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A PHYSICAL INTERPRETATION OF THE IRREDUNDANT PART OF THE FIRST PIOLA-KIRCHHOFF-STRESS TENSOR OF A DISCRETE MEDIUM FORMING A SKIN

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0. Introduction

Deformable continua in an Euclidean space are characterized by the first Piola-Kirchhoff stress tensor α. In doing so it is assumed that the continuum forms a connected, smooth and oriented Riemannian submanifold M of $\mathbb{R}^n$ with boundary ∂M. Taking (covariant) divergence ∇^* of the tensor α (assumed to be smooth) yields the internal force density Φ on M. The internal force density φ caused on ∂M is $\alpha(\mathbf{n})$ with $\mathbf{n}$ the oriented unit normal of ∂M in M.

The question arises as to whether α is the only tensor causing Φ and φ via the mathematical procedure just mentioned. This tensor is not unique at all, as we see as follows: Given any α with $\Phi := \nabla^*\alpha$ and $\varphi := \alpha(\mathbf{n})$ we may pose the Neumann problem

$$\Phi = \Delta\mathcal{H} \qquad \text{with} \quad \varphi = d\mathcal{H}(\mathbf{n}) \ .$$

Here Δ is the Laplacian of the Riemannian submanifold $M \subset \mathbb{R}^n$. This elliptic boundary value problem admits a unique smooth solution $\mathcal{H}$ in $C_0^\infty(M, \mathbb{R}^n)$, the collection of all $\mathbb{R}^n$-valued maps, L_2-orthogonal to the constants. Hence $d\mathcal{H}$ is (in general) another type of a first Piola-Kirchhoff stress tensor causing the same force densities as α does. It satisfies

$$\alpha = d\mathcal{H} + \beta \ ,$$

where $\beta := \alpha - d\mathcal{H}$ is divergence free and vanishes on $\mathbf{n}$. This decomposition is unique. We call $d\mathcal{H}$ hence the irredundant part of α. Since $\mathcal{H}$ is smooth the medium is called smooth. The whole mathematical setting is based on a Dirichlet form, the theorem of Stokes and the solution theory of Neumann problems. We present this formalism in section two based on geometric preliminaries in section one.

In a series of papers (cf. References) we studied $d\mathcal{H}$ in various phenomenological aspects and showed how to set up a dynamics within the frame work of symplectic geometry. What was only hinted at, was the physical nature of $\mathcal{H}$.

Here we present a physical interpretation of $\mathcal{H}$ in a special situation: We consider skins only, expressed by the assumption $\partial M = \emptyset$. These skins are supposed to consist of finitely many particles, each reacting only with its nearest neighbours. We call this kind of media discrete media forming a skin or just discrete media in these notes.

In doing so we introduce in section 3 a connected graph V on an abstract manifold M of which the vertices mark the mean location of massive material particles. We do not specify what sorts of material particles are considered. They can be molecules, clusters etc. Edges are thrown if the particles at the two bounding vertices interact with each other. This graph together with the types of interactions describes the physical nature of the discrete medium. (It hence makes no sense to refine the graph in order to approximate the continuum!) This configuration is kept undisturbed at first.

This situation on the discrete level resembles the physical situation of having a continuous medium on M at a fixed configuration j_0 (a smooth embedding from M to $\mathbb{R}^n$). The next step is hence to imitate the mathematical technique on V and to write internal force densities on V as $\Delta_V \mathcal{H}_V$, where Δ_V is the Laplacian and $\mathcal{H}_V$ is the constitutive $\mathbb{R}^n$-valued map on V describing the discrete medium at the fixed configuration. In fact the discrete geometry (cf. [Ch,St]) on V allows to construct a Dirichlet form $\mathfrak{g}_V$, a metric $\mathcal{G}_V$ and a Laplacian Δ_V on V.

Now we represent any internal force density Φ_V on V as $\Delta_V \mathcal{H}_V$ for a uniquely determined map $\mathcal{H}_V : V \to \mathbb{R}^n$ in $\mathcal{F}_0(V, \mathbb{R}^n)$, the space of all $\mathbb{R}^n$-valued maps of V which are $\mathcal{G}_V$-orthogonal to the constants.

Within this frame work $\mathcal{H}_V$ allows the following physical interpretation: Let q_i be one of the nearest neighbours of q. $\mathcal{H}_V$ restricted to V is then a $\mathbb{R}^n$-valued potential such that the difference $\mathcal{H}(q) - \mathcal{H}(q_i)$ is the interacting force density of the particle at q with the one at q_i, a nearest neighbour of q. The force density $\Phi_V = \Delta_V \mathcal{H}_V(q)$ is hence the resulting force density of the interacting force densities of the particle at q with all its neighbours. The physical quality of the discrete medium is therefore determined if both the graph V and the constitutive map $\mathcal{H}_V$, the interaction potential density, are specified.

