**Idealized skins determined by finitely many particles**

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## 0. Introduction

In the present notes we study skins made up by finitely many material particles in $\mathbb{R}^3$. The picture we have in mind is a very large collection of material particles which interact such that we see a skin from the macroscopic point of view. In particular we are interested in the case where each particle acts only with its nearest neighbours.

The idealized situation we study is an follows: We have a large but finite collection $P'$ of mean locations in $\mathbb{R}^n$ of material particles. The interaction scheme is such that these locations, i.e. these points are all placed on a smooth, compact, oriented, closed manifold $M' \subset \mathbb{R}^n$ of $dim\ M \geq 2$. The manifold $M'$ is called the skin. We choose this dimensional set up because of specific dimensional factors appearing in the forthcoming formulas. At first, we do not specify the interaction scheme any further.

However, along the line of our development we refine the set up by drawing an edge in $M'$ between the location of two interacting particles, i.e. a geodesic segment and require that the graph obtained in this way is a simplicial one-complex in $M'$. This complex reflects the nearest neighbour interaction scheme: Each point $q_i'$ which is connected by an edge with $q$ is a nearest neighbour of $q$.

$M' \subset \mathbb{R}^n$ represents the continuum, the one-complex visualizes the large collection of interacting particles.

The study of this interaction scheme in relation to the geometric and topological properties of the skin is one of the main purposes of these notes. However, we will study at first the interaction between $P'$ and the skin $M'$ without specifying any interaction scheme in order to keep the full generality and to see how the nearest neighbour interaction influences the set up.

In the following part of this introduction we will describe the topological and geometrical frame work more closely.

Since both $M'$ and $P' \subset M'$ will be deformed in $\mathbb{R}^n$ we replace $M'$ and $P'$ by intrinsic objects, this is to say by a smooth, compact, oriented, closed manifold $M$ and a collection of points $P \subset M$. Both $M'$ and $P'$ will be obtained from $M$ and $P$ by a smooth embedding $j : M \longrightarrow \mathbb{R}^n$ namely by $M' = j(M)$ and $P' = j(P)$. Passing from $j$ to another embedding $j_1$ describes a deformation from $j(M)$ to $j_1(M)$.

Thus the configuration space of our medium is $E(M, \mathbb{R}^n)$, the collection of all smooth embeddings from $M$ into $\mathbb{R}^n$. Endowed with the $C^\infty$-topology $E(M, \mathbb{R}^n)$ is a smooth Fréchet manifold (cf. [Bi,Sn,Fi]). It is an open subset of $C^\infty(M, \mathbb{R}^n)$, the $\mathbb{R}$-vector space of all smooth $\mathbb{R}^n$-valued maps of $M$ endowed with the $C^\infty$-topology. Restricting each $j \in E(M, \mathbb{R}^n)$ onto the collection $P$ yields a configuration of $P$. By $E^\infty(P, \mathbb{R}^n)$ we denote the collection of all these restrictions. This configuration space of $P$ is an open set of the finite dimensional space $\mathcal{F}(P, \mathbb{R}^n)$ of all $\mathbb{R}^n$-valued maps of $P$. We will use $E(M, \mathbb{R}^n)$ for the description of the continuum and $E^\infty(P, \mathbb{R}^n)$ for the description of the discrete medium. The link between $E(M, \mathbb{R}^n)$ and $E^\infty(P, \mathbb{R}^n)$ i.e. the restriction map will then be used to link the two different descriptions.

So far we sketched the topological situation. Let us next show how we characterize the medium forming the skin $j(M)$, a continuum.

First of all we assume that no external force densities are present.

The medium considered as a continuum at the configuration $j$ is classified by its internal force density $\Phi(j)$ resisting a deformation $l$. (For simplicity we let $\Phi$ depend on $j$ only). The classification of media with the help of internal force densities is a rather rough scheme. Both $\Phi(j)$ and $l$ are assumed to be smooth, i.e. $\Phi(j), l \in C^\infty(M, \mathbb{R}^n)$. Since $\Phi(j)$ is of internal nature (and hence invariant under the translation group $\mathbb{R}^n$ of $\mathbb{R}^n$) it does not cause any work against a constant distortion $z \in \mathbb{R}^n$. Hence $\int_M < \Phi(j), z > \mu(j) = 0$. Here $\mu(j)$ is the Riemannian volume caused by the Riemannian metric $j^* <,>$, the pull back by $j$ of the fixed scalar product $<,>$ on $\mathbb{R}^n$. Therefore $\int_M \Phi(j)\mu(j) = 0$. This means, however, that

$$\Phi(j) = \Delta(j)\mathcal{H}(j) \tag{0.1}$$

has a solution $\mathcal{H}(j)$, where $\Delta(j)$ is the Laplacian on $M$ determined by $j^* <,>$ and $\mathcal{H}(j) \in C^\infty(M, \mathbb{R}^n)$ is smooth in $j$. Here $j$ varies in an open subset $O \subset E(M, \mathbb{R}^n)$. The virtual work $A$ determined by $\Phi$ is a one-form on $E(M, \mathbb{R}^n)$ introduced in chapter one. We will linearize it and study in particular exact linearized one-forms on $O$ (cf. sections one and four). Here we will see that these sorts of virtual works are characterized by - what we call - the structural capillarity $a$ and the area functional $\mathcal{A}$ both defined on $O$. So far we have neglected $P$.

To elaborate a physical interpretation of $\mathcal{H}(j)$ and to exhibit some of its main properties will be major tasks of our paper.

We will do so in particular within the frame work of nearest neighbour interaction, i.e. we take the simplicial structure of $P$ into account. It will turn out that $\mathcal{H}(j)(q) - \mathcal{H}(j)(q_i)$ is linked to the interaction force within the medium of the particle at $q$ with the one at $q_i$, a nearest neighbour of $q$. This will be seen in section three. As we will see, the geometry may hinder the direct sight to the interaction mechanism.

This interpretation, however, requires that we have a natural way to describe the discrete medium as a continuum. In doing so, we need to understand which part of the formalism requires the nearest neighbour interaction scheme. Therefore we treat first the situation of an arbitrary interaction scheme within the collection of particles and show how to describe naturally the discrete medium as a continuum, i.e. by formalisms associated with the continuum.

To this end we consider in section 2 the restriction map $r : C^\infty(M, \mathbb{R}^n) \longrightarrow \mathcal{F}(P, \mathbb{R}^n)$ and construct a space $\mathcal{F}^\infty(M, \mathbb{R}^n) \subset C^\infty(M, \mathbb{R}^n)$ on which $r$ is an isomorphism. The force density $\Phi(j)$ is then said to be produced by the finitely many particles if $\Phi(j) \in \mathcal{F}^\infty(M, \mathbb{R}^n)$. The finite dimensional vector space $\mathcal{F}^\infty(M, \mathbb{R}^n)$ will be a special choice of a complement to $ker\ r$ (since there is now canonical complement). The motivation of the choice is based on (0.1) and on a fixed configuration $j_0 \in E(M, \mathbb{R}^n)$, called a reference configuration, thought of as an equilibrium configuration. We will rewrite the above equation for the internal force density as

$$\Phi(j) = \Delta(j_0)\widehat{\mathcal{H}}(j). \tag{0.2}$$

Here $\Delta(j_0)$ is fixed, while $\widehat{\mathcal{H}}$ still depends on $j \in O$. The complement $\mathcal{F}^\infty(M, \mathbb{R}^n)$ to $ker\ r$ is such that it is generated by finitely many eigenvectors of $\Delta(j_0)$, implying that $\mathcal{F}^\infty(M, \mathbb{R}^n)$ is preserved by this Laplace operator. The map $r$ restricted to $\mathcal{F}^\infty(M, \mathbb{R}^n)$ is called $r_\infty$.

The link with the discrete regime is made up as follows: Since there is a natural metric $\mathcal{G}_P$ on the space $\mathcal{F}(P, \mathbb{R}^n)$, there is a natural metric on $\mathcal{F}^\infty(M, \mathbb{R}^n)$ namely its pull back $r_\infty^* \mathcal{G}_P$ to $\mathcal{F}^\infty(M, \mathbb{R}^n)$. It has to be compared with the given $L_2$-metric $\mathcal{G}(j_0)$ defined by $j_0^* <,>$ on $M$. We call $j_0$ metrically well fitting if $\mathcal{G}(j_0) = r_\infty^* \mathcal{G}_P$. This kind of equilibrium configuration $j_0$ for low dimensional ambient space $\mathbb{R}^n$ does not exist in general (cf. [G,R]).

The virtual work $A_P$ on a closed neighbourhood $\mathcal{W}(j_P^0)$ of a configuration $j_P^0 \in E^\infty(P, \mathbb{R}^n)$, caused by distorting the finite collection of interacting particles, will be pulled back to $\mathcal{W}^\infty(j_0) \subset E(M, \mathbb{R}^n)$ and there represented by an internal force density in the sense of 0.2. Here $r_\infty(\mathcal{W}^\infty(j_0)) \subset E(M, \mathbb{R}^n)$ with $r_\infty(j_0) = j_P^0$ and $\mathcal{W}^\infty(j_0) - j_0 \in \mathcal{F}^\infty(M, \mathbb{R}^n)$ is a closed neighbourhood of zero. The pull back $A := r_\infty^* A_P$ is hence the virtual work on the continuum; $\mathcal{H}_P^M$ is its constitutive map.

In case of a first neighbour interactions the force $\Phi_P$ causing the virtual work $A_P$ is itself of the form 0.2 on $\mathcal{W}(j_P^0)$; however, $\Delta(j_0)$ has to be replaced by the topological Laplacian $\Delta_T$ determined by the simplicial structure. In addition $\widehat{\mathcal{H}}$ will have to be replaced by $\mathcal{H}_P$, say. Since $\mathcal{H}_P(j_P)(q) - \mathcal{H}_P(j_P)(q_i)$ reflects for any $j_P \in \mathcal{W}(j_P^0)$ the interaction force within the medium between the particle at any $q$ with the one at $q_i$, a nearest neighbour of $q$, the difference $\widehat{\mathcal{H}}_P^M(j)(q) - \widehat{\mathcal{H}}_P^M(j)(q_i)$ hence does so too, for any $j \in \mathcal{W}(j_0)$ provided that $j_0$ is metrically well fitting. Here $\Phi_P^M := \Delta(j_0)\widehat{\mathcal{H}}_P^M$ is the force density of $A$. The internal force $\Phi_P(j_P)(q)$ is the resulting force of the interaction force between the particle at $q$ with all its nearest neighbours; vice versa any internal force has to be of this form. This interpretation holds accordingly for $\Phi_P^M(j)(q)$.

Since $r_\infty^* A$ is defined on a finite dimensional neighbourhood $\mathcal{W}^\infty(j_0)$ we will use the Neumann splitting to exhibit in section 2.2 its exact part $\mathbb{D}\overline{F}$, the differential of what we call the free energy $\overline{F}$ and will see that $\overline{F} = r_\infty^* \overline{F}_P$. Here $F_P$ is the free energy of the discrete regime (constructed with the help of the Neumann boundary value problem, too). In this context a metrically well fitting configuration will be called good fitting if $\mathbb{D}\overline{F}(j_0) = 0$, i.e. if $j_0$ is a stationary configuration of $\overline{F}$.

Fixing a temperature $T$, a Gibbs state $\rho_e$ and an observable $I$ are defined on $\mathcal{W}^\infty(j_0)$, such that the free energy of $I$ is $\overline{F}$. In this sense the term 'free energy' from above has to be understood in these notes. Here again $\mathcal{W}^\infty(j_0)$ is assumed to be that small that any distortion within $\mathcal{W}^\infty(j_0) - j_0$ does not affect $T$ from the physical point of view. A more realistic version of this mechanism would have to be done on $\mathcal{W}^\infty(j_0) \times \mathbb{R}$ (cf. [Bi6]).

In the last chapter we study the whole apparatus in the frame work of the linearized situation and exhibit the influence of the structural capillarity - a constitutive entity - to the equilibrium configuration.

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# 1. Description of deformable continua

## 1.1 The constitutive law on a continuum

Let $M$ be a smooth, connected, oriented and compact manifold. $M$ shall be equipped with a **mass density** $\rho_m$, a smooth real valued function on $M$ (cf. appendix 2). The manifold together with this mass distribution is referred to as the standard body. In what follows we refer to the items [B1], to [Bi6] as well as to [Bi, Fi 2] in the references.

We begin by specifying what we mean by a configuration and the space of configurations. Let $M$ be embeddable into $\mathbb{R}^n$. Any smooth embedding

$$j : M \longrightarrow \mathbb{R}^n$$

is called a configurations of $M$. The space of all configuration is called $E(M, \mathbb{R}^n)$; it shall be endowed with the $C^\infty$-topology. $E(M, \mathbb{R}^n)$ is thus a Fréchet manifold (cf. [Bi,Sn,Fi], [Fr,Kr] and [Bi,Fi1]). In fact it is an open subset of the collection $C^\infty(M, \mathbb{R}^n)$ of all $\mathbb{R}^n$-valued smooth functions of $M$ endowed with the $C^\infty$-topology.

Let us fix a scalar product on $\mathbb{R}^n$ in order to introduce metric concepts on $M$. Each $j \in E(M, \mathbb{R}^n)$ defines a **Riemannian metric** $m(j)$, the pull back of $<,>$ by $j$. Moreover $m(j)$ and the given orientation determine the **Riemannian volume form** $\mu(j)$. For any two $j, j_0 \in E(M, \mathbb{R}^n)$ with fixed $j_0$ the metrics $m(j)$ and $m(j_0)$ respectively their associated volume forms $\mu(j)$ and $\mu(j_0)$ are related by

$$m(j)(v, w) = m(j_0)\big(f^2(j)v, w\big) \quad \forall v, w \in TM$$

and

$$\mu(j) = det\ f(j) \cdot \mu(j_0) \quad \forall v, w \in TM \tag{1.1.1}$$

where $f^2(j)$ is a uniquely determined strong smooth bundle isomorphism on $TM$ selfadjoint with respect to $m(j_0)$ (cf. appendix 1).

Next let us specify what is meant here by a constitutive law. (Throughout the paper we neglect external force densities) By a **constitutive law** of a medium we mean in these notes the prescription of either the **internal force density** $\Phi(j)$ (to be specified below) at a configuration $j$ varying in an open set $O \subset E(M, \mathbb{R}^n)$ or any ingredient out of which $\Phi(j)$ can be derived. For simplicity we let $O = E(M, \mathbb{R}^n)$ in this section.

Therefore, we point out that a medium *is characterized here only in as far as it determines the internal force density.*

By a smooth internal force density $\Phi(j)$ at the configuration $j \in E(M, \mathbb{R}^n)$ we mean a smooth map

$$\Phi(j) : M \longrightarrow \mathbb{R}^n \tag{1.1.2}$$

depending smoothly on $j \in E(M, \mathbb{R}^n)$ and satisfying the following two requirements

$$(i) \qquad \int_M \Phi(j)\mu(j) = 0 \quad \forall j \in E(M, \mathbb{R}^n), \tag{1.1.3}$$

saying that $\Phi(j)$ is $L_2(j)$-orthogonal to the collection of all constant maps and

$$(ii) \qquad \Phi(j+z) = \Phi(j) \quad \forall j \in E(M, \mathbb{R}^n) \quad \text{and} \quad \forall z \in \mathbb{R}^n \tag{1.1.4}$$

reflecting the invariance of $\Phi$ under the translation group $\mathbb{R}^n$ of $\mathbb{R}^n$. Hence an internal force density $\Phi(j)$ at $j$ depends on $dj$ only!

The constraint $(i)$ an internal force density has to satisfy, is directly related to the centre of mass defined with respect to the mass density $\rho_m$ (cf. appendix 2): For a given embedding $j \in E(M, \mathbb{R}^n)$ the **centre $z_m(j)$ of mass** is defined by

$$z_m(j) \cdot \int_M \rho_m(j)\mu(j) = \int_M \rho_m(j) \cdot j \cdot \mu(j). \tag{1.1.5}$$

For any $z \in \mathbb{R}^n$, the map $j + z$ is a smooth embedding and its centre of mass is $z_m(j) + z$. Obviously, an internal force density has to satisfy

$$\int_M < \Phi(j), z_m(j) > \mu(j) = 0 \tag{1.1.6}$$

for $j \in E(M, \mathbb{R}^n)$, implying (1.1.3). In terms of the **$L_2$-metric** $\mathcal{G}(j)$ on $C^\infty(M, \mathbb{R}^n)$ (cf. appendix 1) equation (1.1.6) reads as

$$\mathcal{G}(j)\big(\Phi(j), z_m\big) = 0. \tag{1.1.7}$$

Let $\Phi$ be given internal force density. By (1.1.3) we find a smooth map

$$\mathcal{H} : E(M, \mathbb{R}^n) \longrightarrow C^\infty(M, \mathbb{R}^n) \tag{1.1.8}$$

such that

$$\Delta(j)\mathcal{H}(j) = \Phi(j) \quad \forall j \in E(M, \mathbb{R}^n). \tag{1.1.9}$$

Here $\Delta(j)$ is the Laplace operator on $M$ determined by $m(j)$. (cf. [Ma],[L,M] or [G,H,L]). Vice versa, for any smooth map

$$\mathcal{H} : E(M, I\!R^n) \longrightarrow C^\infty(M, I\!R^n)$$

the map

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

defined by

$$\Phi(j) := \Delta(j)\mathcal{H}(j) \quad \forall j \in E(M, I\!R^n) \tag{1.1.10}$$

is a smooth internal force density. The smooth map $\mathcal{H}$ is called the **constitutive map**.

A constitutive law on $M$ is therefore specified by a constitutive (smooth) map

$$\mathcal{H} : E(M, I\!R^n) \longrightarrow C^\infty(M, I\!R^n).$$

Hence $\Phi(j)$ is an internal force density for all $j \in E(M, I\!R^n)$ iff (1.1.4) and

$$\Phi(j) = \Delta(j)\mathcal{H}(j) \quad \forall j \in E(M, I\!R^n) \tag{1.1.11}$$

hold. The **virtual work** $A(j)(l) \in I\!R$ the internal force density $\Phi(j)$ causes against a distortion $l \in C^\infty(M, I\!R^n)$ at any $j \in E(M, I\!R^n)$ is given by

$$A(j)(l) = \int_M < \Phi(j), l > \mu(j) = \int_M < \Delta(j)\mathcal{H}(j), l > \mu(j). \tag{1.1.12}$$

( The general study of the virtual work can be found in [E,S] and [He]). Using the metric $\mathcal{G}(j)$ in appendix 1 we hence can rewrite $A(j)(l)$ as

$$A(j)(l) = \mathcal{G}(j)\big(d\mathcal{H}(j), d(l)\big) = \int_M d\mathcal{H}(j) \bullet dl\mu(j) \tag{1.1.13}$$

for any $j \in E(M, I\!R^n)$ and any $l \in C^\infty(M, I\!R^n)$.

For convenience $A$ is refered to as a constitutive law, too.

The internal force density $\Phi(j) : M \longrightarrow I\!R^n$ splits pointwise into parts $\Phi_N(j)$ and $\Phi_T(j)$, normal respectively tangential to $j(M)$, this is to say

$$\Phi(j) = \Phi_N(j) + \Phi_T(j); \tag{1.1.14}$$

the normal part $\Phi_N(j)$ is determined via the virtual work $A$ via

$$A(j)(N(j)) = \int_M d\mathcal{H}(j) \bullet dj\ W(j_0)\mu(j) = \int_M < \Phi(j), N(j) > \mu(j) \qquad (1.1.15)$$

Here $N(j) : M \longrightarrow \mathbb{R}^n$ is the pointwise defined unit normal to $T_jTM$ and $W(j_0) \in End\ TM$, the **Weingarten map**, is given by

$$dN(j) = dj\ W(j_0) \qquad (1.1.16)$$

and $\bullet$ is as in appendix 1. $j_0 \in E(M, \mathbb{R}^n)$ is called an **equilibrium configuration** if $A(j_0) = 0$ this is to say if $\Phi(j_0) = 0$. Hence $j_0$ is an equilibrium configuration iff

$$\Phi_T(j_0) = 0 \quad \text{and} \quad \Phi_N(j_0) = 0. \qquad (1.1.17)$$

To perform calculations involving configurations near a fixed one $j_0 \in E(M, \mathbb{R}^n)$ it is convenient to replace the right hand side of $\Phi(j) = \Delta(j)\mathcal{H}(j)$ by an expression involving $\Delta(j_0)$ only. To do so we proceed as follows: Using (1.1.1) we have

$$\int_M \Phi(j)\mu(j) = \int_M \Phi(j) detf(j)\mu(j_0) \qquad (1.1.18)$$

and by (1.1.11) hence

$$\Phi(j) = detf^{-1}(j) \cdot \Delta(j_0) \cdot \widehat{\mathcal{H}}(j) \quad \forall j \in E(M, \mathbb{R}^n). \qquad (1.1.19)$$

The equation admits a solution $\widehat{\mathcal{H}}(j)$ smooth in $j$ and uniquely determined up to a constant and the virtual work associated with $\widehat{\mathcal{H}}$ is

$$\begin{aligned} A(j)(l) = \mathcal{G}(j)(\Phi(j), l) &= \int_M < \Phi(j), l > \mu(j) \\ &= \mathcal{G}(j_0)(\Delta(j_0)\widehat{\mathcal{H}}(j), l) \end{aligned}$$

Let $C^\infty(M, \mathbb{R}^n)_{j_0} := \{l \in C^\infty(M, \mathbb{R}^n) | l \perp_{L_2(j_0)} \mathbb{R}^n\}$ where $\perp_{L_2(j_0)}$ means orthogonal with respect to the $L_2$-metric $\mathcal{G}(j_0)$ assigning to each pair $h, l \in C^\infty(M, \mathbb{R}^n)$ the value

$$\mathcal{G}(j_0)(h, l) = \int_M < h, l > \mu(j_0). \qquad (1.1.20)$$

**Definition 1.1.1:**

*Let $\widehat{\mathcal{H}}$ be called $\mathcal{G}(j_0)$-**normalized** if*

$$\mathcal{G}(j_0)(\widehat{\mathcal{H}}(j), z) = 0 \qquad (1.1.21)$$

*for all $z \in \mathbb{R}^n$ i.e. if $\widehat{\mathcal{H}}(j) \in C^\infty(M, \mathbb{R}^n)_{j_0}$ for all $j$ in the domain of $\widehat{\mathcal{H}}$.*

In summarizing we state (for $\mathcal{g}$ cf. appendix 1):

**Lemma 1.1.2:**

*Let $j_0 \in E(M, \mathbb{R}^n)$ be fixed and $\Phi$ be an internal force density. For each $j \in E(M, \mathbb{R}^n)$ the equation*

$$\widehat{\Phi}(j) := detf(j) \cdot \Phi(j) = \Delta(j_0)\widehat{\mathcal{H}}(j) \tag{1.1.22}$$

*has a unique $\mathcal{G}(j_0)$-normalized solution $\widehat{\mathcal{H}}(j)$ in $C^\infty(M, \mathbb{R}^n)$. Moreover*

$$\begin{aligned} \mathcal{G}(j)(\Phi(j), h) = \int_M < \Phi(j), h > \mu(j) &= \int_M < \widehat{\Phi}(j), h > \mu(j_0) \\ &= \int_M < \Delta(j_0)\widehat{\mathcal{H}}(j), h > \mu(j) \\ &= \mathcal{G}(j_0)\big(\Delta(j_0)\widehat{\mathcal{H}}(j), h\big) \\ &= \mathcal{g}(j_0)\big(d\widehat{\mathcal{H}}(j), dl\big). \end{aligned} \tag{1.1.23}$$

Since (1.1.23) involves a fixed Laplacian we may use **Fourier expansions** associated with $j_0$: Let $\widehat{e}_1, \widehat{e}_2, ...$ be the **eigenvectors** of $\Delta(j_0)$ having **respective eigenvalues** $0 < \lambda_1 \leq \lambda_2 \leq \ldots$. Let $\mathcal{H}$ satisfy (1.1.21). Then

$$\widehat{\mathcal{H}}(j) = \sum_{i=1}^{\infty} \widehat{\kappa}^i(j)\widehat{e}_i \tag{1.1.24}$$

where $\widehat{\kappa}^i$ is the $i^{th}$ Fourier coefficient of $\widehat{\mathcal{H}}(j)$ for all $j$ in the domain of $\widehat{\mathcal{H}}$; obviously

$$\widehat{\Phi}(j) = \sum_{i=1}^{\infty} \lambda_i\widehat{\kappa}^i(j)\widehat{e}_i. \tag{1.1.25}$$

The real number $\widehat{\kappa}^i(j)$ will be called the $i^{th}$ **global coefficients** at the configuration $j$. In general these Fourier coefficients regarded as $\mathbb{R}$-valued maps will not be independent from each other.

