heidelberg, New York (1991)

[Bi3] E. Binz : *On the Irredundant Part of the First Piola-Kirchhoff Stress Tensor*, Rep. on Math. Phys, Vol 32, No.2, (1993)

[Bi4] E.Binz: *A physical Interpretation of the Irredundant part of the First Piola-Kirchhoff Stress Tensor of a Discrete Medium Forming a Skin*, Grazer Mathematische Berichte, No. 320, (1993).

[Bi,Fi] E.Binz, H.R. Fischer : *The Manifold of Embeddings of a closed Manifold*, Differential Geometric Methods in Mathematical Physics, 139, Springer Verlag, Berlin, Heidelberg, New York (1981)

[Bi,Sn,Fi] E.Binz, Sniatycki, H.-R.Fischer : *Geometry of Classical Fields*, Mathematics Studies 154, North-Holland, Amsterdam (1988).

[Ch,St] F.R.K.Chung, S.Sternberg: *Laplacian and Vibrational Spectra of Homogeneous Graphs*, Journal of Graph Theory Vol 16, No.6, John Wiley and Sons Inc. (1992).

[E] B. Eckmann: *Harmonische Funktionen und Randwertaufgaben in einem Komplex*, Comment.Math.Helv. Vol 17 (1944/45).

[Fr,Kr] A.Frölicher, A.Kriegl : *Linear Spaces and Differentiation Theory*, John Wiley and Sons Inc., Chichester, England (1988).

[G,H,V] W.Greub, S. Halperin, J.Vanstone: *Connections, Curvature and Cohomology, I and II*, Academic Press, New York, (1972-73).

[He] E.Hellinger: *Die allgemeinen Ansätze der Medien der Kontinua*, Enzykl. Math. Wiss. 4/4, (1914).

[Hö] L.Hörmander : *The Analysis of Linear Partial Differential Operators III*, Grundlehren der mathematischen Wissenschaften, Vol.274, Springer Verlag Berlin, Heidelberg, New York (1985).

[L,L] L.P.Landau, E.M. Lifschitz: *Lehrbuch der Theoretischen Physik, Vol. VII Elastizitätstheorie*, 4. Auflage, Akademie Verlag (1975).

[Ma] Y. Matsushima: *Vector Bundle Valued Harmonic Forms and Immersions of Riemannian Manifolds*, Osaka Journal of Mathematics, 8 (1971).

[M,H] J.E. Marsden, J.R. Hughes : *Mathematical Foundation of Elasticity*, Prentice - Hall, Inc. Englewood Clifts, New Jersey (1983).

Ernst Binz
Lehrstuhl für Mathematik I
Universität Mannheim
Seminargebäude A5
D-68131 Mannheim