Next we link the smooth and the discrete setups as follows: We exhibit a subspace $\mathcal{F}_0^\infty(M, \mathbb{R}^n)$ of $C_0^\infty(M, \mathbb{R}^n)$ being L_2-orthogonal to the constants in $\mathbb{R}^n$ together with a map ψ onto it and obtain in turn the following commuting diagram

$$\begin{array}{ccc} C_0^\infty(M, \mathbb{R}^n) & \xrightarrow{\Delta \circ \psi} & \mathcal{F}_0^\infty(M, \mathbb{R}^n) \\ {\scriptstyle r}\downarrow & & \downarrow{\scriptstyle r} \\ \mathcal{F}_0(V, \mathbb{R}^n) & \xrightarrow{\Delta_V} & \mathcal{F}_0(V, \mathbb{R}^n) \end{array}$$

where r is the restriction map onto the space $\mathcal{F}_0(V, \mathbb{R}^n)$. The finite dimensional space $\mathcal{F}_0^\infty(M, \mathbb{R}^n)$ is the continuum version of $\mathcal{F}_0(V, \mathbb{R}^n)$ which is stable under Δ, i.e. $\Delta\big(\mathcal{F}_0^\infty(M, \mathbb{R}^n)\big) \subset \mathcal{F}_0^\infty(M, \mathbb{R}^n)$. The map ψ reflects the geometry of the graph V expressed in terms of the geometry of the Riemannian manifold M. Moreover $\Delta \circ \psi$ on $\mathcal{F}_0^\infty(M, \mathbb{R}^n)$ and Δ_V on $\mathcal{F}_0(V, \mathbb{R}^n)$ have the same eigen vectors and eigen values, i.e. the Laplacian Δ_V expressed on M is the operator $\Delta \circ \psi$. Let s_0 be the number of vertices of V. The number of all non vanishing eigenvalues of Δ_V on $\mathcal{F}_0(V, \mathbb{R}^n)$ is s_0. Moreover we express the metric on V by means of the bundle endomorphism φ on TM. The geometric ingredients on V are hence all expressed on M. These constructions allow us to link the description of the smooth and the discrete media.

In fact $\mathcal{H}_V$ has a unique counterpart $\widehat{\mathcal{H}} \in \mathcal{F}_0^\infty(M, I\!R^n)$ on M, namely $\mathcal{H}_V^M := \psi\varphi\mathcal{H}_V$. The map $\Delta\mathcal{H} \in \mathcal{F}_0^\infty(M, I\!R^n)$ is the force density on M. Thus it makes sense to talk about a discrete medium on the manifold M.
If the graph and its geometry are given each constitutive map splits uniquely into its discrete part in $\mathcal{F}_0^\infty(M, I\!R^n)$ and continuum part in the L_2-orthogonal complement $\mathcal{F}_0^\infty(M, I\!R^n)^\perp$ of $\mathcal{F}_0^\infty(M, I\!R^n)$ in $C_0^\infty(M, I\!R^n)$. The discrete part is called the **discretization** of the smooth medium. This shows that there are media on M of which the discretization on a given graph is trivial, namely those of which $\mathcal{H}(j_0) \in \mathcal{F}^\infty(M, I\!R^n)^\perp$. In this context one might consider the problem of discrete approximations, for computational purposes e.g., a task not headed for in these notes.

If we regard $\mathcal{H}_V$ as the constitutive entity deduced from knowledge on the microscopic level then $\mathcal{H}_V^M = \psi\varphi\mathcal{H}_V$ describes the resulting macroscopic structure on M. In this way we pass from the microscopic to the macroscopic level by geometric means rather than statistical ones. It's $\mathcal{H}_V$ which links the levels. What is missing is to find a "best fit" through a graph V in order to obtain a working formalism. We will deal with this much harder problem elsewhere.

Having looked at a discrete medium at a fixed configuration we develop a formalism in section four which allows deformations. These deformations, however, have to be small enough in order to preserve the interacting pattern among the particles. Thus we vary the configuration j only in a small neighbourhood $W(j_0) \subset \mathcal{F}_0(V, I\!R^n)$ of a fixed configuration j_0. The constitutive map $\widehat{\mathcal{H}}_V(j)$ is hence defined for any $j \in W(j_0)$ and characterizes the discrete medium with respect to a reference configuration j_0. Its physical interpretation is of the same nature as the one for $\mathcal{H}_V$; it only depends on an additional parameter, namely j. Its counterpart on M is called $\widehat{\mathcal{H}}_V^M(j)$.

For any configuration $j \in W(j_0) \subset \mathcal{F}_0(V, I\!R^n)$ the map $\widehat{\mathcal{H}}_V(j) : V \to I\!R$ admits a Fourier decomposition

$$\widehat{\mathcal{H}}_V(j) = \sum_{i=1}^{s_0} \kappa^i(j) u_i$$

with respect to a complete eigen system $u_1, \ldots, u_{s_0}$ of Δ_V. Hence the virtual work functional $F_V(j)$ is represented by

$$F_V(j) = \sum_{i=1}^{s_0} \nu^i \kappa^i(j) \cdot d\!l \mathrm{x}_i \ ,$$

where x_i is the coordinate on the axis $I\!R u_i$ and $d\!l$ denotes its differential. ν^i is the eigen value of Δ_V at u_i.
$d\!l_s F_V(j)$, the symmetric differential of F_V at j, is expressed by

$$d\!l_s F_V(j) = \frac{1}{2} \sum_{i=1}^{s_0} \nu^i d\!l \kappa^i(j) \vee d\!l \mathrm{x}_i \ ,$$

with $\vee$ the symmetric product. $\mathrm{d}_s F_V(j)$ is of of physical relevance: As an example we consider a medium given by Hook's law. Its eigenvalues at an equilibrium configuration j of internal force densities i.e. $F_V(j) = 0$ form the vibrational spectrum (cf. [C,St]).