Clearly $\Phi(j_0) = 0$ iff $\widehat{\kappa}(j_0)^i = 0$ for all $i = 1, ..., \infty$.

To prepare the study of the area sensitive part of the virtual work we introduce the **area map**

$$\mathcal{A} : E(M, \mathbb{R}^n) \longrightarrow \mathbb{R}$$

given by

$$\mathcal{A}(j) = \int_M \mu(j) \quad \forall j \in E(M, I\!R^n) \tag{1.1.26}$$

where $\mu(j)$ is the Riemannian volume form. As it is easily seen (cf. appendix 1)

$$I\!D\,\mathcal{A}(j)(h) = \int_M dj \bullet dh\mu(j) = \int_M < \Delta(j)j, h > \mu(j) \quad \forall j \in E(M, I\!R^n) \tag{1.1.27}$$

holds true. In addition we have

$$\Delta(j)j = -tr\ S(j) \quad \forall j \in E(M, I\!R^n) \tag{1.1.28}$$

where $S(j)$ is the second fundamental tensor (cf.[Bi,Sn,Fi] or [G,K,M]). (For the calcules on Fréchet spaces we refer to [Bi,Sn,Fi] or [Fr,Kr].) In case of $1 + dim\ M = n$

$$\Delta(j)j = H(j)N(j) \tag{1.1.29}$$

where $H(j)$ is the **trace of the Weingarten map** $W(j)$ and $N(j)$ is the oriented unit normal of $j(M)$ along $j$ (cf. 1.1.16). This is the motivation for calling $\Delta(j)j$ in (1.1.28) the mean curvature tensor.
Clearly $\Delta(j)j$ (and hence $H(j)N(j)$ in case of $codim\ M = 1$) is the value of the $\mathcal{G}$-gradient $Grad_{\mathcal{G}}\mathcal{A}$ of $\mathcal{A}$ at $j$. For $\mathcal{G}$ consult appendix 1.

Let us study next the component (formed with respect to $\mathcal{G}(j)$) along $dj$ of the differential $d\mathcal{H}(j)$, of any constitutive map $\mathcal{H} : E(M, I\!R^n) \longrightarrow C^\infty(M, I\!R^n)$. To this end we point out that due to (1.1.4) the differential $d\mathcal{H}(j)$ depends on $dj$ only rather than $j$! We form

$$\mathcal{G}(j)\big(d\mathcal{H}(j), dj\big) = \int_M d\mathcal{H}(j) \bullet dj\mu(j) \quad \forall j \in E(M, I\!R^n)$$

(cf. appendix 1). Since the square of the $\mathcal{G}(j)$-norm of $dj$ is

$$\mathcal{G}(j)(dj, dj) = dim\ M \cdot \mathcal{A}(j) \quad \forall j \in E(M, I\!R^n)$$

we write

$$\mathcal{G}(j)\big(d\mathcal{H}(j), dj\big) = a(j) \cdot dim\ M \cdot \mathcal{A}(j) \quad \forall j \in E(M, I\!R^n). \tag{1.1.30}$$

Therefore $d\mathcal{H}(j)$ splits for any $j \in E(M, I\!R^n)$ into

$$d\mathcal{H}(j) = a(j) \cdot dj + d\mathcal{H}_1(j) \tag{1.1.31}$$

with $\mathcal{G}(j)\big(d\mathcal{H}_1(j), dj\big) = 0$. (At this point we have used the $dj$ dependence of $d\mathcal{H}(j)$).

Here $a : E(M, \mathbb{R}^n) \longrightarrow \mathbb{R}$ given by (1.1.31) for all $j \in E(M, \mathbb{R}^n)$ is an $\mathbb{R}^n$-invariant smooth map called the **structural capillarity** (cf. [Bi2] and [Bi3]). (It is the coefficient of the surface tension (Kapillaritätskonstante)). If $A$ and $A_1$ are the virtual works determined by $\mathcal{H}$ and $\mathcal{H}_1$ respectively, then

$$A(j)(h) = a(j) \cdot \mathbb{D}\mathcal{A}(j)(h) + A_1(j)(h) \tag{1.1.32}$$

for all the variables $j$ and $h$, saying that $a \cdot \mathbb{D}\mathcal{A}$ is the **area sensitive part** of $A$ and $A_1$ is not sensitive to the distortion of the volume. If $A(j) = 0$ then

$$a(j) = 0 \quad \text{and} \quad A_1(j) = 0 \tag{1.1.33}$$

since $\mathbb{D}\mathcal{A}(j)(j) = \mathcal{A}(j) \cdot dim\ M$. Hence the structural capillarity $a$ is determined by

$$A(j)(j) = a(j) \cdot \mathbb{D}\mathcal{A}(j)(j). \tag{1.1.34}$$

Clearly (1.1.31) shows that $a$ is of a constitutive nature. The following is obvious:

**Lemma 1.1.3:**

*The area sensitive part of a virtual work $A$ defined on an open neighbourhood $O$ of $j_0 \in E(M, \mathbb{R}^n)$ is determined by the structural capillarity $a$. This capillarity is given by*

$$A(j_0 + l)(j_0 + l) = dim\ M \cdot a(j_0 + l) \cdot \mathcal{A}(j_0 + l) \tag{1.1.35}$$

*Approximating both sides at $j_0$ up to terms of order two yields*

$$\begin{aligned} &A(j_0)(j_0) + A(j_0)(l) + \mathbb{D}A(j_0)(l)(j_0) + \mathbb{D}A(j_0)(l)(l) \\ &= dim\ M \cdot \big(a(j_0) \cdot \mathcal{A}(j_0) + \mathbb{D}(a \cdot \mathcal{A})(j_0)(l) + \frac{1}{2}\mathbb{D}^2(a \cdot \mathcal{A})(j_0)(l, l)\big) \end{aligned} \tag{1.1.36}$$

The **constitutive law** is called **linear** if

$$A(j_0 + l)(h) = A(j_0) + \mathbb{D}A(j_0)(l)(h) \tag{1.1.37}$$

for all $l \in O - j_0$ where $O$ is an open neighbourhood of $j_0 \in E(M, \mathbb{R}^n)$. In this case the constitutive map is given by

$$\widehat{\mathcal{H}}(j_0 + l) = \widehat{\mathcal{H}}(j_0) + \mathbb{D}\widehat{\mathcal{H}}(j_0)(l) \quad \forall\, l \in O - j_0. \tag{1.1.38}$$

Moreover we call a constitutive law $A$ to be exact if $A = I\!D\,\overline{F}$, where $\overline{F}$ is a smooth $I\!R$-valued map defined on some open set of $E(M, I\!R^n)$. (In section 2.2 we will split off the exact part of any virtual work $A$ " caused by finitely many particles ").

If $A = I\!D\,\overline{F}$ with $I\!D\,\overline{F}(j_0) = 0$ saying that $j_0$ is a **stationary configuration** for $\overline{F}$ then the linearity of $A$ implies

$$I\!D\,\overline{F}(j_0 + h)(k) = I\!D^2\overline{F}(j_0)(h,k) \quad \forall\, h,k \in O - j_0.$$

If $A = I\!D\,\overline{F}$ and linear in addition (cf. 1.1.35) then $\overline{F}$ on $O$ is given by

$$\overline{F}(j_0 + h) = \overline{F}(j_0) + \frac{1}{2} I\!D^2\overline{F}(j_0)(h,h) \quad \forall\, h \in O - j_0.$$

Lemma 1.1.3 yields therefore :

**Theorem 1.1.4:**

*Let $\overline{F}$ be a smooth real-valued map defined on some open neighbourhood $O$ of $j_0 \in E(M, I\!R^n)$ for which $I\!D\,\overline{F}$ admits a constitutive map $\mathcal{H}_{\overline{F}} : O \longrightarrow C^\infty(M, I\!R^n)$. Then*

$$I\!D\,\overline{F}(j_0 + l)(j_0 + l) = dim\ M \cdot a(j_0 + l) \cdot \mathcal{A}(j_0 + l) \quad \forall\, l \in O - j_0. \qquad (1.1.39)$$

*Let $I\!D\,\overline{F}$ be linear on $O$ with $I\!D\,\overline{F}(j_0) = 0$. Then*

$$I\!D^2\overline{F}(j_0)(h,k) = \frac{dim\ M}{2} \cdot I\!D^2(a \cdot \mathcal{A})(j_0)(h,k) \quad \forall\, l \in O - j_0 \qquad (1.1.40)$$

*and*

$$I\!D^2\overline{F}(j_0)(j_0,h) = dim\ M \cdot I\!D\,(a \cdot \mathcal{A})(j_0)(h) \quad \forall\, l \in O - j_0 \qquad (1.1.41)$$

*hold true for all $h,k \in C^\infty(M, I\!R^n)$. If $I\!D\,\overline{F}$ is linear on $O$ then $a(j_0) = 0$, provided $I\!D\,\overline{F}(j_0) = 0$; if $I\!D\,\overline{F}(j_0) = 0$ then for each $l \in O - j_0$ the value of $F(j_0 + l)$ is*

$$\overline{F}(j_0 + l) = \overline{F}(j_0) + \frac{1}{2} I\!D^2\overline{F}(j_0)(l,l) = \overline{F}(j_0) + \frac{dim\ M}{4} I\!D^2(a \cdot \mathcal{A})(j_0)(l,l) \quad (1.1.42)$$

*and $a$ is the structural capillarity of $I\!D\,\overline{F}$, i.e.*

$$a(j_0 + l) = \frac{1}{dim\ M \cdot \mathcal{A}(j_0 + l)} \cdot I\!D^2(a \cdot \mathcal{A})(j_0)(l, j_0 + l) \quad \forall\, l \in O - j_0. \qquad (1.1.43)$$

*Since $I\!D\,\overline{F}$ admits a constitutive map, $\mathcal{H}_{\overline{F}}$ say, the $\mathcal{G}$-gradient at $j \in O$ is $Grad_{\mathcal{G}}\overline{F}(j) = \Delta(j)\mathcal{H}_{\overline{F}}(j)$. Therefore $\mathcal{H}_{\overline{F}}(j_0 + l)$ is determined for each $l \in O - j_0$ by*

$$\Delta(j_0 + l)\mathcal{H}_{\overline{F}}(j_0 + l) = \mathcal{A}(j_0) \cdot I\!D\,(Grad_{\mathcal{G}}\ a)(j_0)(l) \qquad (1.1.44)$$

*provided* $I\!D\,\overline{F}(j_0) = 0$ *(since* $a(j_0) = 0$*).*

Theorem 1.1.4 requires us to investigate the relationship between $\overline{F}$ and the structural capillarity $a$ more closely. Let $I\!D\,\overline{F}$ be linear. By (1.1.42) we conclude for $I\!D\,\overline{F}$

$$\begin{aligned} dim\ M(a\cdot\mathcal{A})(j_0+l) &= I\!D^{\,2}\overline{F}(j_0)(l, j_0+l) \\ &= \frac{dim\ M}{2} I\!D^{\,2}(a\cdot\mathcal{A})(j_0)(l, j_0+l) \\ &= \frac{dim\ M}{2} I\!D^{\,2}(a\cdot\mathcal{A})(j_0, l) + \frac{dim\ M}{2} I\!D^{\,2}(a\cdot\mathcal{A})(l, l) \end{aligned}$$

On the other hand the Taylor expansion up to order two of $a\cdot\mathcal{A}$ at $j_0$ implies that no higher order terms are present and that

$$\frac{1}{2} I\!D^{\,2}(a\cdot\mathcal{A})(j_0, l) = I\!D\,(a\cdot\mathcal{A})(j_0)(l) \quad \forall\, l \in O - j_0.$$

Hence

$$\begin{aligned} I\!D^{\,2}a(j_0)(j_0, l)\cdot\mathcal{A}(j_0) + I\!D\,a(j_0)(j_0)\cdot I\!D\,\mathcal{A}(j_0)(l) + dim\ M\cdot I\!D\,a(j_0)(l)\cdot\mathcal{A}(j_0) \\ = 2\cdot I\!D\,(a\cdot\mathcal{A})(j_0)(l). \end{aligned}$$

We therefore have

**Proposition 1.1.5:**

*Let* $\overline{F}$ *be a real-valued smooth map on a neighbourhood* $O$ *of* $j_0 \in E(M, I\!R^n)$*, admitting a constitutive map* $\mathcal{H}_{\overline{F}}$ *and satisfying (1.1.42). The structural capillarity* $a : O \longrightarrow I\!R$ *satisfies then*

$$I\!D^{\,2}(a\cdot\mathcal{A})(j_0, l) = I\!D\,(a\cdot\mathcal{A})(j_0)(l) \quad \forall\, l \in O - j_0 \tag{1.1.45}$$

*implying*

$$I\!D^{\,2}a(j_0)(j_0, l)\cdot\mathcal{A}(j_0) + I\!D\,a(j_0)(j_0)\cdot I\!D\,\mathcal{A}(j_0)(l) = (2 - dim\ M)\cdot I\!D\,a(j_0)(l)\cdot\mathcal{A}(j_0). \tag{1.1.46}$$

*If hence* $dim\ M = 2$ *then*

$$I\!D^{\,2}a(j_0)(j_0, l)\cdot\mathcal{A}(j_0) = -I\!D\,a(j_0)(j_0)\cdot I\!D\,\mathcal{A}(j_0)(l) \tag{1.1.47}$$

*holds for all* $l \in O - j_0$.

The following is an immediate consequence of (1.1.30) and the definition of $B_h$ for any $h \in C^\infty(M, \mathbb{R}^n)$ given in A1.1

**Lemma 1.1.6:**

*The map*

$$a : E(M, \mathbb{R}^n) \longrightarrow \mathbb{R}$$

*in (1.1.30) admits the density assigning to each $j \in O$ the value $\frac{tr\ B_{\mathcal{H}}(j)}{dim\ M \cdot \mathcal{A}(j)}$ i.e.*

$$a(j) = \int_M \frac{tr\ B_{\mathcal{H}}(j)}{dim\ M \cdot \mathcal{A}(j)} \mu(j) \quad \forall j \in E(M, \mathbb{R}^n) \tag{1.1.48}$$

*or*

$$a(j) = \int_M \frac{det\ f(j) \cdot tr\ B_{\mathcal{H}}(j)}{dim\ M \cdot \mathcal{A}(j)} \mu(j_0) \quad \forall j \in E(M, \mathbb{R}^n) \tag{1.1.49}$$

*if $j_0 \in E(M, \mathbb{R}^n)$ is a fixed configuration. Hence $a(j) = 0$ iff $\int_M tr B_{\mathcal{H}}(j)\mu(j) = 0$ or equivalently $a(j) = 0$ iff $\mathbb{D}\mathcal{A}(j)(\mathcal{H}(j)) = 0$.*

Lemma 1.1.6 suggests to write (1.1.39) in the form

$$\mathbb{D}\overline{F}(j_0 + l)(j_0 + l) = a(j_0 + l) \cdot \mathcal{A}(j_0 + l) \cdot dim\ M = \int_M tr\ B_{\mathcal{H}}(j_0 + l)\mu(j_0 + l)$$

or in view of A1.3 as

$$\mathbb{D}\overline{F}(j_0 + l)(j_0 + l) = \int_M tr\ B_{\mathcal{H}}(j_0 + l) \cdot det\ f(j_0 + l) \cdot \mu(j_0).$$

Hence (1.1.42) implies for all $l \in O - j_0$

$$\mathbb{D}^2\overline{F}(j_0)(l, j_0) + \mathbb{D}^2\overline{F}(j_0)(l, l) = \int_M (tr\ B_{\mathcal{H}} \cdot det\ f)(j_0 + l) \cdot \mu(j_0)$$

and therefore

$$2 \cdot \mathbb{D}^2\overline{F}(j_0)(h, k) = \int_M \mathbb{D}^2(tr\ B_{\mathcal{H}} \cdot det\ f)(j_0)(h, k) \cdot \mu(j_0).$$

Thus we have shown the following

**Proposition 1.1.7:**

*If $\overline{F} : O \longrightarrow I\!R$ has the form*

$$\overline{F}(j_0 + l) = \overline{F}(j_0) + \frac{1}{2} I\!D^2 \overline{F}(j_0)(l,l) \quad \forall\, l \in O - j_0$$

*and $I\!D\,\overline{F}$ admits a constitutive map $\mathcal{H}_{\overline{F}} : O \longrightarrow C^\infty(M, I\!R^n)$ then*

$$I\!D\,\overline{F}(j_0 + l)(j_0 + l) = a(j_0 + l) \cdot \mathcal{A}(j_0 + l) \quad \forall\, l \in O - j_0$$

*for some smooth map $a : O \longrightarrow I\!R$ implying*

$$\overline{F}(j_0 + l) = \overline{F}(j_0) + \frac{1}{4} \cdot \int_M I\!D^2(tr\ B_{\mathcal{H}} \cdot det\ f)(j_0)(l,l) \cdot \mu(j_0) \quad \forall\, l \in O - j_0. \tag{1.1.50}$$

*Therefore $\overline{F}$ admits a density $F$ meaning*

$$\overline{F}(j_0 + l) = \int_M F(j_0 + l)\mu(j_0) \quad \forall\, l \in O - j_0. \tag{1.1.51}$$

*with*

$$F(j_0 + l) = \frac{\overline{F}(j_0)}{\mathcal{A}(j_0)} + \frac{1}{4} \cdot I\!D^2(tr\ B_{\mathcal{H}} \cdot det\ f)(j_0)(l,l) \quad \forall\, l \in O - j_0 \tag{1.1.52}$$

*where we may assume that $B_{\mathcal{H}}(j_0) = 0$. Hence*

$$F(j_0 + l) = \frac{\overline{F}(j_0)}{\mathcal{A}(j_0)} + \frac{1}{4}\left(tr\ I\!D^2 B_{\mathcal{H}}(j_0)(l,l) + tr\ B_{\mathcal{H}}(j_0) \cdot tr\ B_l\right) \tag{1.1.53}$$

*for all $l \in O - j_0$, showing that $F$ depends on the symmetric endomorphisms $B_{\mathcal{H}}$ and $B_l$ only.*

From here one obtains the form of the **free energy** in [L,L] if one assumes that $B_{\mathcal{H}}(j_0 + l)$ depends on $B_l$ only. We will investigate the nature of the constitutive map of the type $I\!D\,\overline{F}$ in chapter three.

**1.2 The Ricci-sensitive part and a topological condition for the equilibrium**

Let $dim M = 2$ and $\mathbb{R}^n = \mathbb{R}^3$. 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. [Bi,Sn,Fi] or [G,K,M]) yields for any $j \in E(M, \mathbb{R}^n)$ immediately

$$Ric(j)(X,Y) = m(j)\Big(\big(H(j)W(j) - W^2(j)\big)X, Y\Big) \tag{1.2.1}$$

for all smooth vector field $X, Y$ on $M$. Here $H(j) = trW(j)$ (cf. section 1.1). Let $R(j)$ denote the symmetric operator such that

$$Ric(j)(X,Y) = m(j)\big(R(j), X, Y\big) \tag{1.2.2}$$

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

$$R(j) = H(j)W(j) - W^2(j). \tag{1.2.3}$$

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

$$\boldsymbol{\lambda}(j) = H(j)^2 - trW^2(j). \tag{1.2.4}$$

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

$$\boldsymbol{\kappa}(j) = \frac{\boldsymbol{\lambda}(j)}{2} \tag{1.2.5}$$

where $\boldsymbol{\kappa}(j) := detW(j)$ is the **Gaussian curvature**. Since $M$ is two dimensional we can assume that

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

holds true (cf. [B,G]).

Clearly $\frac{\boldsymbol{\lambda}(j)}{2} \cdot dj$ is in general not a differential. It is easy to see (cf. [Bi3]) that $\frac{\boldsymbol{\lambda}(j)}{2} \cdot dj$ is a differential iff $\boldsymbol{\lambda}(j)$ is a constant map on $M$. Hence $\frac{\boldsymbol{\lambda}(j)}{2} \cdot dj$ is not exact in general. Let us call the **exact part** of $djR(j)$ by $d\mathbf{r}(j)$. We are interested in particular in the component of $djR(j)$ along $dj$ formed with respect to $\mathcal{G}(j)$. This is to say we form

$$\frac{\boldsymbol{\lambda}(j)}{2} dj = K(j) \cdot dj + \gamma(j) \tag{1.2.6}$$

with $K(j) \in \mathbb{R}$ and

$$\int_M \frac{\boldsymbol{\lambda}(j)}{2} \cdot dj \bullet dj \mu(j) = K(j) \int_M dj \bullet dj \; \mu(j), \tag{1.2.7}$$

has to hold for each $j \in E(M, \mathbb{R}^n)$ and $\gamma(j)$ is a $\mathbb{R}^n$-valued one-form on $M$ smoothly depending on $j \in E(M, \mathbb{R}^n)$. Obviously we have $\int_M \frac{\boldsymbol{\lambda}(j)}{2} \cdot 2\mu(j) = 2 \cdot K(j) \cdot \mathcal{A}(j)$ with $\mathcal{A}(j)$ being the area of $M$. By the theorem of Gauss-Bonnet we conclude

$$\frac{1}{4\pi}\mathbf{X} = 2 \cdot K(j) \cdot \mathcal{A}(j) \quad \forall j \in E(M, \mathbb{R}^n) \tag{1.2.8}$$

which determines the map $K : E(M, \mathbb{R}^n) \longrightarrow \mathbb{R}$ as

$$K(j) = \frac{1}{8\pi \cdot \mathcal{A}(j)} \cdot \mathbf{X} \quad \text{or} \quad \mathcal{A}(j) = \frac{\mathbf{X}}{8\pi K(j)} \quad \forall j \in E(M, \mathbb{R}^n) \tag{1.2.9}$$

with $\mathbf{X}$ the **Euler-characteristic** of $M$.

Using (1.2.9) the following is immediate:

**Lemma 1.2.1:**

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

$$K \cdot \mathbb{D}\,\mathcal{A} = \frac{\mathbf{X}}{8\pi} \cdot \mathbb{D}\, ln\mathcal{A} \tag{1.2.10}$$

.