Introducing a thermodynamical (equilibrium) setting (cf. [L,L] and [Str]) in section five, we can represent the Fourier coefficients thermodynamically as

$$\kappa^i(j) = \frac{T}{\nu^i}\frac{\partial S}{\partial \mathrm{x}_i} \qquad i = 1, \ldots, s_0 \ .$$

Here T is the absolute temperature and S is the entropy. At j with $\mathrm{d}T(j) = 0$ these sorts of coefficients can be obtained by

$$\kappa^i(j) = \frac{1}{\nu^i}\frac{\partial \mathrm{Fr}\,(j)}{\partial \mathrm{x}_i} \qquad i = 1, \ldots, s_0$$

with Fr the free energy. In this case the differential dFr coincides with the exact part of F_V in the sense of Hodge theory. Using the partition function Z for the Gibbs distribution in statistical mechanics (at an equilibrium state and constant temperature) the coefficients $\kappa^i(j)$ are of the form

$$\kappa^i(j) = \frac{T}{\nu^i} \left.\frac{\partial \log Z}{\partial \mathrm{x}_i}\right|_j \qquad i = 1, \ldots, s_0$$

out of which one immediately obtains the modes σ_i of dFr at constant T. The modes of dFr are called the modes of F_V or the modes of the medium. In fact

$$\sigma_i = \frac{1}{(\nu^i)^2} \cdot \frac{\partial \kappa^i}{\partial \mathrm{x}_i} = \frac{T}{(\nu^i)^2} \cdot \frac{\partial^2 \log Z}{\partial^2 \mathrm{x}_i} \qquad i = 1 \ldots, s_0 \ .$$

This spectrum determines a linearized model of the medium with exactly the same spectrum.

At this point let us repeat, in other terms, that the spectrum of the discrete medium at ***constant temperature*** and at an equilibrium configuration of internal force densities is entirely determined by the exact part of the virtual work form F_V. This exact part $\mathrm{d}L$ is extracted via Hodge theory (with Neumann data e.g.) on $\mathcal{F}_0(V, \mathbb{R}^n)$. No further thermodynamical entity is needed.

1. Geometric preliminaries and the Fréchet manifold $E(M, \mathbb{R}^n)$

Let M be a compact, oriented, connected and smooth manifold (without boundary) and $\mathbb{R}^n$ be equipped with an orientation and a scalar product $<\ ,\ >$, both fixed throughout the note.

For any $j \in E(M, \mathbb{R}^n)$ we define a Riemannian metric $m(j)$ on M by setting

$$m(j)(X, Y) :=< TjX, TjY >, \qquad \forall X, Y \in \Gamma(TM). \tag{1.1}$$

(More customary is the notation $j^* <\,,\,>$ instead of $m(j)$.) We use $\Gamma(\mathbf{E})$ to denote the collection of all smooth sections of any smooth vector bundle $\mathbf{E}$ over a manifold Q with $\pi_Q : \mathbf{E} \to Q$ the canonical projection. Let $\mu(j)$ be the Riemannian volume on M defined by the given orientation and the metric $m(j)$.

The Levi-Cività connection $\nabla(j)$ of $(M, m(j))$ is obtained as follows: $T\mathbb{R}^n|j(M)$ splits into $Tj(TM)$ and its orthogonal complement $(Tj(TM))^\perp$ (the Riemannian normal bundle of j). Hence any $Z \in \Gamma(T\mathbb{R}^n|j(M))$ has an orthogonal decomposition $Z = Z^\top + Z^\perp$, where the tangential component $Z^\top$ is of the form $Z^\top = TjV$ for a unique $V \in \Gamma(TM)$. For any $Y \in \Gamma(TM)$ the function $TjY : M \to T\mathbb{R}^n$ is smooth. The vector field $\nabla(j)_X Y$ on M, the covariant derivative of Y in the direction of X, is defined by the equation

$$Tj(\nabla(j)_X Y) = d(TjY)(X) - (\nabla_X(TjY))^\perp \tag{1.2}$$

for all $X, Y \in \Gamma(TM)$. Instead of $\left(\nabla_X(TjY)\right)^\perp$ we write $S(j)(X,Y)$ and call $S(j)$ the second fundamental tensor of j.

It is well-known that the set $C^\infty(M, \mathbb{R}^n)$ of smooth maps from M into $\mathbb{R}^n$ endowed with Whitney's C^∞-topology is a Fréchet manifold (cf.e.g.[Bi,Sn,Fi] or [Fr,Kr]). For a given $f \in C^\infty(M, \mathbb{R}^n)$, the tangent space $T_f C^\infty(M, \mathbb{R}^n)$ is the Fréchet space $C^\infty_f(M, T\mathbb{R}^n) := \{l \in C^\infty(M, T\mathbb{R}^n) | \tau_{\mathbb{R}^n} \circ l = f\} \cong \Gamma(f^* T\mathbb{R}^n)$ and the tangent bundle $TC^\infty(M, \mathbb{R}^n)$ is identified with $C^\infty(M, T\mathbb{R}^n)$, the topology again being the C^∞-topology.

The set $E(M, \mathbb{R}^n)$ of all C^∞-embeddings from M to $\mathbb{R}^n$ is open in $C^\infty(M, \mathbb{R}^n)$ and thus is a Fréchet manifold whose tangent bundle we denote by $C^\infty_E(M, T\mathbb{R}^n)$. It is an open submanifold of $C^\infty(M, T\mathbb{R}^n)$, fibred over $E(M, \mathbb{R}^n)$ by "composition with $\pi_{\mathbb{R}^n}$". Moreover, the Fréchet manifold $E(M, \mathbb{R}^n)$ is a principal *Diff* M-bundle under the obvious right *Diff* M-action and the quotient $U(M, \mathbb{R}^n) := E(M, \mathbb{R}^n)/\mathit{Diff}\, M$ is the manifold of "submanifolds of type M" of $\mathbb{R}^n$ (cf. [Bi,Sn,Fi], ch.5, and [Bi,Fi1]).
The set $\mathcal{M}(M)$ of all Riemannian structures on M is a Fréchet manifold since it is an open convex cone in the Fréchet space $S^2(M)$ of smooth, symmetric bilinear forms on M. Moreover, the map

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

is smooth (cf.[Bi,Sn,Fi]).

The Riemannian metric $<\,,\,>$ of $\mathbb{R}^n$ induces a "Riemannian structure" $\mathcal{G}$ on $E(M, \mathbb{R}^n)$ as follows: For any $j \in E(M, \mathbb{R}^n)$ and any two pairs of tangent vectors $l_1, l_2 \in C^\infty_j(M, T\mathbb{R}^n)$ we set

$$\mathcal{G}(j)(l_1, l_2) := \int_M \langle l_1, l_2 \rangle \, \mu(j) \, . \tag{1.3}$$

It is clear that $\mathcal{G}(j)$ is a continuous, symmetric, positive-definite bilinear form on $C^\infty_j(M, T\mathbb{R}^n)$ for each $j \in E(M, \mathbb{R}^n)$. Next we point out some invariance properties of $\mathcal{G}$: Let $\mathit{Diff}^+ M$ be the group of orientation-preserving diffeomorphisms of M. As a subgroup of *Diff* M, it operates freely on the right on $E(M, \mathbb{R}^n)$ by

$$\begin{aligned} \phi : E(M, \mathbb{R}^n) \times \mathit{Diff}^+ M &\longrightarrow E(M, \mathbb{R}^n) \\ (j, \varphi) &\longmapsto j \circ \varphi. \end{aligned} \tag{1.4}$$

Similarly, any group $\mathcal{J}$ of orientation-preserving isometries of $\mathbb{R}^n$ operates on the left on $E(M,\mathbb{R}^n)$ by

$$\begin{aligned} \mathcal{J} \times E(M,\mathbb{R}^n) &\longrightarrow E(M,\mathbb{R}^n). \\ (g,j) &\longmapsto g \circ j \end{aligned} \tag{1.5}$$

One immediately verifies the following (cf. [Bi,Fi2]):

Proposition 1.1

$\mathcal{G}$ is invariant under both $Diff^+M$ and $\mathcal{J}$.

Associated with a deformable medium is a mass distribution on M, a so called **density map**

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

with total mass $m = \int_M \rho(j)\,\mu(j)$. It is supposed to satisfy

$$\rho(j)(p) > 0 \qquad \forall j \in E(M,\mathbb{R}^n) \text{ and } \forall p \in M \;, \tag{1.6}$$

yielding the positivity of mass and which, in addition, is required to obey the **continuity equation**

$$\mathrm{d}\rho(j)(k) = -\frac{\rho(j)}{2} tr_{m(j)} \mathrm{d}m(j)(k) \qquad \forall j \in E(M,\mathbb{R}^n) \text{ and } \forall k \in C_j^\infty(M,T\mathbb{R}^n)\;. \tag{1.7}$$

$tr_{m(j)}$ denotes the trace formed with respect to $m(j)$. The symbol d denotes the differential of maps of which the domain is a Fréchet manifold of maps and which take values in a Fréchet space.
In what follows, we will construct a density map by solving (1.7). Let $j_0 \in E(M,\mathbb{R}^n)$ be fixed. For any $j \in E(M,\mathbb{R}^n)$ we express $m(j)$ via an uniquely determined smooth, strong bundle endomorphism $B(j)$ of TM (selfadjoint with respect to $m(j_0)$) by

$$m(j)(v_p,w_p) = m(j_0)\big(B(j)(p)v_p,w_p\big) \qquad \forall v_p,w_p \in T_pM \text{ and } \forall p \in M \tag{1.8}$$

and observe that the Riemannian volume forms $\mu(j_0)$ and $\mu(j)$ are linked by

$$\mu(j) = \det f(j)\mu(j_0) \tag{1.9}$$

with $f(j) = +\sqrt{B(j)}$. Fixing a map $\rho(j_0) \in C^\infty(M,\mathbb{R})$ satisfying (1.6) then

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

given for any $j \in E(M,\mathbb{R}^n)$ by

$$\rho(j) := \rho(j_0)\det f(j)^{-1} \tag{1.10}$$

satisfies both (1.6) and (1.7). Due to (1.7) the mass $\int \rho(j)\,\mu(j)$ is j-independent.