Given a constitutive map $\mathcal{H}$ we split $d\mathcal{H}$ at $j \in E(M, \mathbb{R}^n)$ with respect to $\mathcal{g}(j)$ into a component along $dj$ and a component $dH_1$ perpendicular to it yielding

$$d\mathcal{H}(j) = a_r(j) \cdot d\mathbf{r} + d\mathcal{H}_2(j) \tag{1.2.11}$$

with

$$a_r : E(M, \mathbb{R}^n) \longrightarrow \mathbb{R}^n$$

being smooth (where $d\mathcal{H}_2(j)$ is determined by the equation just above) since $d\mathbf{r}(j)$ depends on $dj$ rather than $j$ itself. $a_r \cdot d\mathbf{r}$ is the **curvature sensitive** part of $d\mathcal{H}$.for the structural capillarity (cf. 1.1.31)

$$a(j) = a_r(j) \cdot K(j) + u(j)$$

for some smooth map $u : E(M, \mathbb{R}^n) \longrightarrow \mathbb{R}^n$. This shows how the structural capillarity is affected by the map $K$. The force $\Phi_r(j)$ density sensitive to $djR(j)$ is

$$\Phi_r(j) = a_r(j)\Delta(j)\mathbf{r}(j) = a_r \cdot divdjR = -\frac{a_r}{2} \cdot djgrad\, \boldsymbol{\lambda} + \frac{a_r(j)}{2} \cdot \boldsymbol{\lambda}(j) \cdot H(j) \cdot N(j) \tag{1.2.12}$$

Comparing (1.1.14), (1.2.12) with (1.1.17) yields

$$\Phi_T(j) = -\frac{a_r(j)}{2} \cdot dj \; grad\, \boldsymbol{\lambda} + \Phi_T^I(j) \quad \text{and} \quad \Phi_N(j) = \frac{a_r}{2} \cdot \boldsymbol{\lambda}(j) \cdot H(j) \cdot N(j) + \Phi_N^{II}(j). \tag{1.2.13}$$

The gradient is taken with respect to $m(j)$. Here $\Phi_T^I$ and $\Phi_N^{II}$ are defined via (1.2.12), and do not depend on the scalar curvature $\boldsymbol{\lambda}(j)$. In summarizing we state the following lemma and corollary to it:

**Lemma 1.2.2:**

*At each $j \in E(M, I\!R^n)$ the structural capillarity splits into*

$$a(j) = a_r(j) \cdot K(j) + u(j) \tag{1.2.14}$$

*or*

$$a(j) = a_r(j) \cdot \frac{\mathbf{X}}{4\pi \mathcal{A}(j)} + u(j) \tag{1.2.15}$$

*with $d\mathcal{H}(j) = a(j) \cdot dj + d\mathcal{H}_1(j)$ for each $j \in E(M, I\!R^n)$.*

**Corollary 1.2.3:**

*At an equilibrium configuration $j_0 \in E(M, I\!R^n)$ the structural capillarity vanishes, i.e. $a(j_0) = 0$ and therefore $a_r(j_0)$ and $u(j_0)$ are related by*

$$a_r(j_0) \cdot \frac{\mathbf{X}}{8\pi \mathcal{A}(j_0)} = -u(j_0), \tag{1.2.16}$$

*showing that $a_r(j_0) = 0$ iff $u(j_0) = 0$, provided $M$ is not diffeomorphic to a torus. If $M$ is a torus then $u(j_0) = 0$. Moreover the equilibrium condition for $j_0$ reads in terms of the force densities as*

$$\Phi_T^I(j_0) = -\frac{a_r(j_0)}{2} \cdot dj \; grad\, \boldsymbol{\lambda}(j_0) \quad \text{and} \quad \Phi_N^{II}(j_0) = -\frac{a_r(j_0)}{2} \cdot \boldsymbol{\lambda}(j_0) \cdot H(j_0) \cdot N(j_0) \tag{1.2.17}$$

# Description of a discrete medium on a continuum

## 2.1 Internal force densities on the contiuum caused by finitely many particles

Let $P \subset M$ be a collection of finitely many points on $M$. We think of the elements of $P$ as the mean location of material particles on $M$. On the other hand $M$ is regarded as a manifold passing through $P$.

We suppose furthermore that some of this particles interact with each other, but we do not specify any sort of interactions, yet. (We will do so in sections three and four.) These particles, together with a presupposed interaction scheme will be called a **discrete medium**, here. No exterior forces shall be present.

The space of configuration of these particles is $E(P, I\!R^n)$, the collection of all injective maps from $P$ to $I\!R^n$. The set $E(P, I\!R^n)$ is an open subset of the finite dimensional linear space $\mathcal{F}(P, I\!R^n)$, the collection of all maps from $P$ to $I\!R^n$. Moreover $r\big(E(M, I\!R^n)\big) \subset E(P, I\!R^n)$ is open as well, we denote it by $E^\infty(P, I\!R^n)$.

The principle of virtual work on $M$ presented in section 1 is easily transferred to $P \subset M$. This is done as follows: Let $\mathcal{W}(j_P^0) \subset E^\infty(P, I\!R^n)$ be an open neighbourhood of some $j_P^0 \in E^\infty(P, I\!R^n)$ and

$$A_P : \mathcal{W}(j_P^0) \times \mathcal{F}(P, I\!R^n) \longrightarrow I\!R \tag{2.1.1}$$

be a smooth one-form. Clearly

$$A_P(j_P)(h_P) = \mathcal{G}_P\big(\Phi_P(j_P), h_P\big) \quad \forall\, j_P \in E^\infty(P, I\!R^n) \tag{2.1.2}$$

for some well defined map

$$\Phi_P : \mathcal{W}(j_P^0) \longrightarrow \mathcal{F}(P, I\!R^n), \tag{2.1.3}$$

called the **internal force**. Here $\mathcal{G}_P$ is the metric defined in appendix 3 on the collection of all $I\!R^n$-valued zero cochains (cf. A3.18), i.e. on $\mathcal{F}(P, I\!R^n)$. In particular we require that for all $z \in I\!R^n$ the constant map $z : P \longrightarrow I\!R^n$ does not cause any work, i.e.

$$A_P(j_P)(z) = 0.$$

and moreover that $A_P$ is $\mathbb{R}^n$-invariant, this is to say that

$$A_P(j_P + z)(l_P) = 0 \quad \forall\, z \in \mathbb{R}^n \quad \text{and} \quad \forall\, l_P \in \mathcal{F}(P, \mathbb{R}^n)$$

has to hold.

If $\Phi_P$ is an internal force caused by the interaction of the material particles we call $A_P$ the **virtual work** of this **discrete medium**. As in the previous section we characterize this discrete medium in as far only, as it affects the virtual work, i.e. we classify the medium by its internal force density only. Clearly this is a rather rough classification.

To describe the discrete medium on $M$, we would like to form $r^*A_P$ the pull back of $A_P$ by $r$ to $r^{-1}\mathcal{W}(j_P^0)$ and interpret this one-form as a virtual work on the continuum. Having this approach in mind we pose the question as to whether $r^*A_P$ admits a force density in $C^\infty(M, \mathbb{R}^n)$.

Let therefore $j_0 \in r^{-1}\mathcal{W}(j_P^0) \subset E(M, \mathbb{R}^n)$ be such that $r(j_0) = j_P^0$ and $\Phi : r^{-1}\mathcal{W}\big(r(j_P^0)\big) \longrightarrow C^\infty(M, \mathbb{R}^n)$ be a smooth map such that

$$r^*A_P(j)(h) = \mathcal{G}(j_0)\big(\Phi(j), h\big) \quad \forall\, j \in r^{-1}\mathcal{W}\big(r(j_P^0)\big) \quad \forall\, h \in C^\infty(M, \mathbb{R}^n). \tag{2.1.4}$$

$\Phi(j)$, if it exists, is uniquely determined for any $j$ in the domain of $\Phi$ and characterizes the discrete medium as a continuum. This kind of force density, however, does not exist in general as we see as follows: Let $z_1, \dots, z_n$ be the canonical basis of $\mathbb{R}^n$. Then $\Phi(j)$, if it were existent, would decompose for each $j \in r^{-1}\mathcal{W}(j_P^0)$ into

$$\Phi(j) = \sum_{i=1}^{n} \Phi^i(j) \cdot z_i$$

where $\Phi^i(j) \in C^\infty(M, \mathbb{R})$ for all $i$. Hence $\Phi(j)$ exists iff $\Phi^i(j)$ exists for all $i$. Therefore we may assume that $n = 1$. For simplicity let $P = \{q\}$ for some $q \in M$. Without loss of generality we may assume that

$$r^*A_P(j) : C^\infty(M, \mathbb{R}^n) \longrightarrow \mathbb{R}$$

has the form

$$r^*A_P(j)(h) = h(q) \quad \forall\, h \in C^\infty(M, \mathbb{R}^n).$$

Thus $r^*A(j)$ is a point evaluation, i.e. a $\delta$-functional. As it is well known such linear maps do not admit a density (cf. [Bi,Sn,Fi]). Hence there is no $\Phi(j) \in C^\infty(M, \mathbb{R}^n)$ satisfying (2.1.4) in general.

This shows that we have to give up the idea that internal force densities $\Phi(j)$ are in the $\mathcal{G}(j_0)$-orthogonal complement of the kernel *ker r* of the restriction map $r : C^\infty(M, \mathbb{R}^n) \longrightarrow \mathcal{F}(P, \mathbb{R}^n)$ as (2.1.4) would require. Therefore, if we intend to describe internal force densities on the continuum produced by finitely many particles, we have to proceed differently. We base our procedure on (1.1.22) and (1.1.25).

To begin with, we assume that $\Phi : r^{-1}\mathcal{W}(j_P^0) \longrightarrow C^\infty(M, \mathbb{R}^n)$ is a smooth internal force density in the sense of section one. We know by (1.1.19) and (1.1.25) that

$$\Phi(j) = \Delta(j_0)\, \widehat{\mathcal{H}}(j) = \sum_{i=1}^{\infty} \lambda_i \widehat{\kappa}^i(j)\widehat{e}_i \quad \forall j \in \mathcal{W}(j_P^0) \tag{2.1.5}$$

where $\widehat{e}_1, \ldots$ are those ($\mathcal{G}(j_0)$-orthonormed) eigenvectors in $C^\infty(M, \mathbb{R}^n)$ admitting non-vanishing eigenvalues. Here $j_0 \in r^{-1}\mathcal{W}(j_P^0)$ is such that $r(j_0) = j_P^0$.
Since $r : C^\infty(M, \mathbb{R}^n) \longrightarrow \mathcal{F}(P, \mathbb{R}^n)$ is continous

$$r\big(\Phi(j)\big) = \sum_{i=1}^{\infty} \lambda_i \widehat{\kappa}^i(j) \cdot r(\widehat{e}_i) \quad \forall j \in r^{-1}\mathcal{W}(j_P^0) \tag{2.1.6}$$

Clearly $\{r(\widehat{e}_i) | i = 1, \ldots\}$ generates $\mathcal{F}(P, \mathbb{R}^n)$ since $r$ is surjective. Hence, we can choose a basis among $\{r \cdot \widehat{e}_i |\ i = 1, \ldots\}$.

The motivation of the construction below is that the eigenvalues of $\Delta(j_0)$ grow to infinity as $i$ does so; hence the contributions of $\widehat{\kappa}^i(j)$ to $\Phi(j)$ have to diminish. In addition we have to consider only finitely many terms in the series (2.1.6) since $dim\ \mathcal{F}(P, \mathbb{R}^n) < \infty$. Here is how we proceed further:
We will define a finite dimensional subspace $\mathcal{F}^\infty(M, \mathbb{R}^n) \subset C^\infty(M, \mathbb{R}^n)$ generated by $\mathbb{R}^n$ and by eigenvectors of the Laplacian $\Delta(j_0)$ of a fixed $j_0 \in E(M, \mathbb{R}^n)$ such that

$$a) \quad \Delta(j_0)\mathcal{F}^\infty(M, \mathbb{R}^n) \subset \mathcal{F}^\infty(M, \mathbb{R}^n)$$

$$b) \quad r : \mathcal{F}^\infty(M, \mathbb{R}^n) \longrightarrow F^\infty(P, \mathbb{R}^n) \qquad \text{is an isomorphism}$$

for a given embedding $j_0 \in E(M, \mathbb{R}^n)$.

This subspace is obtained as follows: The eigenvectors $\widehat{e}_1, \widehat{e}_2, \ldots$ in $C^\infty(M, I\!R^n)$ of $\Delta(j_0)$ on $C^\infty(M, I\!R^n)$ are ordered such that the respective eigenvalues of $\Delta(j_0)$ satisfy $0 < \lambda_1 \leq \lambda_2 \leq \ldots$. Let $\widehat{e}_{i_1}$ be the first among the above eigenvectors for which $\widehat{e}_{i_1}|P \neq 0$. At this point we have to make a choice. Next we chose $\widehat{e}_{i_2}$, among the complement of $\{\widehat{e}_{i_1}\}$ in $\{\widehat{e}_1, \ldots, \widehat{e}_{i_1+1}, \ldots\}$ with the smallest index for which $\widehat{e}_{i_2}|P$ and $\widehat{e}_{i_1}|P$ are linearly independent.

Continuing this way we obtain a linearly independent set

$$\{\widehat{e}_{i_1}, \ldots, \widehat{e}_{i_{(s_0-1)\cdot n}}\} \subset C^\infty(M, I\!R^n)$$

where $s_0$ is the number of all points in $P$. Let us replace the symbol $\widehat{e}_{i_s}$ by $e_s$ for simplicity. The eigenvectors $e_1, \ldots, e_{(s_0-1)\cdot n}$ of $\Delta(j_0)$ with respective eigenvalues $0 < \lambda_1 \leq \ldots \leq \lambda_{(s_0-1)\cdot n}$ generate a subspace $\mathcal{F}_0^\infty(M, I\!R^n) \subset C^\infty(M, I\!R^n)$. By construction

$$r : \mathcal{F}_0^\infty(M, I\!R) \oplus I\!R^n \longrightarrow \mathcal{F}(P, I\!R^n) \tag{2.1.7}$$

is an isomorphism. Let us denote $\mathcal{F}_0^\infty(M, I\!R^n) \oplus I\!R^n$ by $\mathcal{F}^\infty(M, I\!R^n)$. Moreover the map in (2.1.7) will be denoted by $r_\infty$ in the sequel. The space $\mathcal{F}^\infty(M, I\!R^n)$ will be our smooth analogon to $\mathcal{F}(P, I\!R^n)$. Clearly $\mathcal{F}^\infty(M, I\!R^n)$ will not be $\mathcal{G}(j_0)$-orthogonal to $ker\, r$, in general. The metrics $\mathcal{G}(j_0)$ and $r^*\mathcal{G}_P$ on $\mathcal{F}^\infty(P, I\!R^n)$ will differ, in general. Having related them, we will prepare the study of the notion of virtual work on both $\mathcal{F}(P, I\!R^n)$ and $\mathcal{F}^\infty(P, I\!R^n)$.

But first we have to construct the analogon of $\mathcal{W}\big(r(j_0)\big) \subset E^\infty(P, I\!R^n)$ on $E(M, I\!R^n)$. To this end we introduce

$$\mathcal{K} := \{\{j\} \times \mathcal{F}^\infty(P, I\!R^n) | j \in E(M, I\!R^n) \subset E(M, I\!R^n) \times C^\infty(M, I\!R^n) = TE(M, I\!R^n)\},$$

a distribution on $E(M, I\!R^n)$ (cf. [Bi,Sn,Fi]).

This distribution is integrable, since $j + O \subset E(M, I\!R^n)$ for all $j \in E(M, I\!R^n)$ for any closed small enough neighbourhood $O'$ of zero in $\mathcal{F}^\infty(M, I\!R^n)$. Let

$$\mathcal{W}(j_P^0) := r^{-1}\mathcal{W}(j_P^0) \cap (j_0 + O').$$

Clearly $\mathcal{W}(j_P^0)$ is a closed neighbourhood of $j_0 \in \mathcal{F}^\infty(M, I\!R^n)$ and is a slice in $r^{-1}\big(\mathcal{W}(j_P^0)\big) = \mathcal{W}^\infty(j_0) + ker\ r$. The whole formalism in section 1.1 can be transfered to $\mathcal{W}^\infty(j_0)$ in a straight forward manner.

We begin the investigation of the relation between the scalar products $\mathcal{G}_P$ on $\mathcal{F}(P, I\!R^n)$ and $\mathcal{G}(j_0)$ on $\mathcal{F}^\infty(M, I\!R^n)$ by exhibiting a natural basis on $\mathcal{F}(P, I\!R^n)$. For each basis vector $z_\nu$ of the natural basis in $I\!R^n$ let

$$z_\nu^q : P \longrightarrow I\!R^n$$

be the map assigning $z_\nu$ on $q \in P$ and zero elsewhere. Clearly

$$\{z_\nu^q | \nu = 1, \ldots, n; q \in P\} \tag{2.1.8}$$

is a $\mathcal{G}_P$-orthonormed basis of $\mathcal{F}(P, I\!R^n)$.

Now $r_\infty^* \mathcal{G}_P$, the pull back of $\mathcal{G}_P$ to $\mathcal{F}^\infty(M, I\!R^n)$, is a scalar product related with $\mathcal{G}(j_0)$ by

$$r_\infty^* \mathcal{G}_P(h, l) = \mathcal{G}(j_0)\big(\Theta(j_0)h, l\big) \quad \forall\, h, l \in \mathcal{F}^\infty(P, I\!R^n) \tag{2.1.9}$$

where $\Theta(j_0)$ is a $\mathcal{G}(j_0)$-selfadjoint isomorphism. Since the vectors in (2.1.8) are all orthonormed $\{r_\infty^{-1} z_\nu^q | \nu = 1, \ldots, n; q \in P\}$ is an $r_\infty^* \mathcal{G}_P$-orthonormed eigensystem of $\Theta(j_0)$. Hence

$$\Theta(j_0) r_\infty^{-1} z_\nu^q = \xi_\nu^2(q) z_\nu^q. \tag{2.1.10}$$

Associated with $\Theta(j_0)$ are thus the functions

$$\xi_\nu^2 : P \longrightarrow I\!R \qquad \nu = 1, \ldots, n.$$

Clearly, the $\mathcal{G}(j_0)$-norm $||z_\nu^q||_{\mathcal{G}(j_0)}$ of each $z_\nu^q$ is

$$||z_\nu^q||_{\mathcal{G}(j_0)} = \xi_\nu(q)^{-1}$$

The following is crucial for our further studies:

**Lemma 2.1.1:**

*There is a real-valued function $\xi \in \mathcal{F}(P, I\!R^n)$ such that*

$$\xi_\nu = \xi \quad \forall\, \nu = 1, ..., n. \tag{2.1.11}$$

<u>Proof:</u> At first we observe that

$$z_\nu^q = \mathbf{1}_q \cdot z_\nu \quad \forall\, q \in P \quad \text{and} \quad \nu = 1, ..., n$$

where $\mathbf{1}_q$ is the characteristic function of $\{q\}$ (cf. appendix 3). Moreover we have

$$\mathcal{F}^\infty(M, I\!R^n) = \oplus_{\nu=1}^n \mathcal{F}^\infty(M, I\!R) \cdot z_\nu \qquad (2.1.12)$$

where $\mathcal{F}^\infty(M, I\!R) \subset C^\infty(M, I\!R^n)$ is constructed exactly in an analogous way as we obtained $\mathcal{F}^\infty(P, I\!R^n)$; hence $\mathcal{F}^\infty(M, I\!R^n) = \mathcal{F}_0^\infty(M, I\!R^n) \oplus I\!R^n$ (cf. 2.1.7). The restriction map defined on $\mathcal{F}^\infty(M, I\!R)$ onto $\mathcal{F}(P, I\!R)$ is denoted by $r_\infty$, too. Hence

$$r_\infty^{-1} z_\nu^q = (r_\infty^{-1} \mathbf{1}_q) \cdot z_\nu \quad \forall \nu = 1, ..., n \quad \text{and} \quad \forall q \in P.$$

Since $C^\infty(M, I\!R^n) = \oplus_{\nu=1}^n C^\infty(M, I\!R) \cdot z_\nu$ we have due to (2.1.12)

$$\mathcal{G}(j_0)(g_\nu \cdot z_\nu, g_{\nu'} \cdot z_{\nu'}) = \Big( \int_M g_\nu \cdot g_{\nu'} \mu(j) \Big) \cdot \delta_{\nu,\nu'}$$

for any choices of $g_\nu, g_{\nu'} \in C^\infty(M, I\!R^n)$ and $z_\nu, z_{\nu'} \in I\!R^n$. Accordingly,

$$\delta_{\nu,\nu'} = r^* \mathcal{G}_P(r_\infty^{-1} z_\nu^q, r_\infty^{-1} z_{\nu'}^q) = \Big( \int_M \Theta_{I\!R}(j_0) r^{-1} \mathbf{1}_q \cdot r_\infty^{-1} \mathbf{1}_q \mu(j_0) \Big) \cdot \delta_{\nu,\nu'}$$

has to hold for some endomorphism $\Theta_{I\!R}(j_0)$ on $\mathcal{F}^\infty(M, I\!R)$. Thus $r_\infty^{-1} \mathbf{1}_q$ where $q$ varies in $P$, is an eigensystem of $\Theta_{I\!R}$ on $\mathcal{F}^\infty(P, I\!R)$ with respective eigenvalue $\xi^2(q)$, say. Hence

$$\Theta(j_0) = \oplus_1^n \Theta_{I\!R}(j_0)$$

and

$$\xi_\nu^2(q) = \xi^2(q) \quad \forall q \in P$$

showing our claim.

We now choose some $\overline{\rho} \in C^\infty(M, I\!R)$, positive everywhere but such that

$$r(\overline{\rho}^2) = \xi^2.$$

Then

$$r(\overline{\rho}^2 \cdot r_\infty^{-1} z_\nu^q) = r(\overline{\rho}^2) \cdot z_\nu^q = \xi^2 z_\nu^q = \xi^2(q) z_\nu^q \quad \forall \nu = 1, ..., n \quad \forall q \in P.$$

Thus if $h = \sum_{\nu,q} \alpha_\nu^q r_\infty^{-1} z_\nu^q$ then

$$r(\overline{\rho}^2 h) = \sum \alpha_\nu^q \overline{\rho}^2 r_\infty^{-1}(z_\nu^q) = \sum \alpha_\nu^q \xi_\nu^2(q) z_\nu.$$

Hence we may write on $\mathcal{F}^\infty(P, I\!R^n)$

$$r^* \mathcal{G}_P(h, l) = \mathcal{G}(j_0)(\overline{\rho}^2 \cdot h, l) \quad \forall h, l \in C^\infty(M, I\!R^n).$$

This establishes the following lemma, basic to our investigations. (For a density map and the metric $B(\rho)$ we refer to A2.4 and A2.5 respectively in appendix 2).

**Lemma 2.1.2:**

*There is a density map*

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

*such that*

$$r^*\mathcal{G}_P(h,l) = \mathcal{G}(j_0)\big(\rho(j_0)\cdot h, l\big) \quad \forall\, h,l \in \mathcal{F}^\infty(P, \mathbb{R}^n). \tag{2.1.13}$$

*This is to say that*

$$r^*\mathcal{G}_P = B(\rho) \quad \text{on} \quad \mathcal{F}^\infty(M, \mathbb{R}^n) \tag{2.1.14}$$

*along the foliation defined by the distribution $\mathcal{K}$. Moreover $\rho$ can be chosen such that $\int_M \rho(j_0)\mu(j_0) = (s_0 - 1)\cdot n$ holds true.*

The nature of $\rho$ will become evident as we study the virtual work below.