We close this construction of a density map by revisiting it with respect to technics used in statistical mechanics (cf. sec.5). Equations (1.7) and (1.10) allow us to write

$$d\!\!\!\,d \log \rho(j)(h) = -\operatorname{tr} f^{-1}(j) d\!\!\!\,d f(j)(h) \qquad \forall h \in C^\infty(M, \mathbb{R}^n) \tag{1.11}$$

for any $j \in E(M, \mathbb{R}^n)$. Let j be near j_0. If $b(j) \in EndTM$ is such that $\exp b(j) = f(j)$ and if we write

$$b(j) = \log f(j) \tag{1.12}$$

then

$$\rho(j) = \rho(j_0) \cdot e^{-\operatorname{tr} \log f(j)} = \rho(j_0) \cdot \det f^{-1}(j) \ , \tag{1.13}$$

a well known type of formula (cf. (5.21)).

Associated with a density map ρ on $E(M, \mathbb{R}^n)$ is a natural, j-independent metric $\mathcal{B}$ given by

$$\mathcal{B}(l_1, l_2) := \int_M \rho(j) < l_1, l_2 > \mu(j) \tag{1.14}$$

for each $j \in E(M, \mathbb{R}^n)$ and for each pair $l_1, l_2 \in C^\infty(M, T\mathbb{R}^n)$. This metric depends smoothly on all of its variables. For its covariant derivative and its geodesics see [Bi2].

2. The principle of virtual work and the first Piola-Kirchhoff stress tensor

In this section we will repeat the characterization of a medium via a first Piola-Kirchhoff stress tensor. Moreover, in the absence of external force densities, we will investigate the virtual work depending on any configuration and any infinitesimal virtual distortion. This work is a one-form on $E(M, \mathbb{R}^n)$, denoted by F. However, not all one forms on $E(M, \mathbb{R}^n)$ will serve as virtual works.

We assume that the medium moves and deforms in $\mathbb{R}^n$, equipped with a fixed scalar product. The configuration of the medium may vary rapidly.

At each configuration $j \in E(M, \mathbb{R}^n)$ we characterize the quality of the medium by the smooth first Piola-Kirchhoff stress tensor (cf. [M,H], p.135)

$$\alpha(j) : TM \longrightarrow T\mathbb{R}^n \ = \ \mathbb{R}^n \times \mathbb{R}^n \ .$$

Clearly $\alpha(j)$ is a smooth $\mathbb{R}^n$-valued one-form if the values will be projected onto the second factor (which is done throughout the paper).

Let us assume from now on that

$$\alpha : E(M, \mathbb{R}^n) \longrightarrow \mathcal{A}^1(M, \mathbb{R}^n)$$

is smooth (the range carries the C^∞-topology). The medium characterized by α is thus called a **smoothly deformable medium**. The virtual work determined by α and an (infinitesimal) virtual distortion l will be nothing else but the classical Dirichlet integral:

Given any two form $\alpha, \beta \in \mathcal{A}(M, I\!R^n)$ we can both represent uniquely as

$$\begin{aligned} \alpha &= c(\alpha, dj) \cdot dj \,+\, dj \cdot A(\alpha, dj) \\ \beta &= c(\beta, dj) \cdot dj \,+\, dj \cdot A(\alpha, dj)\ , \end{aligned} \tag{2.1}$$

cf [Bi2].

Now we set

$$\alpha \cdot \beta \;=\; -\tfrac{1}{2}\mathrm{tr}\, c(\alpha, dj) \circ c(\beta, dj) \;+\; \mathrm{tr}\, A(\alpha, dj) \circ A^{\star}(\beta, dj)$$

with $\star$ denoting the adjoint of $A(\beta, dj) : TM \to TM$ formed fibre wise with respect to $m(j)$ and

$$\mathcal{G}(dj)(\alpha, \beta) := \int_M \alpha \cdot \beta \, \mu(j) \qquad \forall \alpha, \beta \in \mathcal{A}(M, I\!R^n)\ .$$

In fact $\mathcal{G}(dj)$ is the Dirichlet integral.
Any (infinitesimal) distortion $l \in C^\infty(M, I\!R^n)$ yields the one-form

$$dl : TM \longrightarrow I\!R^n\ ,$$

which admits according to (2.1) the representation

$$dl \;=\; c(dl, dj) \cdot dj \,+\, dj \cdot A(dl, dj)\ . \tag{2.2}$$

The virtual work F at j is then given by the Dirichlet integral

$$F(j)(l) := \int_M \alpha(j) \bullet dl \, \mu(j) \equiv \mathcal{G}(dj)(\alpha(j), dl) \tag{2.3}$$

for any virtual distortion $l \in C^\infty(M, I\!R^n)$. A routine calculation shows (cf. [Bi2])

$$F(j)(l) = \int \langle \nabla^* \alpha(j), l \rangle \, \mu(j)$$

with ∇^* the covariant divergence given by the Levi Cività connection $\nabla(j)$.

Remark:

(i) If we fix a reference configuration $j_0 \in E(M, I\!R^n)$ then $\mu(j) = \det f(j)\, \mu(j_0)$ and

$$\int_M \alpha(j) \bullet dl \, \mu(j) \;=\; \int_M \big(\det f(j) \alpha(j)\big) \bullet dl \, \mu(j_0)$$

for all $j \in E(M, I\!R^n)$ and all $l \in C^\infty_j(M, TI\!R^n)$. In fact $\alpha(j) \det f(j)$ is usually called the first Piola-Kirchhoff stress tensor. However, since we work in this formalism without reference configurations in general, we call α the first Piola-Kirchhoff stress tensor.

(ii) For the sake of shortness we will frequently use the term "stress form" for $\alpha(j)$ rather than "a first Piola-Kirchhoff stress tensor".

Next let us investigate the virtual work

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

from the point of view of translational invariance. To see what one-forms on $E(M, \mathbb{R}^n)$ are virtual works, in absence of the external force densities, we first point out the following observation: Any virtual work F enjoys two special independent properties reading for any $j \in E(M, \mathbb{R}^n)$ and any $l \in C_j^\infty(M, T\mathbb{R}^n)$ as

$$\text{and} \quad \begin{aligned} F(j+z)(l) &= F(j)(l) \qquad \forall z \in \mathbb{R}^n \\ F(j)(l+z) &= F(j)(l) \qquad \forall z \in \mathbb{R}^n . \end{aligned} \tag{2.4}$$

The first one is certainly the invariance under the obvious action on $E(M, \mathbb{R}^n)$ of the translation groups $\mathbb{R}^n$ of the vector space $\mathbb{R}^n$. Factoring out this action on $E(M, \mathbb{R}^n)$ yields again a Fréchet manifold, called $E(M, \mathbb{R}^n)/_{\mathbb{R}^n}$ (the **reduced configuration space**). It admits a natural visualization via the center of mass as seen as follows (cf. [Bi2]):

Specifying a density map ρ (cf. section 2) on $E(M, \mathbb{R}^n)$ we introduce the **center z_m of mass** by

$$z_m(j) \cdot \int_M \rho(j)\, \mu(j) := \int_M \rho(j)\, j\, \mu(j) \tag{2.5}$$

for any $j \in E(M, \mathbb{R}^n)$. Fixing the center of mass at zero, then

$$\begin{aligned} \{\, j \in E(M, \mathbb{R}^n) \mid z_m(j) = 0 \,\} &\longrightarrow E(M, \mathbb{R}^n)/_{\mathbb{R}^n} \\ j \quad &\longmapsto \quad [j] \end{aligned} \tag{2.6}$$

is a diffeomorphism. Here $[j]$ denotes the equivalence class of j formed with respect to the action of the translation group $\mathbb{R}^n$ on $E(M, \mathbb{R}^n)$.

Clearly the differential

$$d : E(M, \mathbb{R}^n) \longrightarrow \{\, dj \mid j \in E(M, \mathbb{R}^n) \,\}$$

(the second factor carries the C^∞-topology) induces a diffeomorphism

$$\begin{aligned} \tilde{d} : E(M, \mathbb{R}^n)/_{\mathbb{R}^n} &\longrightarrow \{\, dj \mid j \in E(M, \mathbb{R}^n) \,\} \\ [j] \quad &\longmapsto \quad dj \end{aligned} \tag{2.7}$$

since $[j] = \{\, j + z \mid z \in \mathbb{R}^n \,\}$ for any $[j] \in E(M, \mathbb{R}^n)/_{\mathbb{R}^n}$. Obviously the differential

$$\{\, j \in E(M, \mathbb{R}^n) \mid z_m(j) = 0 \,\} \xrightarrow{d} \{\, dj \mid j \in E(M, \mathbb{R}^n) \,\}$$

is a (smooth) diffeomorphism too. Therefore, the reduced configuration space of the action of the translation group $\mathbb{R}^n$ on $E(M,\mathbb{R}^n)$ can be described in either way by

$$E(M,\mathbb{R}^n)/_{\mathbb{R}^n} \quad \text{or} \quad \{\, j \in E(M,\mathbb{R}^n) \mid z_m(j) = 0 \,\} \quad \text{or} \quad \{\, dj \mid j \in E(M,\mathbb{R}^n) \,\} .$$

Consequently we identify all the three and will use either symbol according to our convenience. The reduced phase space is hence

$$E(M,\mathbb{R}^n)/_{\mathbb{R}^n} \times C^\infty(M,\mathbb{R}^n)/_{\mathbb{R}^n} ,$$

the second factor being the usual factor space of $C^\infty(M,\mathbb{R}^n)$ modulo $\mathbb{R}^n$ (identified with $\{\, dl \mid l \in C^\infty(M,\mathbb{R}^n) \,\}$) endowed with the C^∞-topology.