Let us pause to study the freedom in choosing $\rho(j_0)$. To this end let $\widetilde{\rho} : M \longrightarrow \mathbb{R}$ be a smooth map such that

$$\rho' = \rho(j_0) + \widetilde{\rho}$$

where $\rho'$ satisfies (2.1.14) as well. Hence $\widetilde{\rho}|P = 0$. Obviously we have the following :

**Lemma 2.1.3:**

*In order that $\rho' > 0$ the map $\widetilde{\rho}$ has to vary in an open set $O_\rho \subset \ker r$. If we require in addition that $\int_M \rho(j_0)\mu(j_0) = \int_M \big(\rho(j_0) + \widetilde{\rho}(j_0)\big)\mu(j_0) = const.$ Then $\int_M \widetilde{\rho}(j_0)\mu(j_0) = 0$, this is to say $\widetilde{\rho}$ varies in $O_\rho \cap \ker \int_M \ldots \mu(j_0)$.*

Now let us turn back to the virtual work (2.1.1). The internal force density $\Phi_P : \mathcal{W}(j_P^0) \longrightarrow \mathcal{F}(P, \mathbb{R}^n)$ lifts to $\mathcal{W}^\infty(j_0)$ as

$$r_\infty^{-1} \circ \Phi_P \circ r_\infty : \mathcal{W}^\infty(j_0) \longrightarrow \mathcal{F}^\infty(P, \mathbb{R}^n)$$

(here we assumed that $r(j_0) = j_P^0$ and that $r\big(\mathcal{W}^\infty(j_0)\big) = \mathcal{W}(j_P^0)$). Hence for all $j \in \mathcal{W}^\infty(j_0)$ and any $h \in \mathcal{F}^\infty(P, I\!R^n)$

$$\begin{aligned}
&\mathcal{G}_P\Big(\Phi_P\big(r(j)\big), r(h)\Big)\\
&= A_P(j)\big(r(h)\big)\\
&= r_\infty^* A_P(j)(h)\\
&= B(\rho)\Big(r_\infty^{-1}\Phi_P\big(r(j)\big), h\Big).
\end{aligned}$$

Instead of $r_\infty^{-1} \circ \Phi_P \circ r$ we will write $r_\infty^* \Phi_P$ as a shorthand. Clearly $r_\infty^* \Phi_P(j) \in \mathcal{F}^\infty(M, I\!R^n)$ for all $j \in \mathcal{W}^\infty(j_0)$. Since for any $j \in \mathcal{W}^\infty(j_0)$ and any $h \in \mathcal{F}^\infty(P, I\!R^n)$

$$\mathcal{G}_P\big(\Phi_P\big(r_\infty(j)\big), r_\infty(h)\big) = B(\rho)\big(r_\infty^* \Phi_P(j), h\big) = \mathcal{G}(j_0)\big(\rho(j_0) \cdot r_\infty^* \Phi_P(j), h\big)$$

we first observe that $\rho(j_0) \cdot r_\infty^* \Phi_P(j)$ is $\mathcal{G}(j_0)$-orthogonal to the constant maps in $C^\infty(M, I\!R^n)$. Therefore $\rho(j_0) \cdot r_\infty^{-1} \circ \Phi_P \circ r_\infty$ is an internal force density on $\mathcal{W}^\infty(j_0)$ with values in $C^\infty(M, I\!R^n)$. Next let us take the component $\Phi_P^M(j)$ in $\mathcal{F}_0^\infty(P, I\!R^n)$ of $\rho(j_0) \cdot r_\infty^{-1} \Phi_P(j)$ for each $j \in \mathcal{W}^\infty(j_0)$ defined by

$$r_\infty^* A_P(j)(h) = \mathcal{G}(j_0)\big(\Phi_P^M(j), h\big) \quad \forall\, h \in \mathcal{F}^\infty(M, I\!R^n). \tag{2.1.15}$$

Since $\mathcal{G}_P$ is defined via a sum and $\mathcal{G}(j_0)$ via an integral, $\rho$ converts the force $r_\infty^{-1} \circ \Phi_P \circ r_\infty$ into a force density $\rho(j_0) \cdot r_\infty^{-1} \circ \Phi_P \circ r$. This fact reveals the nature of $\rho$; in particular $\rho$ can not be thought of as being a mass density. Equation (2.1.15) shows that $\Phi_P^M$ does not depend on the particular choice of $\rho(j_0)$.

$\Phi_P^M(j) \in \mathcal{F}_0^\infty(M, I\!R^n)$ is represented by some well defined $\mathcal{G}(j_0)$-normalized constitutive map $\widehat{\mathcal{H}}_P^M(j) \in \mathcal{F}^\infty(M, I\!R^n)$ for any $j \in \mathcal{W}^\infty(j_0)$ as

$$\Phi_P^M(j) = \Delta(j_0)\mathcal{H}_P^M(j). \tag{2.1.16}$$

It will be convenient to work also with the Fourier expansion of $\mathcal{H}_P^M(j)$, namely

$$\mathcal{H}_P^M(j) = \sum_{i=1}^{(s_0-1)\cdot n} \widehat{\kappa}_\infty^i(j) e_i \quad \forall\, j \in \mathcal{W}^\infty(j_0). \tag{2.1.17}$$

Hence the uniquely determined force density $\Phi_P^M : \mathcal{W}^\infty(j_0) \longrightarrow \mathcal{F}^\infty(M, \mathbb{R}^n)$ is given by

$$\Phi_P^M(j) = \sum_{i=1}^{(s_0-1)\cdot n} \lambda_i \cdot \widehat{\kappa}_\infty^i(j) e_i \quad \forall j \in \mathcal{W}^\infty(j_0). \tag{2.1.18}$$

Clearly

$$r^* A_P(j) | \mathcal{F}^\infty(M, \mathbb{R}^n) = r_\infty^* A_P(j). \tag{2.1.19}$$

However, $\Delta(j_0) ker\, r \not\subset ker\, r$.

Referring to appendix 2 for $B(\rho)$ once more we therefore state:

**Theorem 2.1.4:**

*Given an internal force density $\Phi_P$ then $\Phi_P^M$ and $r_\infty^* \Phi_P : \mathcal{W}^\infty(j_0) \longrightarrow \mathcal{F}^\infty(M, \mathbb{R}^n)$ satisfy*

$$\begin{aligned} r_\infty^* A_P(j)(h) &= \mathcal{G}_P\Big(\Phi_P\big(r_\infty(j)\big), r_\infty h\Big) \\ &= B(\rho)\big(r_\infty^* \Phi_P(j), h\big) \\ &= \mathcal{G}(j_0)\big(\Phi_P^M(j), h\big) \quad \forall h \in \mathcal{F}^\infty(P, \mathbb{R}^n) \end{aligned} \tag{2.1.20}$$

*on $\mathcal{W}^\infty(j_0)$. Hence*

$$\Phi_P^M = Pr \circ \rho(j_0) \cdot r_\infty^* \circ \Phi_P \tag{2.1.21}$$

*holds true. Here $Pr$ denotes the $\mathcal{G}(j_0)$-orthogonal projection onto $\mathcal{F}^\infty(M, \mathbb{R}^n)$.*

Both force densities $\Phi_P^M$ and $r_\infty^* \Phi_P$ in (2.1.20) admit constitutive maps, namely $\widehat{\mathcal{H}}_P^M$ and $\widehat{\mathcal{H}}$, both map into the $\mathcal{G}(j_0)$-orthogonal complement of $\mathbb{R}^n \subset \mathcal{F}^\infty(M, \mathbb{R}^n)$ that is into $\mathcal{F}_0^\infty(M, \mathbb{R}^n)$. The force density $\Phi_P^M(j)$ on $\mathcal{W}^\infty(j_0)$ does not depend on the particular choice of $\rho$ for any $j \in \mathcal{W}^\infty(j_0)$.

The following corollary is immediate:

**Corollary 2.1.5:**

*A smooth map $\Phi : \mathcal{W}^\infty(j_0) \longrightarrow \mathcal{F}^\infty(P, \mathbb{R}^n)$ satisfies*

$$r_\infty^* A_P(j)(h) = \mathcal{G}(j_0)\big(\Phi(j), h\big)$$

*for all $h \in \mathcal{F}^\infty(P, \mathbb{R}^n)$ iff $\Phi = \Phi_P^M$.*

Corollary 2.1.5 motivates the following

**Definition 2.1.6:**

*$r_\infty^* A_P$ is the virtual work and $\Phi_P^M$ its associated internal force density on $\mathcal{W}^\infty(j_0) \subset E(M, \mathbb{R}^n)$ caused by the smooth medium made up by finitely many particles which is characterized by either one $A_P$, its internal force $\Phi_P$ or by $\mathcal{H}_P^M$.*

Since $\mathcal{F}^\infty(M,\mathbb{R}^n) + ker\ r = C^\infty(M,\mathbb{R}^n)$, we extend $A = r_\infty^* A_P$ to all of $r^{-1}\big(\mathcal{W}(j_P^0)\big)$ by setting

$$A(j)(l+k) := A\Big(r_\infty^{-1}\big(r(j)\big)\Big)(l)$$

for all $j \in r^{-1}\mathcal{W}(j_P^0)$ all $l \in \mathcal{F}^\infty(M,\mathbb{R}^n)$ and all $k \in ker\ r$. Clearly $r^* A \neq A$. In the sequel we will work on the slice $\mathcal{W}^\infty(j_0)$ of $r^{-1}\big(\mathcal{W}(j_P^0)\big)$ exclusively, however.

We conclude this section by investigating $\rho \cdot r_\infty^* \Phi_P$ a little further.

Equation (2.1.20) shows that there is a uniquely determined $\mathcal{F}_0^\infty(M,\mathbb{R}^n)$-valued constitutive map $\widehat{\mathcal{H}}_P^M$ on $\mathcal{W}^\infty(j_0)$ such that

$$Pr \circ \rho(j_0) \cdot r_\infty^* \Phi_P = \Delta(j_0)\widehat{\mathcal{H}}_P^M \quad \text{on} \quad \mathcal{W}^\infty(j_0),$$

saying that

$$\mathcal{G}(j_0)\big(Pr \circ \rho(j_0) \cdot r_\infty^* \Phi_P(j), j\big) = \mathcal{G}(j_0)\big(\Delta(j_0)\widehat{\mathcal{H}}_P^M(j), h\big)$$
$$\forall\, j \in \mathcal{W}^\infty(j_0) \quad \forall\, h \in \mathcal{F}^\infty(M,\mathbb{R}^n).$$

In the special case $dimM = 2$ we rewrite (2.1.14) on $\mathcal{W}^\infty(j_0)$ for each $j \in \mathcal{W}^\infty(j_0)$

$$\begin{aligned} r_\infty^* A(j)(h) = B(\rho)\big(r_\infty^* \Phi_P(j), h\big) &= \int_M < r_\infty^* \Phi_P(j), h > \rho(j_0)\mu(j_0) \\ &= \int_M < \Delta_\rho \widehat{\mathcal{H}}_\rho(j), h > \mu_\rho \end{aligned}$$

for any $h \in \mathcal{F}^\infty(M,\mathbb{R}^n)$. The Riemannian metric $m_\rho := \rho^{\frac{1}{2}}(j_0)m(j_0)$ with $\mu_\rho$ as its volume form has $\rho(j_0)^{\frac{-1}{2}}\Delta$ as its Laplacian $\Delta_\rho$. Since $r_\infty^* A(j)(z) = 0$ for each $z \in \mathbb{R}^n$ we conclude the following:

**Proposition 2.1.7:**

*There is a constitutive map $\widehat{\mathcal{H}}_P^M$ on $\mathcal{W}^\infty(j_0)$ such that for all $j \in \mathcal{W}^\infty(j_0)$*

$$Pr\rho(j_0)r_\infty^*\Phi_P(j) = \Delta(j_0)\widehat{\mathcal{H}}_P^M(j) \tag{2.1.22}$$

*holds true. If dim $M = 2$ there is a constitutive map $\widehat{\mathcal{H}}_\rho : \mathcal{W}^\infty(j_0) \longrightarrow \mathcal{F}^\infty(M, I\!R^n)$ with*

$$r_\infty^*\Phi_P(j) = \Delta_\rho\widehat{\mathcal{H}}_\rho(j) = \rho(j_0)^{\frac{-1}{2}} \cdot \Delta(j_0)\widehat{\mathcal{H}}_\rho(j) \quad \forall\, j \in \mathcal{W}^\infty(j_0),$$

*where $\Delta_\rho$ is the Laplacian of the Riemannian metric $m_\rho$ given by*

$$m_\rho(v,w) =< \rho(j_0)^{\frac{1}{4}} dj_0 v, \rho(j_0)^{\frac{1}{4}} dj_0 w > \quad \forall\, v,w \in TqM \quad \text{and} \quad \forall\, q \in M.$$

Let $dim\ M = 2$. In general $(M, m_\rho)$ can not be globally and smoothly embedded, i.e. in general there is no embedding $j_1 \in E(M, I\!R^n)$ such that

$$m_\rho = m(j_1) \tag{2.1.23}$$

for small $n$. More explicitly $m_\rho$ is a pull back by a $C^\infty$-embedding if $n = 10$ (cf.[G,R]). If, however, the scalar curvature $\lambda_\rho$ of $m_\rho$ is strictly positive, then $M$ has to be isometric to an embedded sphere in $I\!R^3$ (cf.[B,G]). If $M$ is diffeomorphic to a sphere then $j_1$ exists if $n = 7$ (cf. [G,R]). For the local embedding of $(M, m_\rho)$ confirm [G,S].

If $n$ is large enough however, then $j_1 \in E(M, I\!R^n)$ exists. Therefore proposition 2.1.7 motivates us to call a configuration $j_1 \in E(M, I\!R^n)$ to **fit metrically well** if

$$m_\rho = m(j_1) \quad \text{and hence} \quad r^*\mathcal{G}_P = \mathcal{G}(j_1) \tag{2.1.24}$$

along $\mathcal{W}(j_P^0)$.

It is easy to see that if $j_0$ is an equilibrium configuration then $j_1$ is one too and vice versa. If $j_1$ exists we may hence assume, without loss of generality, that $j_1 = j_0$.

## 2.2 The exact part of the virtual work of a smooth medium made up by finitely many particles and the free energy associated with it

The goal of this section is to split off in a geometric fashion an exact part $\mathbb{D}\overline{F}$ of the virtual work. This part is called the exact part of the virtual work of a smooth medium made up by finitely many particles. It will be interpreted as the differential of the free energy $\overline{F}$ associated to an adapted statistics (cf. [B,St],[Bi6],[Str],[L,L] and [M,H]).

The geometric setting based on theorem 2.1.4 yielding this exact part (via a Neumann splitting) is the following one:

Let $j_0 \in E(M, \mathbb{R}^n)$ be fixed and $\mathcal{W}^\infty(j_0) \subset E(M, \mathbb{R}^n)$ be a closed ball centred about $j_0$. The motivation of restricting us to $\mathcal{W}^\infty(j_0)$ is clearly the Neumann splitting, however it will become entirely clear from a physical point of view in chapter three. Moreover to prepare the geometric tool we let $\rho$ denote a density map such that the scalar product $B(\rho)$ on $\mathcal{F}^\infty(M, \mathbb{R}^n)$ (cf. A2.5)
satisfies

$$r^*\mathcal{G}_P(h,k) = B(\rho)(h,k) = \int_M \rho(j_0) < h, k > \mu(j_0) \tag{2.2.1}$$

for any $h, k \in \mathcal{F}^\infty(M, \mathbb{R}^n)$. This kind of density exists by (2.1.14) in lemma 2.1.2. We set $\rho(j_0) = \rho_0$, for simplicity.

Next let $A$ be virtual work, i.e. a one-form $A$ on $\mathcal{W}^\infty(j_0)$. This one-form is assumed to be of the form $r_\infty^* A_P$ for some one-form $A_P$ on $r_\infty\big(\mathcal{W}^\infty(j_0)\big) = \mathcal{W}(j_P^0)$; here $r(j_0) = j_P^0$. We decompose $A$ on $\mathcal{W}^\infty(j_0)$ into

$$A = \mathbb{D}\overline{F} + \Psi$$

in the sense of Neumann by solving the following elliptic boundary value problem:

$$\mathbb{d}iv_B A = \Delta\!\!\!\!/_B \overline{F}$$

$$A(\mathbf{n}_B) = \mathbb{D}\overline{F}(\mathbf{n}_B)$$

where $\mathbf{n}_B$ is the oriented normal to the sphere bounding $\mathcal{W}^\infty(j_0)$, formed with respect to the scalar product $B(\rho)$. The operators $\mathbb{d}iv_B$ and $\Delta\!\!\!\!/_B$ are respectively the divergence and the Laplacian of $B(\rho)$ on $\mathcal{F}^\infty(M, \mathbb{R}^n)$. Next we will construct a $\mathcal{G}(j_0)$-normalized constitutive map $\widehat{\mathcal{H}}_{\overline{F}}$ of $\mathbb{D}\overline{F}$.

The gradient $Grad_{\mathcal{G}(j_0)}\overline{F}$ of $\overline{F}$ formed with respect to $\mathcal{G}(j_0)$ can be represented as

$$Grad_{\mathcal{G}(j_0)}\overline{F} = Grad_{\mathcal{G}(j_0)}\overline{F}_0 + z_F$$

where $z_{\overline{F}}$ is a constant $I\!R^n$-valued function on $\mathcal{W}^\infty(j_0)$, and $Grad_{\mathcal{G}(j_0)}\overline{F}_0$ is perpendicular to the constant maps on $\mathcal{W}^\infty(j_0)$ formed with respect to $\mathcal{G}(j_0)$.

Similarly, we may represent the one-form $\Psi$ as

$$\Psi = \mathcal{G}(j_0)(\mathbf{V}_\Psi, \ldots)$$

for some well defined vector field $\mathbf{V}_\Psi$ on $\mathcal{W}^\infty(j_0)$ and split it into

$$\mathbf{V}_\Psi = \mathbf{V}^0_\Psi + z_\Psi$$

for $z_\Psi \in I\!R^n$. Since $A(j)(z) = 0$ for all $j \in \mathcal{W}^\infty(j_0)$ and $z \in I\!R^n$ we find

$$z_\Psi = -z_{\overline{F}},$$

therefore we can assume $z_{\overline{F}} = z_\Psi = 0$ and set $\overline{F} = \overline{F}_0$ respectively $\mathbf{V}_\Psi = \mathbf{V}^0_\Psi$. Hence $Grad_{\mathcal{G}(j_0)}\overline{F} : \mathcal{W}^\infty(j_0) \longrightarrow \mathcal{F}^\infty(M, I\!R^n)$ satisfies

$$\big(Grad_{\mathcal{G}(j_0)}\overline{F}\big)(j) = \Delta\widehat{\mathcal{H}}_{\overline{F}}(j) \quad \forall j \in \mathcal{W}^\infty(j_0) \tag{2.2.2}$$

for some well defined smooth $\mathcal{G}(j_0)$-normalized map $\widehat{\mathcal{H}}_F : \mathcal{W}^\infty(j_0) \longrightarrow \mathcal{F}^\infty(M, I\!R^n)$ fulfilling the boundary condition

$$\mathcal{G}(j_0)\big(Grad_{\mathcal{G}(j_0)}\overline{F}|_{\partial\mathcal{W}^\infty(j_0)}, \mathbf{n}_B\big) = I\!D\,\widehat{\mathcal{H}}_{\overline{F}}(\mathbf{n}_B). \tag{2.2.3}$$

Thus we have :

**Theorem 2.2.1:**

*Let $A_P$ be any virtual work on $r_\infty\big(\mathcal{W}^\infty(j_0)\big) \subset E^\infty(P, I\!R^n)$, and $\mathcal{F}^\infty(M, I\!R^n)$ be equipped with the metric $B(\rho)$, satisfying (2.2.1). Moreover let $\rho_0 := \rho(j_0)$ for some $j_0 \in E^\infty(P, I\!R^n)$.*

*The virtual work $A := r^*_\infty A_P$ splits uniquely on a closed ball $\mathcal{W}^\infty(j_0)$ centred about $j_0$ into*

$$A = I\!D\,\overline{F} + \Psi \tag{2.2.4}$$

*where $\overline{F}$ satisfies*

$$d\!\!\!\;iv_B A = \Delta\!\!\!\!/_B\overline{F} = d\!\!\!\;iv_B \frac{1}{\rho_0}\Delta\widehat{\mathcal{H}}_{\overline{F}} \quad \text{and} \quad A(\mathbf{n}_B) = I\!D\,\overline{F}(\mathbf{n}_B). \tag{2.2.5}$$

*Moreover, $Grad_B\overline{F}$, the gradient of $\overline{F}$ formed with respect to $B(\rho)$ and $Grad_{\mathcal{G}(j_0)}$ are related by*

$$Grad_{\mathcal{G}(j_0)}\overline{F} = Pr \cdot \rho_0 \cdot Grad_B\overline{F} = \Delta\widehat{\mathcal{H}}_{\overline{F}} \tag{2.2.6}$$

*where $Pr$ is the $\mathcal{G}(j_0)$-orthogonal projection onto $\mathcal{F}^\infty(M, I\!R^n)$ and $\widehat{\mathcal{H}}_{\overline{F}}(j) \in \mathcal{F}^\infty(M, I\!R^n)$ for each $j \in \mathcal{W}^\infty(j_0)$. The operators $d\!\!\!\!\;div_B$ and $\not\!\Delta_B$ are the divergence and Laplacian on $\mathcal{F}^\infty(M, I\!R^n)$ formed with respect to $B(\rho)$. Both $\widehat{\mathcal{H}}$ and $\overline{F}$ depend smoothly on $j \in \mathcal{W}^\infty(j_0)$.*

Now we turn to the discrete level again. $A_P$ splits on $\mathcal{W}(j_P^0) := r_\infty\big(\mathcal{W}^\infty(j_0)\big)$ accordingly into

$$A_P = I\!D\,\overline{F}_P + \Psi_P$$

i.e.

$$d\!\!\!\!\;div_P A_P = \not\!\Delta_P \overline{F}_P$$

and

$$A(\mathbf{n}_P) = I\!D\,\overline{F}(\mathbf{n}_P)$$

have to hold. Here $d\!\!\!\!\;div_P$, $\not\!\Delta_P$ and $(\mathbf{n}_P)$, the outward directed unit normal field of $\mathcal{W}(j_P^0)$, are all formed with respect to $\mathcal{G}_P$ (cf.[Ma]). Due to (2.2.1) we immediately deduce:

**Theorem 2.2.2:**

*Let $A = r_\infty^* A$ on $\mathcal{W}^\infty(j_0)$. Then*

$$\overline{F} = r_\infty^* \overline{F}_P + const. \quad \text{and} \quad \Psi = r_\infty^* \Psi_P. \tag{2.2.7}$$

Next we will construct a natural **density** $F : \mathcal{W}^\infty(j_0) \longrightarrow C^\infty(M, I\!R^n)$ for $\overline{F}$ exhibited in the theorem above, i.e.

$$\overline{F}(j) = \int_M F(j)\mu(j_0) \quad \forall\, j \in \mathcal{W}^\infty(j_0).$$