The second property in (2.4) means that constant virtual distortions cause no virtual work. The two properties in (2.4) allow our work F, defined on $TE(M,\mathbb{R}^n) = E(M,\mathbb{R}^n) \times C^\infty(M,\mathbb{R}^n)$ to factor to $\overline{F}$, as shown in the following diagram:

$$\begin{tikzcd} E(M,\mathbb{R}^n) \times C^\infty(M,\mathbb{R}^n) \arrow[r, "F"] \arrow[d, "d\times d"'] & \mathbb{R} \\ \{dj | j \in E(M,\mathbb{R}^n)\} \times \{dl | l \in C^\infty(M,\mathbb{R}^n)\} \arrow[ur, "\overline{F}"'] & \end{tikzcd}$$

(In the sequel we will write F instead of $\overline{F}$.) These considerations reversed yield immediately those one forms on $E(M,\mathbb{R}^n)$ which are virtual works(cf. [Bi2]):

Lemma 2.1

There is a surjection from $C^\infty\big(E(M,\mathbb{R}^n), A^1(M,\mathbb{R}^n)\big)$ to the collection $A^1_{\mathcal{g}}\big(E(M,\mathbb{R}^n),\mathbb{R}\big)$ of all one-forms $F : E(M,\mathbb{R}^n) \times C^\infty(M,\mathbb{R}^n) \to \mathbb{R}$ characterized by the following properties:

1) F is invariant under the action of the translation group $\mathbb{R}^n$ on $E(M,\mathbb{R}^n)$.

2) $F(j)(l+z) = F(j)(l) \quad \forall j \in E(M,\mathbb{R}^n),\ \forall l \in C^\infty(M,\mathbb{R}^n)$ and $\forall z \in \mathbb{R}^n$.

3) F admits an integral representation of the form

$$F(j)(l) = \int \alpha(j) \bullet dl\, \mu(j) = \mathcal{g}(dj)(\alpha(j), dl) \tag{2.8}$$

for all variables of F where $\alpha : E(M,\mathbb{R}^n) \to \mathcal{A}^1(M,\mathbb{R}^n)$ is a smooth density.

The characterization by α of the medium is rather general. However, the question arises from (2.8) as to whether the virtual work is uniquely represented by the stress form α or not. In fact it is not:
Solving

$$\nabla^*(j)\alpha(j) = \Delta(j)\mathcal{H}(j) \qquad \forall j \in E(M,\mathbb{R}^n)$$

such that $\mathcal{G}(j)\big(\mathcal{H}(j), z\big) = 0$ for all $z \in \mathbb{R}^n$ shows immediately the unique decomposition

$$\alpha(j) = d\mathcal{H}(j) + \beta(j) \qquad \text{with } \nabla^*(j)\beta(j) = 0 .$$

$d\mathcal{H}(j)$ is therefore called the **irredundant part** of the first Piola-Kirchhoff stress tensor for any $j \in E(M, \mathbb{R}^n)$. This yields now the following main theorem in this section:

Theorem 2.2

Any deformable medium can be uniquely characterized by a smooth map $\mathcal{H} : E(M, \mathbb{R}^n) \to C^\infty(M, \mathbb{R}^n)$ with $\mathcal{G}(j)\big(\mathcal{H}(j), z\big) = 0$ for any $z \in \mathbb{R}^n$. The internal force density $\Phi(j)$ causing the virtual work against a deformation is

$$\Delta(j)\mathcal{H}(j) = \Phi(j) \qquad \forall j \in E(M, \mathbb{R}^n) . \tag{2.9}$$

Moreover

$$F(j)(l) = \mathcal{g}(dj)(d\mathcal{H}(j), dl) = \int_M d\mathcal{H}(j) \cdot dl\, \mu(j) = \int_M \langle \Delta(j)\mathcal{H}(j), l\rangle\, \mu(j) \tag{2.10}$$

holds for any $j \in E(M, \mathbb{R}^n)$ and any (virtual) deformation $l \in C^\infty(M, \mathbb{R}^n)$.

The question we will partially answer in the next section is: What is the physical nature of $\mathcal{H}$? The answer will be given only for media which consist of finitely many particles each interacting only with its nearest neighbours.

3. A discrete model with nearest neighbour interaction and a discretization formalism

Here we will develop a physical interpretation of the irredundant part of the first Piola-Kirchhoff stress tensor within the frame work of the nearest neighbour interaction in a graph.

To this end let $j_0 \in E(M, \mathbb{R}^n)$ be fixed throughout the rest of the paper. We fix a finite collection $V \subset M$ of points and form $j_0(V) \subset \mathbb{R}^n$. These points are the mean location of the material particles in $\mathbb{R}^n$. (These material particles could be molecules, clusters etc.) The total number of all points in V is denoted by s_0. If two of these particles interact the underlying locis in $j_0(V) \subset \mathbb{R}^n$ are connected with an edge. In this way $j_0(V)$ is turned into a graph (a one dimensional complex) in $\mathbb{R}^n$, assumed to be connected. We will generalize this situation in the following way:

The collection $V \subset M$ will be turned into a graph in M as follows: Let U_q be a neighbourhood of q on which $\exp_q^{-1}$ is bijective. Let s_0, the number of points in V, be such that $\bigcup_q U_q = M$. If $q' \in V \cap U_q$ then q' and q are connected by a geodesic segment (with respect to $m(j_0)$) provided $j_0(q)$ and $j_0(q')$ are connected by an edge in $\mathbb{R}^n$. In this way $V \subset M$ is a one dimensional complex in M. In addition we require that the graph is connected and oriented, i.e. the geodesic segments are directed. We moreover take a triangulation $\mathbf{t}$ of M subordinated to the covering $\{\, U_q \mid q \in M \,\}$ and such that each simplex contains exactly one vertex in its interior.