Obviously $\overline{F}$ admits many densities, e.g.$F := \frac{\overline{F}}{A}$ is one. We will construct one which is based on the gradient of $\overline{F}$, and hence differs from $\frac{\overline{F}}{A}$ in general: To this end we will write

$$I\!D\,\overline{F} = \mathcal{G}(j_0)(Grad_{\mathcal{G}(j_0)}\overline{F}, ...)$$

which implies the Fourier decomposition

$$Grad_{\mathcal{G}(j_0)}\overline{F} = \sum_i \frac{\partial \overline{F}}{\partial \overline{\mathbf{x}}_i} \cdot e_i \tag{2.2.8}$$

where $\overline{\mathbf{x}}_i$ is the $i^{th}$ coordinate function defined by $e_i \in \mathcal{F}_0^\infty(M, I\!R^n)$. The one-form $w$ with

$$w(h) :=< Grad_{\mathcal{G}(j_0)}\overline{F}, h > \quad \forall\, h \in \mathcal{F}^\infty(P, I\!R^n)$$

on $\mathcal{W}^\infty(j_0)$ (having values in the finite dimensional subspace of $C^\infty(M, I\!R^n)$ generated by $\{< e_i, e_r > |i, r = 1, ..., (s_0 - 1) \cdot n\}$) splits into

$$w = I\!D\, F + \Psi_{Gr}$$

in the sense of Neumann on $\mathcal{W}^\infty(j_0)$. This is to say both equation

$$d\!\!\!\!\!\;div_{\mathcal{G}(j_0)}\; w = \Delta\!\!\!\!\!\;\Delta \overline{F}$$

and

$$w(N) = I\!D\, F(N)$$

hold true, where $N$ is the oriented (outward directed) $\mathcal{G}(j_0)$-unit normal along $\partial\mathcal{W}^\infty(j_0)$ and $\Delta\!\!\!\!\!\;\Delta$ and $d\!\!\!\!\!\;div_{\mathcal{G}(j_0)}$ are the Laplacian and divergence both formed with respect it $\mathcal{G}(j_0)$ (cf. [Ma]). Clearly

$$d\!\!\!\!\!\;div_{\mathcal{G}(j_0)}\; w = \sum_i \frac{\partial^2 \overline{F}}{\partial \overline{\mathbf{x}}_i^2} < e_i, e_i > .$$

Thus

$$\Delta\!\!\!\!\!\;\Delta \overline{F} = \Delta\!\!\!\!\!\;\Delta \int_M F\mu(j_0) = \int_M \Delta\!\!\!\!\!\;\Delta F\mu(j_0)$$

showing that $\overline{F}$ and $\int_M F\mu(j_0)$ differ by a constant. Moreover

$$I\!D\, \overline{F} = \int_M I\!D\, F\mu(j_0) = \int_M < Grad\, \overline{F}, ... > \mu(j_0)$$

which implies in particular

$$\frac{\partial \overline{F}(j)}{\partial \overline{\mathbf{x}}_i} = \int_M I\!D\, F(j)(e_i)\mu(j_0) \quad \forall\, i = 1, ..., (s_0 - 1) \cdot n$$

on all of $\mathcal{W}^\infty(j_0)$. This shows that

$$\int_M \Psi_{Gr}(h)\mu(j_0) = 0 \quad \forall\, h \in \mathcal{F}^\infty(M, I\!R^n).$$

We therefore have

**Proposition 2.2.3:**

*The function* $\overline{F} \in C^\infty(\mathcal{W}^\infty(j_0), I\!R)$ *of the exact part* $I\!D\overline{F}$ *admits a density* $F$, *i.e.*

$$\overline{F} = \int_M F\mu(j_0) \tag{2.2.9}$$

*satisfying*

$$I\!D\overline{F} = \int_M I\!D F\mu(j_0) = \int_M < Grad\overline{F}, ... > \mu(j_0). \tag{2.2.10}$$

*on* $\mathcal{W}^\infty(j_0)$. *Moreover the following equations hold:*

$$< Grad_{\mathcal{G}(j_0)}\overline{F}, ... >= I\!D F + \Psi_{Gr}$$

$$< Grad_{\mathcal{G}(j_0)}\overline{F}, N >= I\!D F(N) \tag{2.2.11}$$

$$\Delta\overline{F} = \mathrm{div}_{\mathcal{G}(j_0)}(< Grad_{\mathcal{G}(j_0)}\overline{F}, ... >)$$

$$\int_M \Psi_{Gr}(h)\mu(j_0) = 0. \tag{2.2.12}$$

$\forall\, h \in \mathcal{F}^\infty(M, I\!R^n)$. *Here* $N$ *is the outward directed* $\mathcal{G}(j_0)$ *unit normal along* $\partial\mathcal{W}^\infty(j_0)$.

Next we will show that $\overline{F}$ admits an observable $I \in C^\infty(\mathcal{W}^\infty(j_0), I\!R)$ at a fixed prescribed **temperature** $T$ such that the partition function $Z$, formed with respect to an equilibrium state $\rho_e$ (cf. appendix 2, A2.16), will satisfy

$$ln\ Z := -\frac{1}{T}\overline{F}. \tag{2.2.13}$$

The state $\rho_e$ has to be determined. To this end let $F$ be a density of $\overline{F}$. To relate the density $F$ with the observable we set

$$\rho_e \cdot ln\ Z = -\frac{1}{T}F \tag{2.2.14}$$

$$\frac{e^{-\frac{1}{T}\cdot I}}{Z} ln\ Z = -\frac{1}{T}F$$

or

$$e^{-\frac{1}{T}\cdot I} = e^{-\frac{1}{T}\cdot\overline{F}} \cdot \frac{F}{\overline{F}}$$

if $\overline{F}$ is nowhere zero. Hence (2.2.14) implies obviously (2.2.13). We therefore have the following :

**Theorem 2.2.4:**

*Associated with the map $\overline{F}$, for which $I\!D\overline{F}$ is the exact part of a constitutive law $A : \mathcal{W}^\infty(j_0) \times \mathcal{F}(M, I\!R^n) \longrightarrow I\!R$ made up by finitely many particles and any a density $F$ of $\overline{F}$, i.e. a map $F : \mathcal{W}^\infty(j_0) \longrightarrow C^\infty(M, I\!R)$ with*

$$\overline{F} = \int_M F\mu(j_0), \tag{2.2.15}$$

*there is an observable $I$ such that $\overline{F}$ is the free energy of the Gibbs state*

$$\rho_e := \frac{e^{-\frac{1}{T}I}}{\int_M e^{-\frac{1}{T}I}\mu(j_0)} \tag{2.2.16}$$

*at a fixed temperature $T$; Hence*

$$\rho_e = e^{\frac{1}{T}(\overline{F}-I)}. \tag{2.2.17}$$

*This observable $I$ is given by*

$$I := \frac{\overline{F} + T\ ln\ \overline{F}}{F}. \tag{2.2.18}$$

*The density $F$ is related to $\overline{F}$ by*

$$F = \rho_e \cdot \overline{F}. \tag{2.2.19}$$

*(2.2.18) shows that $I$ depends on the choice of the density $F$.*

The above theorem motivates us to call $\overline{F}$, a real-valued function on $\mathcal{W}^\infty(j_0)$, the **free energy** of the medium (cf. appendix 2). Here again $\mathcal{W}(j_0)$ has to be small in order to fit reality some what.

Let us point out that if the second law in thermodynamics holds, then the free energy defined in a thermodynamical setting satisfies (2.2.4) (cf.[Bi6]).

From (2.2.14) and (2.2.19) we immediately deduce

$$T \cdot \rho_e \cdot ln\ Z = -\rho_e \cdot I - T \cdot \rho_e ln\ \rho_e \tag{2.2.20}$$

or equivalently

$$F = \rho_e \cdot I - T \cdot S$$

with $S := -\rho_e ln\ \rho_e$ the **entropy density** associated with $I$ and $T$ (cf. appendix 2). Integrating both sides yields

$$\overline{F} = \overline{I} - T \cdot \overline{S}. \tag{2.2.21}$$

This formula shows that $\overline{I}$ can be identified with the **internal energy** (cf.[B,St] or [L,L]). In fact we have $\frac{\partial ln Z}{\partial \frac{1}{T}} = -\overline{I}$, saying again that $\overline{I}$ is the internal energy (cf. [B,St]). On the other hand (2.2.21) implies

$$I\!D\, F = I\!D\,(\rho_e \cdot I) - T \cdot I\!D\, S \tag{2.2.22}$$

and hence (2.2.10) yields

$$< Grad_{\mathcal{G}(j_0)}\overline{F}, ... >= I\!D\,(\rho_e \cdot I) - T \cdot I\!D\, S + \Psi_{Gr}. \tag{2.2.23}$$

Since moreover

$$Grad_{\mathcal{G}(j_0)}\overline{F} = \sum \lambda_i \widehat{\kappa}^i_{\overline{F}} \widehat{e}_i = \sum \frac{\partial \overline{F}}{\partial \overline{\mathbf{x}}_i} \cdot \widehat{e}_i.$$

We therefore have shown the following:

**Proposition 2.2.5:**

*At a fixed temperature $T$ the densities $F$,$I$ and $S$ of the free energy, the internal energy and the entropy are related by*

$$F = \rho_e \cdot I - T \cdot S \tag{2.2.24}$$

*implying*

$$\overline{F} = \int_M \rho_e I \mu(j_0) - T \cdot \int_M \rho_e ln\ \rho_e \mu(j_0) = \overline{I} - T \cdot \overline{S} \tag{2.2.25}$$

*and therefore*

$$A = I\!D\,\overline{F} + \Psi = I\!D\,\overline{I} - T \cdot I\!D\,\overline{S} + \Psi \tag{2.2.26}$$

*for fixed $T$. Since the gradient $Grad_{\mathcal{G}(j_0)}\overline{F}$ of $\overline{F}$ formed with respect to $\mathcal{G}(j_0)$ is*

$$Grad_{\mathcal{G}(j_0)}\overline{F} = \sum_i \lambda_i \widehat{\kappa}^i_{\overline{F}} e_i = \sum_i \frac{\partial \overline{F}}{\partial \overline{\mathbf{x}}_i} \cdot e_i \tag{2.2.27}$$

*saying that*

$$\lambda_i \widehat{\kappa}^i_{\overline{F}} = \frac{\partial \overline{F}}{\partial \overline{\mathbf{x}}_i} \quad \forall\, i = 1, ..., (s_0 - 1) \cdot n \tag{2.2.28}$$

*we have in addition for each $i = 1, ..., (s_0 - 1) \cdot n$*

$$\widehat{\kappa}^i_{\overline{F}} < e_i, e_i >= \frac{\partial(I - TS)}{\partial \overline{\mathbf{x}}_i} + < \Psi e_i, e_i > \quad \text{or} \quad \widehat{\kappa}^i_{\overline{F}} = \frac{\partial(\overline{I} - T\overline{S})}{\partial \overline{\mathbf{x}}_i}. \tag{2.2.29}$$

*In particular, if $I\!D\,\overline{F}(j_0) = 0$*

$$\widehat{\kappa}^i_{\overline{F}}(j_0) = 0 \quad \text{or equivalently} \quad \frac{\partial \overline{I}}{\partial \overline{\mathbf{x}}_i} = T \cdot \frac{\partial \overline{S}}{\partial \overline{\mathbf{x}}_i} \quad \forall\, i = 1, ..., (s_0 - 1) \cdot n \tag{2.2.30}$$

Now we turn to the statistical set up on the discrete level. Here too $\overline{F}_P$ admits a natural density $F_P$:

**Proposition 2.2.6:**

*The constitutive law $A_P$ has a uniquely determined exact part $I\!D\,\overline{F}_P$. The map $\overline{F}_P$ : $\mathcal{W}(j_P^0) \longrightarrow I\!R$ admits a density map*

$$F_P : \mathcal{W}(j_P^0) \longrightarrow \mathcal{F}(P, I\!R)$$

*smoothly depending on $j_P \in \mathcal{W}(j_P^0)$ such that*

$$\overline{F}_P(j_P) = \sum_{q \in M} F_P(j_P)(q) \quad \forall j \in \mathcal{W}(j_P^0) \tag{2.2.31}$$

*and $I\!D\,F$ is the exact part of $< Grad\overline{F}_P, \ldots >$ for which*

$$\Delta\!\!\!\!/\,\overline{F}(j_P) = \sum_{q \in P} \Delta\!\!\!\!/_P F_P(j_P) \tag{2.2.32}$$

*holds. Here $\Delta\!\!\!\!/_P$ is the Laplacian determined $\mathcal{G}_P$ on $\mathcal{F}(P, I\!R^n)$.*

<u>Proof:</u> The proof follows exactly the same pattern as the one of proposition (2.2.3). $\overline{F}$ admits a gradient $Grad_P\overline{F}_P$. The divergence of

$$< Grad_P\overline{F}_P, \ldots >: \mathcal{W}(j_P^0)_P \longrightarrow \mathcal{F}(P, I\!R)$$

yields for each $j_P \in \mathcal{W}(j_P^0)$ a map $F_P(j_P) : \mathcal{W}(j_P^0)_P \longrightarrow \mathcal{F}(P, I\!R^n)$ which can be chosen such that $F_P(j_P)$ is perpendicular to $I\!R^n \subset \mathcal{F}(P, I\!R^n)$ for all $j_P \in \mathcal{W}(j_P^0)$. Thus $F_P$ is uniquely determined and satisfies $\Delta\!\!\!\!/_P\overline{F}(j_P) = \Delta\!\!\!\!/_P \sum_P F(j_P)(q)$, showing the lemma.

Let us point out here, that theorem 2.2.4 holds accordingly for $A_P$ and $\overline{F}_P$ exhibited in theorem 2.2.2; the respective maps on $\mathcal{W}(j_P^0)$ are denoted by $I_P, \overline{I}_P, S_P$ and $\overline{S}_P$. The integral $\int_M$ has to be replaced by $\sum_{q \in P}$.

Therefore we have the following:

**Theorem 2.2.7:**

*To* $\overline{F}_P : \mathcal{W}_P(j_P^0) \longrightarrow I\!R$ *and any density* $F_P : \mathcal{W}(j_P^0) \times P \longrightarrow I\!R$*, there is an observable* $I_P : \mathcal{W}_P(j_P^0) \times P \longrightarrow I\!R$ *such that*

$$\rho_e^P \cdot F_P = -\frac{1}{T} ln\ Z_P = \overline{F}_P \qquad (2.2.33)$$

*where* $Z_P(q) = \sum e^{-\frac{1}{T} I_P}(q)$ and $\rho_e^P := \frac{e^{-\frac{1}{T} I_P}}{Z_P}$*. Moreover* $\overline{F}_P = -\frac{1}{T} \cdot ln\ Z_P$ *is the free energy of* $I_P$ *at a fixed temperature* $T$*. The observable* $I_P$ *is given by*

$$I_P := \overline{F}_P + T\ ln\ \overline{F}_P / F_P. \qquad (2.2.34)$$

Again as in the continuum case, the above theorem motivates us to call $\overline{F}_P$ the **free energy** of the virtual work of the discrete medium.

The functions $\overline{F}, Z, \overline{F}_P$ and $Z_P$ are linked by construction in the following manner

**Corollary 2.2.8:**

*Let* $\overline{F}_P$ *be the free energy associated with a virtual work* $A_P$*. The free energy* $\overline{F}$ *and the partition function* $Z$ *on* $\mathcal{W}^\infty(j_0)$ *are related to* $F_P$ *and* $Z_P$ *on* $\mathcal{W}\big(r_\infty(j_0)\big)$ *by*

$$\overline{F} = r^* \overline{F}_P \quad \text{and hence} \quad Z = r^* Z_P \qquad (2.2.35)$$

*for fixed temperature* $T$*.*

Finally let us make examples to the statistical set up on $M$:

**Example:** 1) We consider the area function

$$\mathcal{A}(j) := \int_M \mu(j) = \int_M det\ f(j) \mu(j_0) \quad \forall j \in \mathcal{W}^\infty(j_0).$$

Here $\mathcal{A} = \overline{F}$ and $det\ f(j) = F$, in the sense of theorem 2.2.4.

If $j$ and $j_0$ are close to each other then

$$det\ f(j) = e^{tr \varphi(j)} \qquad (2.2.36)$$

Hence the density $F$ is *det* $f(j)$. Let $T$ be fixed. Then

$$Z(j) = e^{-\frac{1}{T}\mathcal{A}(j)} \quad \forall j \in \mathcal{W}^{\infty}(j_0). \tag{2.2.37}$$

Hence

$$I = \mathcal{A}(j) - T \cdot ln\ \mathcal{A}(j) - T \cdot tr\varphi(j). \tag{2.2.38}$$

To compute the Fourier coefficients of $\widehat{H}_{\mathcal{A}}$, the constitutive map of $\mathcal{A}$ we use (2.2.27) and get

$$\widehat{\kappa}^i_{\mathcal{A}} = \frac{1}{\lambda_i}\frac{\partial \mathcal{A}}{\partial \overline{\mathbf{x}}_i}.$$

On the other hand we have in case of $n = 1 + dim\ M$

$$Grad_{\mathcal{G}}\mathcal{A} = H \cdot N$$

where $H$ is as in (1.1.29) and $N$ is the oriented $m(j_0)$-unit normal vector field along the embedded manifold (cf.(1.1.29)). Thus

$$\widehat{\kappa}^i_{\mathcal{A}} = \mathcal{G}(j_0)(H \cdot N, e_i) \quad \forall i = 1, ...(s_0 - 1) \cdot n$$

(cf. section 2.1) showing

$$\frac{\partial \mathcal{A}}{\partial \overline{\mathbf{x}}_i} = H \cdot \mathcal{G}(j_0)(N, e_i) \quad \forall i = 1, ...(s_0 - 1) \cdot n.$$

2) We consider the $i^{th}$ coordinate function

$$\overline{\mathbf{x}}_i : \mathcal{W}^{\infty}(j_0) \longrightarrow I\!R$$

determined by $e_i$. Clearly

$$\begin{aligned} d\overline{\mathbf{x}}_i &= \int_M < e_i, ... > \mu(j_0) = \mathcal{G}(j_0)(Grad_{\mathcal{G}(j_0)}\overline{\mathbf{x}}_i, ...) \\ &= \int_M \rho_0 < \rho_0^{-1} e_i, ... > \mu(j_0) = B(\rho_0)(\rho_0^{-1} e_i, ...) \end{aligned}$$

Thus $Pr\rho_0^{-1}e_i$ is the gradient of $\overline{\mathbf{x}}_i$ with respect to $B(\rho)$, and $d\overline{\mathbf{x}}_i(l)$ is the $i^{th}$ Fourier coefficient of $l \in \mathcal{F}^{\infty}(M, I\!R^n)$. Here $Pr$ is the $\mathcal{G}(j_0)$-orthogonal projection onto $\mathcal{F}^{\infty}(M, I\!R^n)$. The density map $\mathbf{x}_i$ of $\overline{\mathbf{x}}_i$ is given by

$$\overline{\mathbf{x}}_i := < e_i, ... >$$

Therefore we have

$$\overline{\mathbf{x}}_i = \int_M \mathbf{x}_i \mu(j_0)$$

and obviously $\mathbb{d}\overline{\mathbf{x}}_i = \int_M \mathbb{d}\mathbf{x}_i \mu(j_0)$. Given any $\overline{F} : \mathcal{W}^\infty(j_0) \longrightarrow I\!R$ we have

$$I\!D\,\overline{F} = \sum_i \frac{\partial \overline{F}}{\partial \mathbf{x}_i} \mathbb{d}\overline{\mathbf{x}}_i = \sum_i \int_M \frac{\partial \overline{F}}{\partial \mathbf{x}_i} \mathbb{d}\overline{\mathbf{x}}_i$$

Hence the density map $F$ of $\overline{F}$ in theorem 2.2.3 satisfies

$$\sum_i \int_M \frac{\partial \overline{F}}{\partial \mathbf{x}_i} \mathbb{d}\mathbf{x}_i \mu(j_0) = \int_M I\!D\, F \mu(j_0).$$

Following the construction of $F$ out of $\overline{F}$ we may set

$$\not\Delta F_i = \mathbb{d}iv_{\mathcal{G}(j_0)} \frac{\partial \overline{F}}{\partial \mathbf{x}_i} \mathbb{d}\overline{\mathbf{x}}_i = - \sum_{i=1}^{(s_0-1)\cdot n} \frac{\partial^2 \overline{F}}{\partial \mathbf{x}_r \partial \mathbf{x}_i} < e_i, e_r > .$$

In all the formulas the coordinate system $e_1, ..., e_{(s_0-1)\cdot n}$ can be replaced by any other $\mathcal{G}(j_0)$-orthonormed one.

Moreover $\overline{F}$ and $F$ in (2.2.15) have the form

$$\overline{F} = \sum_i \overline{F}_i \quad \text{and} \quad F = \sum_i F_i$$

with $\overline{F}_i(j) := \int_M F_i(j)\mu(j_0)$ for all $j \in \mathcal{W}^\infty(j_0)$ due to the construction of $F$. Then $\overline{F} = \sum \overline{F}_i$ and

$$\not\Delta \overline{F}_i = - \frac{\partial^2 \overline{F}}{\partial \mathbf{x}_\mathbf{i}^2}$$

This equation has a solution $F_i$ up to a constant. To associate a component $I_i$ of the observable $I$ given by $F$ via (2.2.17) we set

$$Z_i := e^{-\frac{1}{T}\overline{F}_i} \quad \text{and} \quad \rho_e^i := \frac{e^{-\frac{1}{T}I_i}}{Z_i} \quad \forall\, i = 1, ..., (s_0 - 1)\cdot n$$

Then $Z = \prod_i Z_i$ and $\rho_e = \prod_i \rho_e^i$; therefore

$$I_i := -T(ln\ Z_i + ln\ \rho_0^i)$$

implying

$$I = \sum I_i \quad \forall\, i = 1, ..., (s_0 - 1)\cdot n$$

## 3) Nearest neighbour interaction

### 3.1 Nearest neighbour interaction

So far we did not specify any interaction type among the material particles of which the mean locations are the points of $P \subset M$. In this section we implement an interaction structure as follows: Let $\mathbf{L} \subset M$ be a connected simplicial complex consisting of zero- and one-simplices only, the zero simplices being the points in $P$ and the one-simplices being segments connecting points in $P$. In the terminology of appendix 3 we have $P = \mathbf{L}_0$. Our $\mathbb{R}^n$-valued cochain complex associated with $\mathbf{L}$ has the form

$$\mathbb{R} \xrightarrow{\partial^0} C^0(\mathbf{L}) \xrightarrow{\partial^1} C^1(\mathbf{L}).$$

All points $q_i$ which are connected with $q \in P$, say, are called **nearest neighbours** of $q$. Instead of $C^0(\mathbf{L})$ we write $\mathcal{F}(P, \mathbb{R}^n)$. The number of nearest neighbours of $q$ is called $k(q)$. Furthermore we assume that all nearest neighbours of any $q \in P$ are within the domain of a Riemannian normal chart about $q$. The Riemannian metric being $m(j_0)$ for some fixed $j_0 \in E(M, \mathbb{R}^n)$, a reference configuration. The distances between $q$ and its nearest neighbours shall all be extremely small, which means that $s_0$, the number of points in $P$ is rather large for a large diameter of $M$. Any $q \in P$ is supposed to interact only with its nearest neighbours, i.e. we have a nearest **neighbour interaction**.

No external fields shall be present at all.

Let $\mathcal{W}(j_P^0)$ be a closed ball in $E^\infty(P, \mathbb{R}^n)$ centred about $j_P^0 := r(j)$ and let us assume that

$$\Phi_P : \mathcal{W}(j_P^0) \longrightarrow \mathcal{F}(P, \mathbb{R}^n)$$

is an internal force, i.e. the following holds for all $j_P \in \mathcal{W}(j_P^0)$:

$$\sum_{q \in \mathbf{L}_0} \Phi_P(j_P)(q) = 0 \quad \text{and} \quad \Phi_P(j_P + z) = \Phi_P(j_P) \quad \forall\, z \in \mathbb{R}^n. \tag{3.1.1}$$

Hence there is a map $\mathcal{H}_P : \mathcal{W}(j_P^0) \longrightarrow \mathcal{F}(P, \mathbb{R}^n)$ such that

$$\Phi_P(j_P) = \Delta_T \mathcal{H}_P(j_P) \quad \forall\, j_P \in \mathcal{W}(j_P^0), \tag{3.1.2}$$

where $\Delta_T$ is the Laplacian associated with the complex $\mathbf{L}$ on the level of $\mathcal{F}(P, \mathbb{R}^n)$ (cf. appendix3, [B], compare also [Ch,St]).

We call $\mathcal{H}_P$ the **constitutive map**.
$\mathcal{H}_P$ is $\mathcal{G}_P$-normalized provided that $\mathcal{G}_P(\mathcal{H}(j_P), z) = 0$ for all $z \in \mathbb{R}^n$ and all $j_P \in \mathcal{W}(j_P^0)$. Clearly (3.1.2) admits a unique $\mathcal{G}_P$-normalized solution $\mathcal{H}_P$.

By the definition of $\Delta_T$ (cf. appendix 3) we observe that $\mathcal{H}_P(q) - \mathcal{H}_P(q_i)$ is the **interaction force within the medium** of the particle at $q$ with its nearest neighbour at $q_i$ for all $i = 1, ..., k(q)$ and each $q \in P$. These interaction forces might be given by potentials (cf. lemma 3.1.1 below)

Let $e_1^T, ..., e_{(s_0-1)\cdot n}^T$ be the $\mathcal{G}_P$-orthogonal eigenvectors of $\Delta_T$ in $\mathcal{F}(P, \mathbb{R}^n)$ having eigenvalues $0 < \lambda_1^T \leq \lambda_2^T \leq \ldots \leq \lambda_{(s_0-1)\cdot n}^T$. Then

$$\mathcal{H}_P(j_P) = \sum_{i=1}^{(s_0-1)\cdot n} \zeta^i(j_P) \cdot e_i^T \quad \forall\, j_P \in \mathcal{W}(j_P^0) \tag{3.1.3}$$

and

$$\Phi_P(j_P) = \sum_{i=1}^{(s_0-1)\cdot n} \lambda_i^T \zeta^i(j_P) \cdot e_i^T \quad \forall\, j_P \in \mathcal{W}(j_P^0); \tag{3.1.4}$$

here $\zeta^i : \mathcal{W}(j_P^0) \longrightarrow \mathbb{R}$ are smooth for each $i = 1, ..., (s_0 - 1) \cdot n$.

Proceeding as in the previous section we verify that associated with $\overline{F}_P$ and a fixed temperature $T$ there is an equilibrium state (as already pointed out in section 2.2).

Let us assume that the interaction force between the particle at $q$ and the one at $q_i$ is derivable from a potential in the ambient space $\mathbb{R}^n$. This is to say that we assume a **potential**

$$V : P \times \mathbb{R}^n \backslash \{0\} \longrightarrow \mathbb{R}$$

which is smooth in the variable $z \in \mathbb{R}^n \backslash \{0\}$ and which does not depend on $j_P \in \mathcal{W}(j_P^0)$.
Therefore the interaction force $\mathcal{H}_P(j_P)(q) - \mathcal{H}_P(j_P)(q_i)$ has the form

$$\mathcal{H}_P(j_P)(q) - \mathcal{H}_P(j_P)(q_i) = grad_{\mathbb{R}^n} V\big(j_P(q) - j_P(q_i)\big) \quad \forall\, j_P \in \mathcal{W}(j_P^0) \tag{3.1.5}$$

where $grad_{\mathbb{R}^n}$ means the gradient formed in $\mathbb{R}^n \backslash \{0\}$. Hence

$$\Delta_T \mathcal{H}_P(j)(q) = \sum_{i=1}^{k(q)} grad_{\mathbb{R}^n} V\big(j_P(q) - j_P(q_i)\big). \tag{3.1.6}$$

Therefore we have the following

**Lemma 3.1.1:**

*Let $V : P \times I\!R^n \backslash \{0\} \longrightarrow I\!R$ be a potential for the interaction forces. The constitutive map satisfies*

$$\mathcal{H}_P(j_P)(q) - \mathcal{H}_P(j_P)(q_i) = \big(grad_{I\!R^n} V\big)\big(j(q) - j(q_i)\big)$$

$$\forall\, q \in P \quad \text{and} \quad \forall\, i = 1, ..., k(q), \forall\, j_P \in \mathcal{W}(j_P^0).$$

*Moreover the Fourier coefficients and their derivatives are determined by*

$$\zeta_i(j_P) = \frac{1}{\lambda_i^T} \sum_{q \in P} \sum_{i=1}^{k(q)} DV\big(j_P(q) - j_P(q_i)\big)\big(e_i^T(q_i)\big)$$

*for all $j_P \in \mathcal{W}(j_P^0)$, for all $i = 1, ..., k(q)$ and for all $q \in P$. Hence*

$$\frac{\partial \zeta_i(j_P)}{\partial \mathbf{y}_s} = \frac{1}{\lambda_i^P} \sum_{q \in P} \sum_{i=1}^{k(q)} D^2V\big(j_P(q) - j_P(q_i)\big)\Big(\big(e_i^T(q), e_s^T(q)\big)\Big)$$

$$\forall\, i, s = 1, ..., k(q) \quad \text{and} \quad \forall\, q \in P$$

*where $\mathbf{y}_i$ is the coordinate function defined of $e_i^T$. Here $D$ denotes the Fréchet derivative in $I\!R^n$.*

The presence of a potential requires us to restrict the constitutive map $\mathcal{H}_P$ to a neighbourhood $\mathcal{W}(j_P^0)$ of some configuration of $j_P^0 \in E(P, I\!R^n)$. To show this let us assume that $V|q \times I\!R^n \backslash \{0\}$ grows rapidly to infinite near zero. Then the nearest neighbours of $q \in P$ react with $q$ only. Let $j_P^0(q_i), ..., j_P^0(q_{k(q)})$ be these nearest neighbours. If the distances between $j_P(q)$ and $j_P(q_1), ..., j_P(q_{k(q)})$ are made sufficiently large, then at least some of $j_P(q_1), ..., j_P(q_{k(q)})$ need not to be nearest neighbours $j_P(q)$ any more. This is precisely why we restrict us to $\mathcal{W}(j_P^0)$ from the beginning on. In presence of a potential , $\mathcal{W}(j_P^0)$ is supposed to consist of those configuration $j_P$ only for which $j(q_i)$ are the nearest neighbours of $j(q)$ for all $i = 1, ..., k(q)$ and all $q \in P$.

### 3.2 Nearest neighbour interactions described on a smooth manifold

In this section we will relate the description of the nearest neighbour interaction on a one-complex **L** considered in section 3.1 with the description on a smooth manifold $M$ containing the one-complex.

In contrast to section 2.1 we have a Laplacian $\Delta_T$ on $\mathcal{F}(P, I\!R^n)$ given by the interaction pattern. Hence we have constitutive maps, as seen in section 3.1.

One goal of this section will therefore be to relate the constitutive map on $P$ namely $\mathcal{H}_P : \mathcal{W}(j_P^0) \longrightarrow \mathcal{F}^\infty(M, I\!R^n)$, constructed in section 3.1, with the constitutive map on the continuum $M$, this is to say with $\mathcal{H}_P^M$, considered in section 2.1.

The relation of these two descriptions will be established via the restriction map

$$r : C^\infty(M, I\!R^n) \longrightarrow \mathcal{F}(P, I\!R^n).$$

In particular we will use $r_\infty : \mathcal{F}^\infty(M, I\!R^n) \longrightarrow \mathcal{F}(P, I\!R^n)$, a surjection (cf. sec 2.1) given by $r^\infty := r|\mathcal{F}^\infty(M, I\!R^n)$. We therefore consider again the integrable distribution

$$\mathcal{K} := \{j + \mathcal{F}^\infty(M, I\!R^n) | j \in E(M, I\!R^n)\}.$$

In particular we consider a leaf $\mathcal{W}^\infty(j) = j + O$ where $O$ is a closed ball in $\mathcal{F}^\infty(M, I\!R^n)$ centred about $j_0$ such that $r_\infty(\mathcal{W}^\infty(j_0)) = \mathcal{W}(j_P^0)$. Here $j_0 \in E(M, I\!R^n)$ a reference configuration such that $r^\infty(j_0) = j_P^0$. Again $\Delta(j_0)$ will be denoted by $\Delta$.

Throughout this section we assume that $j_P^0$ is an equilibrium configuration for the virtual work $A_P$ on $\mathcal{W}(j_P^0)$ or at least a stationary point of the free energy $\overline{F}_P$ (cf. section 2.1).

We assume furthermore that all nearest neighbours of any $q$ are within a distance smaller than the injectivity radius determined by the metric $m(j_0)$. In fact we require that there is a covering $(U_q | q \in P)$ of $M$ of open sets each of which has a diameter smaller than $\epsilon$ which itself is smaller than the injectivity radius of $exp$ at $q$ and suppose that $U_q$ contains all the nearest neighbours of $q$ in $P$. The real number $\epsilon$ itself shall be extremely small.

Finally let $\rho$ be a density map satisfying

$$r^*\mathcal{G}_P = B(\rho) \tag{3.2.1}$$

on the leaf $\mathcal{W}^\infty(j_0)$, (cf. lemma 2.1.2). Again we write $\rho_0$ instead of $\rho(j_0)$.

No external forces shall be present on $\mathcal{W}(j_P^0)$.

We begin by an internal force

$$\Phi_P : \mathcal{W}(j_P^0) \longrightarrow \mathcal{F}(P, I\!R^n)$$

which by definition is pointwise $\mathcal{G}_P$-orthogonal to $I\!R^n$. This force determines a virtual work $A_P$, say. Hence

$$\Phi_P = \Delta_T \mathcal{H}_P \tag{3.2.2}$$

for an uniquely determined smooth map $\mathcal{H}_P : \mathcal{W}(j_P^0) \longrightarrow \mathcal{F}(P, I\!R^n)$, pointwise $\mathcal{G}_P$-orthogonal to $I\!R^n$ as seen in the previous section. Since

$$\mathcal{G}(j_0)(\rho_0 r_\infty^{-1}\Phi_P r_\infty, l \ldots) = B(\rho)(r_\infty^{-1}\Phi_P r_\infty, l \ldots) = r^*\mathcal{G}_P(r_\infty^{-1}\Phi_P r_\infty, l \ldots)$$

for all $l \in \mathcal{F}(P, I\!R^n)$ we know by proposition 2.1.7 that

$$Pr \circ \rho_0 r_\infty^{-1} \circ \Phi_P \circ r_\infty = \Delta \widehat{\mathcal{H}}_P^M$$

for an uniquely determined smooth $\widehat{\mathcal{H}}_P^M$ pointwise $\mathcal{G}_P$-orthogonal to $I\!R^n$ with $Pr$ the $\mathcal{G}(j_0)$-orthogonal projection to $\mathcal{F}^\infty(M, I\!R^n)$. Clearly $\widehat{\mathcal{H}}_P^M$ is uniquely determined by $\mathcal{H}_P$. Thus

$$\Phi_P^M := Pr \circ \rho_0 \cdot r_\infty^{-1} \circ \Phi_P \circ r_\infty$$

is the uniquely determined force density on $\mathcal{W}^\infty(j_0)$(with $rj_0 = j_P^0$) for which $r_\infty^* A_P$ is the virtual work. Vice versa if we start with an internal force density

$$\Phi : \mathcal{W}^\infty(j_0) \longrightarrow \mathcal{F}^\infty(M, I\!R^n)$$

for which the virtual work is $A_M$, say. Then

$$\Phi_P := r_\infty \circ \; Pr \circ \frac{1}{\rho_0} \Phi \circ r_\infty^{-1}$$

is an internal force density causing a virtual work $A_P$, say, for which $A_M = r^* A_P$. We therefore have:

**Theorem 3.2.1:**

*There is a one to one correspondence between constitutive $\mathcal{G}_P$-normalized constitutive maps $\mathcal{H}_P$ on $\mathcal{W}(j_P^0)$ and $\mathcal{G}(j_0)$-normalized constitutive maps $\widehat{H}_P^M$ on $\mathcal{W}^\infty(j_0)$ such that the internal force densities on $\mathcal{W}^\infty(j_0)$ are related by*

$$Pr \circ \rho_0 r_\infty^{-1} \circ \Delta_T \mathcal{H}_P \circ r_\infty = \Delta \widehat{\mathcal{H}}_P^M \tag{3.2.3}$$

*where $Pr$ is the $\mathcal{G}(j_0)$ orthogonal projection onto $\mathcal{F}(M, I\!R^n)$. The virtual works $A_P$ and $A$ determined by $\mathcal{H}_P$ and $\widehat{\mathcal{H}}_P^M$ respectively satisfy*

$$A = r^* A_P. \tag{3.2.4}$$

This theorem shows that a medium determined by finitely many particles are equivalently described on $\mathcal{W}^\infty(j_0)$ and $\mathcal{W}\big(r_\infty(j_0)\big)$ by $\mathcal{H}_P^M$ and $\mathcal{H}_P$ respectively.

Now let us show that both $\overline{F}$ and $\overline{F}_P$ associated with $r_\infty^* A_P$ and $A_P$ respectively (both exhibited in section 2.2) admit constitutive maps and show how these maps are related to each other. Let us consider a smooth constitutive map

$$\mathcal{H}_P : \mathcal{W}(j_P^0) \subset \mathcal{F}(P, I\!R^n) \longrightarrow I\!R^n.$$

We form the virtual work $A_P$ and exhibit the free energy $\overline{F}_P$ on $\mathcal{W}(j_P^0)$ as in (theorem 2.2.2). Then we set $\overline{F} := r_\infty^* \overline{F}_P$ on $\mathcal{W}^\infty(j_0)$. Since $r_\infty^* \mathcal{G}_P = B(\rho)$ the map $\overline{F}$ is the free energy of $r_\infty^* A_P$. The gradient $Grad_{\mathcal{G}(j_0)} \overline{F}$ of $\overline{F}$ formed with respect to $\mathcal{G}(j_0)$ allows us to determine the constitutive map $\widehat{\mathcal{H}}_{\overline{F}}$ of $\overline{F}$ as follows: The one-form

$$I\!D\, \overline{F} : \mathcal{W}^\infty(j_0) \times \mathcal{F}^\infty(M, I\!R^n) \longrightarrow I\!R$$

vanishes on $I\!R^n$ since $I\!D\, \overline{F}_P$ does so. Hence $Grad_{\mathcal{G}(j_0)} \overline{F}$ is $\mathcal{G}(j_0)$-perpendicular to the constants $I\!R^n$ implying

$$Grad_{\mathcal{G}(j_0)} \overline{F}(j) = \Delta \widehat{\mathcal{H}}_{\overline{F}}(j)$$

with $\widehat{\mathcal{H}}_{\overline{F}}(j) \in C^\infty(M, I\!R^n)$ and in turn

$$I\!D\, \overline{F}(j)(h) = \mathcal{G}(j_0)\big(\Delta \widehat{\mathcal{H}}_{\overline{F}}(j), h\big)$$

for all $j \in \mathcal{W}^\infty(j_0)$ and all $h \in \mathcal{F}^\infty(M, I\!R^n)$. On the other hand $Grad_{r^*\mathcal{G}_P} \overline{F}$ satisfies for any $j \in \mathcal{W}^\infty(j_0)$ and $h \in \mathcal{F}^\infty(M, I\!R^n)$.

$$B(\rho)\big(Grad_{r^*\mathcal{G}_P} \overline{F}, h\big) = \mathcal{G}(j_0)\big(\rho(j_0) Grad_{r^*\mathcal{G}_P} \overline{F}, h\big) = \mathcal{G}(j_0)\big(\Delta \widehat{\mathcal{H}}_{\overline{F}}(j), h\big)$$

(cf. 3.2.1). If $Pr$ denotes the $\mathcal{G}(j_0)$-orthogonal projection onto $\mathcal{F}^\infty(M, I\!R^n)$ then

$$Pr \circ \rho(j_0) \cdot Grad_{r^*\mathcal{G}_P} \overline{F} = \Delta \widehat{\mathcal{H}}_{\overline{F}} \tag{3.2.5}$$

or due to $r^*\mathcal{G}_P = B(\rho)$

$$Pr \circ \rho(j_0) \cdot r_\infty^{-1} \circ \Delta_T \widehat{\mathcal{H}}_{\overline{F}_P} \circ r_\infty = \Delta \widehat{\mathcal{H}}_{\overline{F}}$$

where $\mathcal{H}_{\overline{F}_P}$ is the constitutive map of $I\!D\overline{F}_P$.

The theorem above together with the theorems 2.1.4, 2.2.1, and lemma 2.2.3 immediately yield the following:

**Corollary 3.2.2:**

*Let $\overline{F}_P$ be the free energy associated with a virtual work $A_P$. The free energy $\overline{F}$ and $\overline{F}_P$ on $\mathcal{W}^\infty(j_0)$ respectively on $\mathcal{W}(rj_0)$ related by $\overline{F} = r^*\overline{F}_P$ and both admit constitutive maps $\mathcal{H}_{\overline{F}}$ and $\mathcal{H}_{\overline{F}_P}$ respectively. These maps are related by*

$$Pr \circ \rho(j_0) r_\infty^{-1} \circ \Delta_T \mathcal{H}_{\overline{F}_P} \circ r_\infty = \Delta \widehat{\mathcal{H}}_{\overline{F}} \tag{3.2.6}$$

*and are such that*

$$Pr \circ \rho(j_0) Grad_{r^*\mathcal{G}} \overline{F} = \Delta \widehat{\mathcal{H}}_F = Grad_{\mathcal{G}(j_0)} \overline{F} \tag{3.2.7}$$

*or equivalently*

$$Pr \circ \rho(j_0) \cdot r_\infty^{-1} \circ \Delta_T \mathcal{H}_{\overline{F}_P} \circ r_\infty = \Delta \widehat{\mathcal{H}}_{\overline{F}} \tag{3.2.8}$$

Now let $dim\ M = 2$. By proposition (2.1.7) we conclude (cf. proposition 2.1.7)

$$\begin{aligned} \mathcal{G}_P\big(\Delta_T r(\mathcal{H}_P(j)), h\big) &= B(\rho)\big(r_\infty^* \Phi_P(j), h\big) \\ &= \int_M < r_\infty^* \Phi_P(j), h > \mu_\rho \\ &= \int_M < \Delta_\rho \mathcal{H}_\rho(j), h > \mu_\rho \\ &= B(\rho)\big(\Delta_\rho \mathcal{H}_\rho(j), h >\big) \end{aligned} \tag{3.2.9}$$

and hence

$$\Delta_\rho \mathcal{H}_\rho(j) = r_\infty^* \Delta_T \mathcal{H}_P(j) \quad \forall j \in \mathcal{W}^\infty(j_0) \tag{3.2.10}$$

have to hold for some smooth map $\mathcal{H}_\rho : \mathcal{W}^\infty(j_0) \longrightarrow C^\infty(M, I\!R^n)$.

Furthermore, as we have shown in appendices 1 and 3

$$d^* d = \Delta_\rho$$

formed with respect to $m_\rho$ ( cf. section 2.1) and

$$d_T^* d_T = \Delta_T.$$

Since $d = d_T$+higher order terms we have on $\mathcal{W}^\infty(j_0) \subset \mathcal{F}^\infty(M, I\!R^n)$ the equation $d^* = d_T^*$ up to higher order terms. Both sides are formed with respect to $r_\infty^* \mathcal{G}_P = B(\rho)$. Therefore the following holds:

**Theorem 3.2.3:**

*In case of dim* $M = 2$ *the Laplacians* $r_\infty^{-1} \circ \Delta_T \circ r_\infty$ *and* $\Delta_\rho$ *on* $\mathcal{F}^\infty(M, I\!R^n)$ *are related on* $\mathcal{W}^\infty(j_0)$ *by*

$$\Delta_\rho = r_\infty^{-1} \circ \Delta_T \circ r_\infty \quad \text{+higher order terms.} \tag{3.2.11}$$

*Therefore the* $\mathcal{G}_P$ *respectively the* $B(\rho)$*-normalized constitutive maps* $\mathcal{H}_P$ *on* $\mathcal{W}(j_P^0)$ *and* $\mathcal{H}_\rho$ *on* $\mathcal{W}^\infty(j_0)$ *of* $\Phi_P$ *and* $r^*\Phi_P$ *respectively, both formed with respect to* $\Delta_T$ *and* $\Delta_\rho$ *satisfy*

$$\mathcal{H}_P = r_\infty \circ \mathcal{H}_\rho \quad \text{+higher order terms.} \tag{3.2.12}$$

*Similarly* $\overline{F}$ *admits a* $B(\rho)$*-normalized constitutive map* $\widehat{\mathcal{H}}_{\overline{F}}^\rho$ *such that*

$$I\!D\,\overline{F}(j)(h) = B(\rho)\big(\Delta_\rho \widehat{\mathcal{H}}_\rho(j), h\big) \quad \forall\, j \in \mathcal{W}^\infty(j_0) \quad \forall\, h \in \mathcal{F}^\infty(M, I\!R^n) \tag{3.2.13}$$

*which is related to* $\mathcal{H}_{\overline{F}_P}$ *by*

$$\mathcal{H}_{\overline{F}_P} = r \circ \mathcal{H}_\rho \quad \text{+higher order terms on } \mathcal{W}^\infty(j_0). \tag{3.2.14}$$

**Definition 3.2.4:**

*In case of dim* $M = 2$ *we call a configuration* $j_0$ *a* **good fit** *for the discrete medium if*

$$m(j_0) = m_\rho \quad \text{and} \quad I\!D\,\overline{F}(j_0) = 0 \tag{3.2.15}$$

*where* $\overline{F} := r_\infty^* \overline{F}_P$.

Theorem 3.2.3 implies the following:

**Corollary 3.2.5:**

*Let dim $M = 2$ and $j_0 \in E(M, I\!R^n)$ with $r_\infty(j_0) = j_P^0$ be a good fit for the discrete medium. The Laplacians $\Delta_T \circ r$ and $\Delta$ are related on $\mathcal{W}^\infty(j_0)$ by*

$$\Delta_T \circ r_\infty = r_\infty \circ \Delta \quad +\text{higher order terms.} \tag{3.2.16}$$

*The constitutive maps $\mathcal{H}_P^M$ and $\mathcal{H}_\rho$ as well as $\mathcal{H}_{\overline{F}_P}$ and $\widehat{\mathcal{H}}_{\overline{F}}$ are related by*

$$\mathcal{H}_{\overline{F}_P}\big(r_\infty(j_0)\big) = r_\infty\big(\widehat{\mathcal{H}}_{\overline{F}}(j_0)\big) \quad +\text{higher order terms on } \mathcal{W}^\infty(j_0) \tag{3.2.17}$$

*and*

$$\mathcal{H}_P^M\big(r_\infty(j_0)\big) = r_\infty\big(\mathcal{H}_\rho(j_0)\big) \quad +\text{higher order terms on } \mathcal{W}^\infty(j_0). \tag{3.2.18}$$

The above corollary has the following consequences :

**Theorem 3.2.6:**

*Let $j_0$ be a good fit. Then the internal force*

$$r_\infty\big(\Delta\mathcal{H}_P^M(j)\big)(q) = \Delta_T\mathcal{H}_T\big(r_\infty(j)\big)(q) \quad \text{up to higher order terms}$$

*can be interpreted in first order as the interaction force between $q$ and all its nearest neighbours for any $q \in P$. Vice versa any internal force on $P$ is of this form.*

**Remark**

*If $j_0$ is not a good fit corollary 3.2.5 is not valid. The geometry on $M$ inherited by $j_0$ disturbs the direct sight to the physical situation, even though this situation is equivalently described as shown by theorem 2.1.4 or theorem 3.2.1.*

Corollary 3.2.5 and equation (1.1.29) together yield

**Corollary 3.2.7:**

*Let $j_0$ fit metrically well then 1.1.29 applied to any $q \in P$ reads as*

$$H(j_0)(q) \cdot N(j_0)(q) = k(q)j_0(q) - \sum_i^{k(q)} j_0(q^i) \quad \forall\, q \in P$$

*up to higher order terms, with $H(j_0)$ being the mean curvature of $j_0$, (the trace of the Weingarten map).*

# 4) Linearizations

## 4.1 Linearized virtual work

In this section we will determine the free energy $\overline{F}^{lin}$ of the linearization $A^{lin}$ of the virtual work $A$, presented in (1.1.35) in lemma 1.1.3. Here we assume that $A = r^* A_P$, where $A_P$ is a virtual work on $\mathcal{W}(j_P^0) \subset E^\infty(P, \mathbb{R}^n)$.

Again we will work on $\mathcal{W}^\infty(j_0)$ as in the previous section. $j_0 \in E(M, \mathbb{R}^n)$ is assumed to be an equilibrium configuration of $A$, i.e. $A(j_0) = 0$. Let $j_P^0 = r(j_0)$. Hence $A_P(j_P^0) = 0$ as well.

The **linearization** $A^{lin}$ of $A$ reads hence for each $l \in \mathcal{W}^\infty(j_0) - j_0$

$$A(j_0 + l)(h) = \mathbb{D}\, A(j_0)(l)(h) \quad \forall\, h \in \mathcal{F}^\infty(M, \mathbb{R}^n), \tag{4.1.1}$$

(cf. 1.1.35).

To determine the free energy $\overline{F}^{lin}$ of $A^{lin}$ we derive from (2.2.4) and (2.2.5) by differentiation at $j_0$

$$\mathbb{D}\, A(j_0)(l)(h) = \mathbb{D}^2\overline{F}(j_0)(l,h) + \mathbb{D}\,\Psi(j_0)(l)(h) \tag{4.1.2}$$

together with

$$\mathbb{D}\, A(j_0)(l)(\mathbf{n}_B) = \mathbb{D}^2\overline{F}(j_0)(l, \mathbf{n}_B) \tag{4.1.3}$$

for each $l \in \mathcal{W}^\infty(j_0) - j_0$, all $h \in \mathcal{F}^\infty(M, \mathbb{R}^n)$. Here $\overline{F}$ is the free energy of $A$, (cf. theorem 2.4.2).

Applying $\mathrm{d\!l}iv_B$ (cf. section 2.2) on both sides of (2.5.2) yields

$$-\sum_i \mathbb{D}\, A(j_0)(u_i)(u_i) = -(\sum_i \mathbb{D}^2\overline{F}(j_0)(u_i)(u_i) + \sum_i \mathbb{D}\,\Psi(j_0)(u_i)(u_i))$$

or

$$(\mathrm{d\!l}iv_B A)(j_0) = \Delta\!\!\!\!/_B \overline{F}(j_0) \quad \text{and} \quad \mathrm{d\!l}iv_B \Psi(j_0) = 0 \tag{4.1.4}$$

where $u_1, \ldots u_{(s_0-1)\cdot n}$ is a $B(\rho)$-orthonormal frame on $\mathcal{W}^\infty(j_0)$, i.e. a $B(\rho)$-orthonormal basis in $\mathcal{F}_0^\infty(M, \mathbb{R}^n)$ (cf. 2.1.7). Due to the definition of the free energy (cf. section 2.2) the following is therefore immediate:

**Theorem 4.1.1:**

*Let $A = r_\infty^* A_P$ on $\mathcal{W}^\infty(j_0)$, where $A_P$ is a virtual work on $\mathcal{W}(j_P^0)$ with $r_\infty(j_0) = j_P^0$. The linearization $A^{lin}$ of $A$ at the equilibrium $j_0$ is for each $l \in \mathcal{W}^\infty(j_0) - j_0$*

$$A^{lin}(j_0 + l)(h) = \mathbb{D} A(j_0)(l)(h) \quad \forall h \in \mathcal{F}^\infty(M, \mathbb{R}^n).$$

*Its free energy $\overline{F}$ is given by*

$$\overline{F}^{lin}(j_0 + l) = \overline{F}(j_0) + \frac{1}{2}\mathbb{D}^2\overline{F}(j_0)(l,l) \quad \forall l \in \mathcal{W}^\infty(j_0) - j_0. \tag{4.1.5}$$

*Here $\overline{F}$ is the free energy of $A$ and is of the form $\overline{F} = r^*\overline{F}_P$, where $\overline{F}_P$ is the free energy of $A_P$ on $\mathcal{W}(j_P^0)$. Hence $A^{lin}(j_0) = 0$ implies $\mathbb{D}\overline{F}^{lin}(j_0) = 0$. Moreover*

$$\not{\Delta}_B \overline{F}^{lin}(j_0 + l) = (\not{\Delta}_B \mathbb{D}^2\overline{F})(j_0)(l) \tag{4.1.6}$$

*(The constant $\overline{F}(j_0)$ is arbitrarily chosen).*

The structures of $A^{lin}$ and $\overline{F}^{lin}$ are determined by lemma 1.1.3 and theorem 1.1.4.

The eigenvalues of $\mathbb{D}^2\overline{F}(j_0)$ are called the **modes** of the **medium made up by finitely many particles** (cf. [Ch,St]). These modes are obviously of a global and classical nature.

To show the roles of this sort of modes let $G \in End\mathcal{F}_0^\infty(M, \mathbb{R}^n)$ be such that

$$\frac{1}{2} \cdot \mathbb{D}^2\overline{F}^{lin}(j_0)(l,l) = \mathcal{G}(j_0)(G\, l, l) \quad \forall l \in \mathcal{W}^\infty(j_0). \tag{4.1.7}$$

The following is obvious:

**Lemma 4.1.2:**

*Let $\mathbf{w}_1, ..., \mathbf{w}_{(s_0-1)\cdot n}$ be an orthonormed system of eigenvectors of $G$ and $\gamma_1, ..., \gamma_{(s_0-1)\cdot n}$ be the respective eigenvalues of $G$, this is to say the modes. Moreover if $\overline{\mathbf{z}}_i$ denotes the coordinate function defined by $\mathbf{w}_i$, then*

$$\overline{F}^{lin}(j_0 + l) = \overline{F}_0 + \sum_s^{(s_0-1)\cdot n} \gamma_s \cdot l_s^2 \quad \forall l \in \left(\mathcal{W}^\infty(j_0) - j_0\right) \tag{4.1.8}$$

*where $h = \sum h_s \mathbf{w}_s$, provided that $\mathbb{D}\overline{F}(j_0) = 0$. Moreover*

$$\frac{\partial^2 \overline{F}(j_0)}{\partial \overline{\mathbf{z}}_i^2} = \gamma_s \quad \text{and} \quad \frac{\partial^2 \overline{F}(j_0)}{\partial \overline{\mathbf{z}}_i \partial \overline{\mathbf{z}}_s} = \delta_{i,s} \quad \forall i, s = 1, ..., (s_0 - 1)\cdot n. \tag{4.1.9}$$

Combining theorem 4.1.1 with lemma 4.1.3 and theorem 2.4.3 yields immediately:

**Corollary 4.1.3:**

*Let* $a_{\overline{F}^{lin}}$ *be the structural capillarity of* $I\!D\,\overline{F}^{lin}$. *The constitutive map* $\mathcal{H}_{\overline{F}^{lin}}$ *assigning to each* $l \in \mathcal{W}^\infty(j_0) - j_0$ *the value*

$$\widehat{\mathcal{H}}_{\overline{F}^{lin}}(j_0 + l) = I\!D\,\widehat{\mathcal{H}}_{\overline{F}}(j_0)(l)$$

*satisfies*

$$I\!D^2(a_{\overline{F}^{lin}} \cdot \mathcal{A})(j_0)(l,h) = \mathcal{G}(j_0)\big(\Delta(j_0) I\!D\,\widehat{\mathcal{H}}_{\overline{F}}(j_0)(l), h\big)$$

*for each* $h \in \mathcal{F}^\infty(M, I\!R^n)$, *implying that*

$$I\!D\,\big(Grad_{\mathcal{G}(j_0)}(a_{\overline{F}^{lin}} \cdot \mathcal{A})\big)(j_0)(l) = I\!D\,\widehat{\mathcal{H}}_{\overline{F}}(j_0)(l).$$

*In case of dim* $M = 2$ *and if* $j_0$ *is a good fit (cf. def 2.4.4) then*

$$r\big(I\!D\,Grad_{\mathcal{G}(j_0)}(a_{\overline{F}^{lin}} \cdot \mathcal{A})(j_0)\big) = I\!D\,\mathcal{H}_{\overline{F}_P}\big(r_\infty(j_0)\big)\big(r_\infty(l)\big).$$

*If in addition* $\mathcal{H}_{\overline{F}_P}$ *is given by a potential (cf. section 3.1) then*

$$\begin{aligned} r_\infty I\!D\,Grad_{\mathcal{G}(j_0)}(a_{\overline{F}^{lin}} \cdot \mathcal{A})(j_0)(q) &= I\!D\,\mathcal{H}_{\overline{F}_P}\big(r_\infty(j_0)\big)\big(r_\infty(l)\big)(q) \\ &= \sum_{i=1}^{k(q)} I\!D\,grad_{I\!R^n} V\big(j_0(q) - j_0(q_i)\big)\big(l(q_i)\big) \quad \forall\, q \in P. \end{aligned}$$

Finally let us express the constitutive map $\widehat{\mathcal{H}}_{\overline{F}^{lin}}$ in terms of the modes of $\overline{F}^{lin}$. At first we observe by corollary 4.1.3 that $\widehat{\mathcal{H}}_{\overline{F}^{lin}}(j_0 + l)$ depends linearly on $l$ because of which we write

$$\widehat{\mathcal{H}}_{\overline{F}^{lin}}(j_0 + l) = \mathcal{L}(l) \quad \forall\, l \in \mathcal{W}^\infty(j_0) - j_0 \tag{4.1.10}$$

with $\mathcal{L} \in End\mathcal{F}^\infty(M, I\!R^n)$. Clearly $\mathcal{L} = I\!D\,\widehat{\mathcal{H}}_{F^{lin}}(j_0)$. By (4.1.7) we deduce hence

$$2Gl = \Delta(j_0)\mathcal{L}(l) \tag{4.1.11}$$

The equations (1.1.25) and (1.1.24) imply therefore (cf. 2.1.17)

$$\lambda_i \cdot \widehat{\kappa}^i_\infty(j_0 + l) = 2\mathcal{G}(j_0)(Gl, e_i) \tag{4.1.12}$$

and in turn for all $i, s = 1, ..., (s_0 - 1) \cdot n$

$$\widehat{\kappa}^i_\infty(j_0 + \mathbf{w}_s) = \frac{2}{\lambda_i} \cdot \gamma_s \cdot \mathcal{G}(j_0)(\mathbf{w}_s, e_i) \tag{4.1.13}$$

Therefore we may summarizing this little analysis by the following two lemmata:

**Proposition 4.1.4:**

*The constitutive map* $\widehat{\mathcal{H}}_{F^{lin}}$ *of* $\overline{F}^{lin}$ *is given by*

$$\widehat{\mathcal{H}}_{\overline{F}^{lin}}(j_0 + l) = 2 \cdot \Delta^{-1}(j_0) \circ Gl \tag{4.1.14}$$

*and the Fourier coefficients are hence*

$$\kappa_i^{\overline{F}^{lin}}(j_0 + \mathbf{w}_s) = \frac{2}{\lambda_i} \cdot \gamma_s \cdot \mathcal{G}(j_0)(\mathbf{w}_s, e_i) \quad \forall\, i, s = 1, ..., (s_0 - 1) \cdot n.$$

*If in particular* $\frac{\partial \widehat{\kappa}_i^{\overline{F}^{lin}}(j_0)}{\partial \overline{\mathbf{x}}_s} = \delta_{i,s} \quad \forall\, i, s = 1, ..., (s_0 - 1) \cdot n$ *then*

$$\widehat{\kappa}_i^{\overline{F}^{lin}}(j_0 + l) = 2 \cdot \frac{\gamma_i}{\lambda_i} \cdot l_i \quad i, s = 1, ..., (s_0 - 1) \cdot n. \tag{4.1.15}$$

**Lemma 4.1.5:**

*The constitutive map* $\widehat{\mathcal{H}}_{\overline{F}^{lin}}$ *of* $\overline{F}^{lin}$ *is given by*

$$\widehat{\mathcal{H}}_{\overline{F}^{lin}}(j_0 + l) = 2 \cdot \Delta^{-1}(j_0) \circ Gl \tag{4.1.16}$$

*showing*

$$I\!D\, \widehat{\mathcal{H}}_{\overline{F}^{lin}}(j_0) = 2 \cdot \Delta^{-1}(j_0) \circ G. \tag{4.1.17}$$

*Hence the modes of* $\overline{F}^{lin}$ *the medium determines the constitutive map of* $\overline{F}^{lin}$ *entirely and vice versa. Therefore the Fourier coefficients are for each* $i = 1, ..., (s_0 - 1) \cdot n$

$$\widehat{\kappa}_i^{\overline{F}^{lin}}(j_0 + l) = \frac{2}{\lambda_i} \sum_{i}^{(s_0-1)\cdot n} \gamma_s l_s \cdot \mathcal{G}(j_0)(\mathbf{w}_s, e_i) \tag{4.1.18}$$

*and hence*

$$\frac{\partial \widehat{\kappa}_i^{\overline{F}^{lin}}(j_0)}{\partial \overline{\mathbf{x}}_r} = \frac{2}{\lambda_i} \cdot \sum_s \gamma_s e_r^s \cdot \mathcal{G}(j_0)(\mathbf{w}_s, e_i) \quad \forall\, r = 1, ..., (s_0 - 1) \cdot n \tag{4.1.19}$$

*with* $e_r = \sum_s e_r^s \mathbf{w}_s$. *If* $\frac{\partial \widehat{\kappa}_i^{\overline{F}^{lin}}(j_0)}{\partial \overline{\mathbf{x}}_r} = \delta_{r,i} \quad \forall\, i, r = 1, ..., (s_0 - 1) \cdot n$, *i.e. if the Fourier coefficients are all decoupled from each other. Therefore*

$$\widehat{\kappa}_i^{\overline{F}^{lin}}(j_0 + l) = \frac{2\gamma_i}{\lambda_i} \cdot l_i$$

*and*

$$\frac{\partial \widehat{\kappa}_i^{\overline{F}^{lin}}(j_0)}{\partial \mathbf{x}_i} = 2\frac{\gamma_i}{\lambda_i} \quad i = 1, ..., (s_0 - 1) \cdot n \tag{4.1.20}$$

*hold in addition. If hence all Fourier coefficients are decoupled from each other, then* $\mathcal{L}$ *diagonalizes with respect to the eigenbasis* $e_1, ..., e_{(s_0-1)\cdot n}$ *of* $\Delta(j_0)$*, this is to say*

$$\mathcal{L} = \begin{pmatrix} 2 \cdot \frac{\gamma_1}{\lambda_i} & & 0 \\ & \ddots & \\ 0 & & 2 \cdot \frac{\gamma_{(s_0-1)\cdot n}}{\lambda_{(s_0-1)\cdot n}} \end{pmatrix}$$

*holds showing that* $\mathcal{L}$ *and* $\Delta(j_0)$ *commute.*

The link between the modes of $I\!D^2\overline{F}^{lin}$ at an equilibrium configuration $j_0$ and the structural capillarity is made via (1.1.41), i.e. by equation

$$I\!D^2 F^{lin}(j_0)(l, j_0) = dim\ M \cdot I\!D(a \cdot \mathcal{A})(j_0)(l)$$

yielding

$$I\!D\overline{F}(l_0 + l)(j_0) = dim\ M \cdot I\!D(a \cdot \mathcal{A})(j_0)(l) = 2 \cdot \mathcal{G}(j_0)(Gl, j_0) = 2 \cdot \sum_{s=1}^{(s_0-1)\cdot n} \gamma_s l_s j_0^s$$

where index $s$ indicates the component formed with respect $\mathbf{w}_s$. Therefore we find

**Theorem 4.1.6:**
*The modes of* $I\!D^2\overline{F}^{lin}$ *affect the structural capillarity by*

$$I\!D\, a_{\overline{F}^{lin}}(j_0)(l) = \frac{2}{dim\ M \cdot \mathcal{A}(j_0)} \sum_s \gamma_s l_s j_0^s \tag{4.1.21}$$

*at an equilibrium configuration* $j_0$*. In particular*

$$I\!D\, a_{\overline{F}^{lin}}(\mathbf{w}_s) = \frac{2}{dim\ M \cdot \mathcal{A}(j_0)} \cdot \gamma_s j_0^s \tag{4.1.22}$$

*has to hold. Hence* $a_{\overline{F}^{lin}}$ *and the modes of* $I\!D\overline{F}^{lin}$ *influence the equilibrium configuration directly.*

*Therefore* $a_{\overline{F}^{lin}}$ *is up to higher order terms*

$$a_{\overline{F}^{lin}}(j_0 + l) = \frac{2}{dim\ M \cdot \mathcal{A}(j_0)} \sum_s \gamma_s l_s j_0^s \tag{4.1.23}$$

*where* $j_0$ *is an equilibrium configuration.*

To link the Fourier coefficients of $\mathcal{H}_{\overline{F}^{lin}}$ formed with respect to $\Delta$ with the structural capillarity we verify

$$\begin{aligned} I\!D\,\overline{F}(j_0+l)(j_0) &= dim\ M \cdot I\!D\,(a_{\overline{F}^{lin}} \cdot \mathcal{A})(j_0)(l) \\ &= \mathcal{G}(j_0)\big(\Delta(j_0)\widehat{\mathcal{H}}^{\overline{F}^{lin}}(j_0+l), j_0\big) \\ &= I\!D\,\mathcal{A}(j_0)\big(\widehat{\mathcal{H}}^{\overline{F}^{lin}}(j_0+l)\big) \\ &= \sum_i \lambda_i \widehat{\kappa}_i^{\overline{F}^{lin}}(j_0+l) \cdot \iota_0^i \end{aligned}$$

with $\iota_0^i$ the $i^{th}$-Fourier coefficient of $j_0$. Therefore we deduce by using proposition 4.1.4

**Theorem 4.1.7:**

*Let $j_0$ be an equilibrium configuration for $I\!D\,\overline{F}^{lin}$. Then*

$$I\!D\,a_{\overline{F}^{lin}}(j_0)(l) = I\!D\,ln\mathcal{A}(j_0)\big(\widehat{\mathcal{H}}^{\overline{F}^{lin}}(j_0+l)\big) \tag{4.1.24}$$

*and thus*

$$I\!D\,a_{\overline{F}^{lin}}(j_0)(l) = \sum_i \frac{\lambda_i \cdot \iota_0^i}{\mathcal{A}(j_0)} \widehat{\kappa}_i^{\overline{F}^{lin}}(j_0+l) \tag{4.1.25}$$

*If all the Fourier coefficients decouple, then*

$$I\!D\,a_{\overline{F}^{lin}}(j_0)(e_i) = 2\gamma_i \cdot \iota_0^i \quad i = 1, ..., (s_0-1)\cdot n, \tag{4.1.26}$$

*in particular if $dim\ M = 2$ and $j_0$ is a good fit then*

$$I\!D\,a_{\overline{F}^{lin}}(j_0)(r_\infty^* e_i^T) = 2\gamma_i \iota_0^i \quad i = 1, ..., (s_0-1)\cdot n \tag{4.1.27}$$

*with $r(j_0) = j_P^0$.*

## Appendix 1

### Dirichlet Integral

Here we will present what is called the **Dirichlet-integral** in to different ways. Let $<,>$ be a fixed scalar product in $\mathbb{R}^n$. 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

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

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

$$dh\ v_q = c_h(q) \cdot dj\ v_q + dj(C_h v_q + B_h v_q)$$

Here $c_h : M \longrightarrow so(n)$ is a smooth map sending vectors in $djT_qM$ into normal vectors in the orthogonal complement $(djT_qM)^\perp$ and vice versa for any $q \in M$; 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 [Bi1],[Bi2],[Bi,Fi2] or [Bi,Sn,Fi]. For any $q \in M$ $c_h^2(q)$ is a selfadjoint endomorphism of $djT_qM$ respectively $(djT_qM)^\perp$. The part of $c_h^2$ mapping $(djT_qM)$ and $c_h^2$ into itself is called $\left(c_h^2(q)\right)^\top$. For any two $h, k \in C^\infty(M, \mathbb{R}^n)$ we define

$$dh \bullet dk := -tr(c_h \circ c_k)^\top - tr\ C_h \circ C_k + tr\ B_h \circ B_k = -\frac{1}{2} tr\ c_h \circ c_k - tr\ C_h \circ C_k + tr\ B_h \circ B_k \tag{A1.2}$$

and observe that

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

where $\mu(j)$ is the Riemannian volume element of $m(j)$. The operator $\Delta(j)$ is the Laplace Beltrami operator associated with $m(j)$. For (A.1.2) and (A.1.3) we refer to [Bi1],[Bi2] or [Bi,Fi2]. Clearly $\mathcal{G}$ 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 Hodge star operator. Clearly $\mathcal{D}$ is a weak Riemannian metric on $E(M, \mathbb{R}^n)/_{\mathbb{R}^n}$.

Next we will represent this integral in a complete different way. It is based on the second derivative of $m(j_0)$ formed with respect to $j_0$.

Let $j_0 \in E(M, I\!R^n)$be fixed and let $h \in C^\infty(M, I\!R^n)$ be such that $j_0 + h \in E(M, I\!R^n)$. Then for any $v, w \in T_qM$ and any $q \in M$

$$m(j_0+h)(v,w) = m(j_0)(v,w) + < dj_0\, v, dh\, w > + < dh\, v, dj_0\, w > + < dh\, v, dh\, w > . \tag{A1.4}$$

Writing

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

for a well defined smooth strong bundle endomorphism $f(j_0 + h)$ of $TM$ positive definite with respect to $m(j_0)$, we observe by (A1.5) that

$$m(j_0 + h) = m(j_0) + I\!D\, m(j_0)(h) + \frac{1}{2} I\!D^2 m(j_0)(h,h) \quad \forall\, h \in C^\infty(M, I\!R^n)$$

and hence

$$\begin{aligned} m(j_0 + h)(v,w) &= m(j_0)\big(f^2(j_0+h)v, w\big) \\ &= m(j_0)(v,w) + m(j_0)\big(I\!D\, f^2(j_0)(h)v, w\big) \\ &+ \frac{1}{2} m(j_0)\big(I\!D^2 f^2(j_0)(h,h)v, w\big) \end{aligned}$$

for all $v, w \in T_qM$ and for all $q \in M$. Using (A.1.1) we conclude that

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

where $\overline{C}_h dj_0$ and $\overline{B}_h dj_0$ are defined by

$$\overline{C}_h dj_0 = dj_0 C_h \qquad \text{and} \qquad \overline{B}_h = dj_0 B_h$$

and the requirement that both $\overline{C}_h$ and $\overline{B}_h$ vanish on the normal bundle of $T_jTM$. By $*$ we mean the adjoint. Therefore the following equation holds

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

Since $c_h^2 dj_0 = (c_h^2)^\top dj_0$ we find for all $h \in C^\infty(M, I\!R^n)$

$$\frac{1}{2} I\!D^2 f^2(j_0)(h,h) = -dj_0^{-1}(c_h^2 dj_0) - C_h^2 + B_h^2 + C_h B_h - B_h C_h$$

and

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

Hence

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

and by polarization

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

Therefore we may state

**Lemma A:**

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

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

*implying*

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

*for all $h, k \in C^\infty(M, I\!R^n)$.* Hence

$$\begin{aligned}\int_M tr\ f(j_0 + h)\mu(j_0) = dim\ M \cdot \mathcal{A}(j_0) &+ \int_M tr\ I\!D f(j)(h)\mu(j_0) \\ &+ \frac{1}{2} \int_M < \Delta(j_0)h, h > \mu(j_0)\end{aligned}$$

has to hold. Here $\mathcal{A}(j_0) := \int_M \mu(j_0)$.

## Appendix 2

### Continuity equation and states

### a) Densities

Let

$$\rho : E(M, I\!R^n) \longrightarrow C^\infty(M, I\!R)$$

be a smooth map for which the value $\int_M \rho(j)\mu(j)$ is constant in $j \in E(M, I\!R^n)$. We call $\rho$ a **density**. A map $\rho$ of this kind is constructed as follows. Let $j_0 \in E(M, I\!R^n)$ be fixed. For each pair $j_0, j \in E(M, I\!R^n)$ with $j_0$ being fixed there is a unique positive smooth and strong bundle isomorphism (cf. [B.G.H], [Bi2] and appendix 1)

$$f(j) : TM \longrightarrow TM$$

for which

$$m(j)(v, w) = m(j_0)\big(f^2(j), v, w\big) \quad \forall\, v, w \in TM. \qquad (A2.1)$$

This bundle isomorphism is fibre wise constructed with the help of the theorem of Fischer-Riesz. Hence we deduce

$$\mu(j) = det f(j)\mu(j_0). \tag{A2.2}$$

Let $\rho(j_0) \in C^\infty(M, I\!R^n)$ be a non-negative map.
Setting

$$\rho(j) := \rho(j_0) \cdot det f^{-1}(j) \quad \forall j \in E(M, I\!R^n)$$

we indeed have

$$\int_M \rho(j)\mu(j) = \int_M \rho(j_0)\mu(j_0) \quad \forall j \in E(M, I\!R^n). \tag{A2.3}$$

A simple calculation shows that

$$I\!D\,\rho(j)(h) = -\rho(j) \cdot tr\ f^{-1}(j) I\!D\, f(j)(h) \quad \forall h \in C^\infty(M, I\!R^n) \tag{A2.4}$$

holds for all $j \in E(M, I\!R^n)$. Here $I\!D$ denotes the derivative on $C^\infty(M, I\!R^n)$ in the sense of [Bi,Sn,Fi]. If $\rho(j_0) > 0$ we call this kind of densities, **density maps**. Equation (A2.4) is called the continuity equation. Associated with each density map $\rho$ is the scalar product $B(\rho)$ on $C^\infty(M, I\!R^n)$ given by

$$B(\rho)(h,k) = \int_M < h,k > \rho(j)\mu(j) = \int_M < h,k > \rho(j_0)\mu(j_0) \quad \forall h,k \in C^\infty(M, I\!R^n). \tag{A2.5}$$

We rewrite a density map as follows: Let us suppose that

$$\rho(j) : M \longrightarrow I\!R$$

assumes only positive values for each $j \in E(M, I\!R^n)$ . In this case (A.2.4) rewrites as

$$I\!D\, ln\rho(j) = -tr f^{-1}(j) I\!D\, f(j). \tag{A2.6}$$

For any $j$ in some neighbourhood $U(j_0) \subset E(M, I\!R^n)$ we write

$$f(j) = exp\varphi(j) \tag{A2.7}$$

where $\varphi(j) : TM \longrightarrow TM$ is a smooth strong bundle endomorphism, depending smoothly on $j$. Hence

$$det f^{-1}(j) = e^{-tr\varphi(j)} \quad \forall j \in U(j_0)$$

and thus

$$\rho(j) = \rho(j_0) \cdot e^{-tr\varphi(j)} \quad \forall j \in U(j_0)$$

yielding

$$I\!D\, ln\rho(j) = -I\!D\, tr\varphi(j) \quad \forall j \in U(j_0). \qquad (A2.8)$$

**b) States, equilibrium states**

In this section we let $\mathcal{W}^\infty(j_0) \subset E(M, I\!R^n)$ be a neighbourhood of $j_0$ and

$$\rho : \mathcal{W}^\infty(j_0) \longrightarrow C^\infty(M, I\!R^n)$$

be any smooth map satisfying

$$\int_M \rho(j_0)\mu(j) = 1 \quad \forall\, j \in \mathcal{W}(j) = \int_M \rho(j) det f^{-1} \mu(j) \qquad (A2.9)$$

where $j_0 \in E(M I\!R^n)$ is fixed. In accordance with [B,St] we call $\rho$ a state. Associated with the smooth maps

$$I : \mathcal{W}^\infty(j_0) \longrightarrow C^\infty(M, V)$$

where $V$ is a given finite dimensional vector space and with a smooth map

$$\gamma : \mathcal{W}^\infty(j_0) \longrightarrow V^*$$

we form

$$\rho_e(I, \gamma)(j) = \frac{e^{-\gamma(j)\cdot I(j)}}{\int_M e^{-\gamma(j)\cdot I(j)}} \quad \forall j \in \mathcal{W}^\infty(j_0). \qquad (A2.10)$$

$I$ corresponds to an **observable,** $\gamma$ produces at each configuration a functional in $V^*$.

$\rho(I, \gamma)$ is called an **equilibrium state** (cf.[B,St]). For simplicity we replace $\int_M e^{-\gamma(j)\cdot I(j)}$ by $Z(I, \gamma)(j)$.

The value

$$\overline{I}(j) := \int_M \rho_e(I, \gamma)(j) \cdot I(j)\mu(j_0) \qquad (A2.11)$$

is the **expectation** value of $I$ at the configuration $j \in \mathcal{W}^\infty(j_0)$.

Defining the **entropy** $S(\rho)(j)$ of $I(j)$ and $\gamma(j)$ at any state by

$$S(I, \gamma)(j) := -\int_S \rho(I, \gamma)(j) ln\rho(I, \gamma)(j)\mu(j_0) \quad \forall\, j \in \mathcal{W}^\infty(j_0) \qquad (A2.12)$$

then $\rho(I, \gamma)(j)$ maximizes the entropy subject to the constraint that the expectation value of

$$\overline{I}(j) := \int_M \rho_e(I, \gamma)(j) I(j)\mu(j_0) \quad \forall\, j \in \mathcal{W}^\infty(j_0) \qquad (A2.13)$$

is kept constant (cf.[B,St]), for each fixed $j \in \mathcal{W}^\infty(j_0)$.

Given an equilibrium state $\rho_e(I, \gamma)$ we set

$$Z(I,\gamma)(j) := \int_M e^{-\gamma(j)I(j)} \mu(j_0). \tag{A2.14}$$

$\overline{I}, S(I,\gamma)$ and $Z(I,\gamma)$ are linked by

$$\overline{\rho}(I,\gamma)(j) = \gamma(j)\overline{I}(j) + lnZ(I,\gamma)(j) \tag{A2.15}$$

as easily deduced from (A2.10). In particular if $\gamma = \frac{1}{T}$ then

$$\overline{F}(I, \frac{1}{T}) := -T \; ln \; Z \tag{A2.16}$$

is the **free energy** associated with the observable $I$. If $\gamma = \frac{1}{T}$ and $I$ are specified we just write $\rho_e$ instead of $\rho_e(I, \frac{1}{T})$.

## Appendix 3

### Topological foundations

*Generalities on simplicial chain and cochain complexes, the Laplacian $\Delta_T$*

Let $\mathbf{L}$ be an oriented connected, finite, **simplicial complex** consisting of finitely many simplices of dimension $\leq m$. A generic $l$-simplex of this complex shall be denoted by $\sigma_l$. If $l = 1$ the initial and final points of $\sigma_1$ (in the sense of the orientation) are denoted by $\sigma_1^+$ and $\sigma_1^-$.

The $\mathbb{R}$-vector space all $l$-**chains** is called $C_l(\mathbf{L})$; the space of $l$-**cochains** is denoted by $C^l(\mathbf{L})$, the $\mathbb{R}$-vector space of all $\mathbb{R}$-valued functions on the collection $\mathbf{L}_l$ of all $l$-simplices. We write $P$ instead of $\mathbf{L}_0$.

The **delta function** associated with any $\sigma_l \in \mathbf{L}_l$ is denoted by $\mathbf{1}_{\sigma_l}$.It is given by

$$\mathbf{1}_l(\sigma'_l) := \begin{cases} 1 & \sigma'_l = \sigma_l \\ 0 & \text{otherwise.} \end{cases} \qquad \forall\, \sigma' \in \mathbf{L}_l \tag{A3.1}$$

Clearly $\mathbf{L}^l := \{\mathbf{1}_{\sigma_0} \mid \sigma_0 \in \mathbf{L}_l\}$ is a basis of $C^l(\mathbf{L})$.

Obviously $C^l(\mathbf{L}) \cong C_l(\mathbf{L})$ as linear spaces. Since $\mathbf{L}_l$ is contained in the dual space $C^l(\mathbf{L})'$ of $C^l(\mathbf{L})$, the vector spaces $C_l(\mathbf{L})$ and $C^l(\mathbf{L})'$ are naturally isomorphic.

The associated chain complex of $\mathbf{L}$ is

$$C_m(\mathbf{L}) \xrightarrow{\partial_m} \ldots \xrightarrow{\partial_2} C_1(\mathbf{L}) \xrightarrow{\partial_1} C_0(\mathbf{L}) \xrightarrow{\partial_0} I\!R\,. \qquad (A3.2)$$

The **boundary operator** $\partial_l$ is defined on the generators as follows. Let the oriented simplex $\sigma_l$ be spanned by $(q_0, \ldots, q_l)$

$$\partial_l \sigma_l = \sum_{s=0}^{l} (-1)(q_1, \ldots, q_s^a, \ldots, q_l) \qquad (A3.3)$$

with $(q_1, \ldots, q_s^a, \ldots, q_l)$ being the $l-1$-simplex spanned by all $q_0, \ldots, q_l$ but $q_s$.

Moreover $\partial_0$ is the zero map, in particular $\partial_1$ is the linear map given on $\mathbf{L}_1$ by

$$\partial_1 \sigma = \sigma^+ - \sigma^- \qquad \forall \sigma \in \mathbf{L}_1\ . \qquad (A3.4)$$

If therefore $\sigma_1^i \in \mathbf{L}_1$ for $i = 1, \ldots, r$ and

$$c := \sum_{i=1}^{r} \alpha^i \sigma_1^i$$

is a one-chain then

$$\partial_1 c = \sum_{i=1}^{r} \alpha^i \partial_1 \sigma_1^i = \sum_{i=1}^{r} \alpha^i \left( (\sigma_1^i)^+ - (\sigma_1^i)^- \right)\ . \qquad (A3.5)$$

The space of $l$-cochains is defined by

$$C^l(\mathbf{L}) := span \mathbf{L}^l.$$

The natural bilinear **evaluation map**

$$ev : C^l(\mathbf{L}) \times C_l(\mathbf{L}) \longrightarrow I\!R\,,$$

assigning to each $\mathbf{1}_{\sigma_l} \in \mathbf{L}^l$ and each $\sigma_l \in \mathbf{L}^l$ the value $\mathbf{1}_{\sigma_l}(\sigma_l)$, yields a **coboundary operation**

$$C^l(\mathbf{L}) \xrightarrow{\partial^{l+1}} C^{l+1}(\mathbf{L})$$

given by

$$ev(\partial^{l+1}\ c^l, c_{l+1}) = ev(c^l, \partial_l\ c_{l+1})$$

for each $c^l \in C^l(\mathbf{L})$ and each $c_{l+1} \in C_{l+1}(\mathbf{L})$. Denoting the collection of zero simplices $L_0$, i.e. the collection of points in $\mathbf{L}$ by $P$, $\partial^1 \mathbf{1}_q$ with $q \in P$ satisfies in particular

$$(\partial^1 \mathbf{1}_q, \sigma) = (\mathbf{1}_q, \partial_1 \sigma) = \mathbf{1}_q(\sigma^+) - \mathbf{1}_q(\sigma^-) \quad \forall\, q \in P. \tag{A3.6}$$

Thus $\partial^1 \mathbf{1}_q$ is determined by

$$\partial^1 \mathbf{1}_q = \Big(\sum_{\sigma^{i+}} \mathbf{1}_q(\sigma_1^{i+}) - \sum_{\sigma^{i-}} \mathbf{1}_q(\sigma_1^{i-})\Big) \cdot \mathbf{1}_{\sigma_1^i} \quad \forall\, q \in P. \tag{A3.7}$$

To get a more handy formula let $k^+(q)$ be the number of + ends matching $q$ of those simplices, connecting $q$ with its **nearest neighbours**, i.e. all $q_i$ linked by a one-simplex. $k^-(q)$ shall be the number of $-$ ends matching $q$ of all those simplices connecting $q$ with its nearest neighbours. Hence

$$\partial^1 \mathbf{1}_q = \big(k^+(q) - k^-(q)\big)\mathbf{1}_q \quad \forall\, q \in P.$$

Let $\mathbf{L}$ be any complex. We define a metric $\mathcal{G}_L^l$ on $C^l(\mathbf{L})$ as follows:
Let $c_1^l$, $c_2^l$ be two cochains which represented as linear combinations of $l$-co-simplices read as

$$c_1^l = \sum_r \beta_1^r(c_1^l) \cdot \mathbf{1}_{\sigma_r^l} \qquad \text{and} \qquad c_2^l = \sum_r \beta_2^r(c_2^l) \cdot \mathbf{1}_{\sigma_r^l}\ .$$

The respective metric is given by

$$\mathcal{G}_{\mathbf{L}}^l(c_1^l, c_2^l) := \sum_{\sigma \in \mathbf{L}_l} \beta_1^r(c_1^l) \cdot \beta_2^r(c_2^l)\ , \tag{A3.8}$$

a scalar product used in [E] (cf. [D], however). The metric on $C^0(\mathbf{L})$ is denotes by $\mathcal{G}_P$.

Associated with the metric $\mathcal{G}_{\mathbf{L}}^l$ we have a **divergence operator** $\delta^l$ given by the formula

$$\mathcal{G}_{\mathbf{L}}^{l-1}(\delta^l\ c^l, c_{l-1}) = \mathcal{G}_{\mathbf{L}}^l(c^l, \partial^l\ c_{l-1}) \tag{A3.9}$$

for each $c^l \in C^l(\mathbf{L})$ and each $c_{l-1} \in C_{l-1}(\mathbf{L})$.

Clearly $\mathcal{G}_{\mathbf{L}}^l$ is a **Dirichlet form**. This is apparent if we introduce the topogical Laplacian $\Delta_T^l$ by

$$\Delta_T^l := \delta^{l+1}\partial^l + \partial^{l-1}\delta^l$$

for which we verify

$$\mathcal{G}_{\mathbf{L}}^l(\Delta_T^l\ c_1^l, c_2^l) = \mathcal{G}_{\mathbf{L}}^{l+l}(\partial^{l+1}\ c_1^l, \partial^{l+1} c_2^l) + \mathcal{G}_{\mathbf{L}}^{l-1}(\delta^l\ c_1^l, \delta^l\ c_2^l)$$

for each pair $c_1^l, c_2^l \in C^l(\mathbf{L})$. This observation immediately yields :

**Lemma A3.1:**

*$\delta^l$ is the adjoint of $\partial^l$ and moreover $\delta^{l+1}\delta^l = 0$.*

Since

$$\begin{aligned} \mathcal{G}_{\mathbf{L}}(\mathbf{1}_{\sigma_l}, \partial^l \mathbf{1}_{\sigma_{l-1}}) &= \sum_{\sigma_l' \in \mathbf{L}_l} \mathbf{1}_{\sigma_l}(\sigma_l') \cdot \partial^l \mathbf{1}_{\sigma_{l-1}}(\sigma_l') \\ &= \sum_{\sigma_l' \in \mathbf{L}_l} \mathbf{1}_{\sigma_l}(\sigma_l') \cdot \mathbf{1}_{\sigma_{l-1}}(\partial_l \sigma_l') \qquad (A3.10) \\ &= \mathbf{1}_{\sigma_l}(\sigma_l) \cdot \mathbf{1}_{\sigma_{l-1}}(\partial_l \sigma_l) = \mathbf{1}_{\sigma_{l-1}}(\partial_l \sigma_l) = \pm 1 \end{aligned}$$

the following holds :

**Lemma A3.2:**

$$\delta^l \mathbf{1}_{\sigma_l} = \sum_{\sigma_{l-1} \in \mathbf{L}_{l-1}} \mathbf{1}_{\sigma_{l-1}}(\partial_l \sigma_l) \cdot \mathbf{1}_{\sigma_{l-1}} \quad \forall\, \sigma_l \in L_l \qquad (A3.11)$$

*holds for each $l$ in particular*

$$\begin{aligned} \delta^1 \mathbf{1}_{\sigma_1} &= \sum_{\sigma_0 \in \mathbf{L}_0} \mathbf{1}_{\sigma^0}(\partial_1 \sigma_1) \cdot \mathbf{1}_{\sigma_0} \qquad (A3.12) \\ &= \mathbf{1}_{\sigma_1^+} - \mathbf{1}_{\sigma_1^-} \qquad (A3.13) \end{aligned}$$

*holds for any $\sigma_1 \in \mathbf{L}_1$. On $c^0 \in C^0(\mathbf{L})$ the Laplacian has the form $\Delta_T c^0 = \delta^1 \partial^1 c^0$ and therefore*

$$\Delta_T c^0(\sigma_0) = k(\sigma_0) c^0(\sigma_0) - \sum_{i=1}^{k} c^0(\sigma_0^i) \qquad \forall \sigma_0 \in \mathbf{L}_0 \qquad (A3.14)$$

*with $k(\sigma_0)$ being the number of nearest neighbours of $\sigma_0$ in $\mathbf{L}$. ($\sigma_0^i$ belongs to the collection of nearest neighbours of $\sigma_0$ iff it is connected by an edge (i.e. a one-simplex) with $\sigma_0$).*

*Moreover (A3.14) immediately shows that*

$$\Delta_T c^0 = 0 \quad \textit{iff} \quad c^0 \in I\!R \ . \qquad (A3.15)$$

As an example let us calculate $\Delta_T \mathbf{1}_q$, with $\mathbf{1}_q$ being the characteristic function on $\mathbf{L}_0$, assuming the value one on $q \in \mathbf{L}_0$ and zero elsewhere. To this end we write

$$\Delta_T \mathbf{1}_q = \sum_{q' \in \mathbf{L}_0} \eta^{q'} \mathbf{1}_{q'}$$

and observe

$$\mathcal{G}_{\mathbf{L}_0}(\Delta_T \mathbf{1}_q, \mathbf{1}_{q'}) = \eta^{q'}.$$

Let $q_1, \ldots, q_{\nu(q)}$ be the nearest neighbours of $q$. Clearly $\eta^{q'} = 0$ for all $q' \in \mathbf{L}_0$ with $q' \neq q_i$ and $q' \neq q_i$ with $i = 1, \ldots, k(q)$ but

$$\eta^q = \nu(q) \quad \text{and} \quad \eta^{q_i} = -1 \quad \forall i = 1, \ldots, \nu(q).$$

Therefore we have :

**Lemma A3.3:**

*For any $q \in \mathbf{L}_0$ and its characteristic map $\mathbf{1}_q$*

$$\Delta_T \mathbf{1}_q = k(q) \cdot \mathbf{1}_q - \sum_{i=1}^{k} \mathbf{1}_{q_i} \tag{A3.16}$$

*holds.*

For any complex $\mathbf{L}$ let $\mathcal{F}(\mathbf{L}^l, I\!R^3)$ denote all the $I\!R^3$-valued maps of $\mathbf{L}^l$. Clearly

$$\mathcal{F}(\mathbf{L}^l, I\!R^3) \cong C^l(\mathbf{L}) \otimes I\!R^3 \tag{A3.17}$$

the isomorphism being canonical.

For a later case we point out here the following observation: We denote by $\mathcal{E}(P_0, I\!R^3)$ the collection of all injective maps from $\mathbf{L}_0 = P$ to $I\!R^3$. One easily verifies the following

**Lemma A3.4:**

$$\mathcal{E}(P_0, I\!R^3) \subset C^0(P, I\!R^3)$$

*is open.*

The metrics $\mathcal{G}^l_{\mathbf{L}}$ on $C^l(\mathbf{L}) \otimes I\!R^3$ are defined by

$$\mathcal{G}^l_{\mathbf{L}}(c^l_1 \otimes v_1, c^l_2 \otimes v_2) = \mathcal{G}^l_{\mathbf{L}}(c^l_1, c^l_2)\langle v_1, v_2 \rangle \qquad \forall l = 0, 1, 2 \tag{A3.18}$$

for all $c^l_1, c^l_2 \in C^l(\mathbf{L})$ and $\forall v_1, v_2 \in I\!R^3$. Since $\mathbf{L}_0$ is denoted by $P$, we will write just $\mathcal{G}_P$ for $\mathcal{G}^0_P$.

Similarly the operators $\partial^l$ and $\delta^l$ and $\Delta_T$ on $C^l(\mathbf{L}) \otimes I\!R^3$ are defined by

$$\partial^l(c^l \otimes v) := \partial^l c^l \otimes v \tag{A3.19}$$

$$\delta^l(c^l \otimes v) := \delta^l c^l \otimes v \tag{A3.20}$$

and

$$\Delta_T(c^l \otimes v) := \Delta_T c^l \otimes v \tag{A3.21}$$

for all $c^l \in C^l(\mathbf{L})$ and all $v \in I\!R$. We proceed for $\mathbf{L}$ accordingly.
Let us observe that the orthogonal $\mathcal{G}^l_{\mathbf{L}}$-complement $(I\!R^3)^\perp$ of $I\!R^3$ within $C^l(\mathbf{L}) \otimes I\!R^3$ is of the form

$$(I\!R^3)^\perp = (I\!R^\perp) \otimes I\!R^3 \tag{A3.22}$$

where $I\!R^\perp$ is the $\mathcal{G}^l_{\mathbf{L}}$ orthogonal complement of $I\!R$ within $C^l(\mathbf{L}, I\!R)$. Since $\Delta_T$ is $\mathcal{G}^0_P$-selfadjoint the equation

$$\Delta_T \mathcal{H}_P = \Phi$$

has a solution (unique up to a constant) for a given $\Phi \in C^0(\mathbf{L})$ iff $\Phi \in (I\!R^3)^\perp$. We therefore have

**Lemma A3.5:**

*Given $\Phi \in C^0(\mathbf{L}) \equiv \mathcal{F}(P, I\!R^n)$ then*

$$\Delta_T \mathcal{H}_P = \Phi \tag{A3.23}$$

*has a solution uniquely determined up to a constant map iff $\Phi \in (I\!R^3)^\perp$. The solution is unique if $\mathcal{H}_P \in (I\!R^3)^\perp$.*

Again these results hold accordingly on the whole cochain complex of $\overline{\mathbf{L}}$. Let us point out that the Laplace equation (A3.23) is of pure topological nature. $\mathcal{H}_P \in (I\!R^3)^\perp$ does not depend on $\langle\ ,\ \rangle$ chosen on $I\!R^3$. This is due to (A3.22). Moreover a Hodge splitting is easily verified in this context.

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