The vertices in V are considered as the mean loci of the material particles in M, too.

We now will make some assumptions of physical nature on this triangulation and this graph:
The volume $|\sigma|$ of any simplex $\sigma \in \mathbf{t}$ given by the Riemannian volume form $\mu(j_0)$ restricted to σ_q shall be a given small constant. This assumption is not very restrictive if the number of edges of the graph is very high and the largest cell is very small, a scenario which we assume to hold.

Let us specify the number of vertices V somewhat further. Let ρ be a density map (cf. sec.1) and call $\rho(j_0)$ restricted to V by $\rho_V(j_0)$. Both $\rho(j_0)$ and $\rho_V(j_0)$ determine respective masses:

$$\mathbf{m} := \int_M \rho(j_0)\,\mu(j_0) \qquad \text{and} \qquad \mathbf{m}_V := \sum_{q\in V} \rho_V(j_0)(q) \cdot |\sigma_q| \ ,$$

where σ_q is the simplex containing q in its interior and $|\sigma_q|$ is the volume of σ_q.
We require

$$\mathbf{m} - \mathbf{m}_V \text{ is very small } .$$

Next we will introduce the Dirichlet-form $\mathcal{g}$ and the Laplacian Δ_V of V. For the sake of simplicity we will often write l instead of its restriction $r(l) \equiv l|_V$ to V for any $l \in C^\infty(M, \mathbb{R}^n)$ (if no confusion will arise). By $\mathcal{F}(V, \mathbb{R}^n)$ we furthermore denote the finite dimensional vector spaces of all $\mathbb{R}^n$-valued maps of V. The dimension of this vector space is $s_0 + n$. Clearly the restriction map $r : C^\infty(M, \mathbb{R}^n) \to \mathcal{F}(V, \mathbb{R}^n)$ is surjective.

We define

$$\mathcal{g}_V : \mathcal{F}(V, \mathbb{R}^n) \times \mathcal{F}(V, \mathbb{R}^n) \longrightarrow \mathbb{R}$$

by

$$\mathcal{g}_V(h,l) := \sum_{q\in V} \sum_{i=1}^{k(q)} \big\langle h(q) - h(q_i), l(q) - l(q_i) \big\rangle |\sigma_q| \tag{3.1}$$

with $k(q)$ the number of nearest neighbours q_i for any pair $h, l \in \mathcal{F}(V, \mathbb{R}^n)$. The number $k(q)$ is called the **degree** of V in q. $\mathcal{g}_V$ is called the **Dirichlet form**. Let

$$\mathcal{G}_V(h,l) := \sum_{q\in V} \big\langle h(q), l(q) \big\rangle\, |\sigma_q| \qquad \forall h, l \in \mathcal{F}(V, \mathbb{R}^n) \ . \tag{3.2}$$

$\mathcal{G}_V$ is a positive-definite bilinear form on $\mathcal{F}(V, \mathbb{R}^n)$. The $\mathcal{G}_V$-orthogonal complement of $\mathbb{R}^n$ in $\mathcal{F}(V, \mathbb{R}^n)$ is called $\mathcal{F}_0(V, \mathbb{R}^n)$. Clearly $\mathcal{g}_V$ is a positive-definite scalarproduct on $\mathcal{F}_0(V, \mathbb{R}^n)$. We define

$$\Delta_V : \mathcal{F}(V, \mathbb{R}^n) \longrightarrow \mathcal{F}(V, \mathbb{R}^n)$$

by

$$\Delta_V h(q) := k(q) \cdot h(q) - \sum_{i=1}^{k(q)} h(q_i) \qquad q_i \in V_q(j) \, , \ \forall h \in \mathcal{F}(V, \mathbb{R}^n) \tag{3.3}$$

(cf. [B]).

For any $h \in \mathcal{F}(V, \mathbb{R}^n)$ we deduce the following analogue of (2.10):

$$\mathcal{G}_V(\Delta_V h, l) = g_V(h, l) \qquad \forall h, l \in \mathcal{F}(V, \mathbb{R}^n) . \tag{3.4}$$

To see that the equation (3.4) is satisfied it is enough to remark that both kinds of the sums

$$\Big(\langle h(q) - h(q_1), l(q)\rangle + \ldots + \langle h(q) - h(q_{k(q)}), l(q)\rangle\Big) |\sigma_q|$$

and

$$\Big(\langle h(q_1) - h(q), l(q_1)\rangle + \ldots + \langle h(q_{k(q)}) - h(q), l(q_{k(q)})\rangle\Big) |\sigma_q|$$

appearing on the right hand side of (3.2) exhaust the double sum of (3.4).
Clearly $\Delta_V h = 0$ if $h \in \mathbb{R}^n$, i.e. if h is a constant map. Moreover all eigen values of Δ_V are non negative.

By the above constructions the following is now obvious:

Proposition 3.1

Δ_V is a linear automorphism of $\mathcal{F}_0(V, \mathbb{R}^n)$. Hence

$$\Delta_V \mathcal{H}_V = \Phi_V$$

has a unique solution in $\mathcal{H}_V \in \mathcal{F}_0(V, \mathbb{R}^n)$ for any $\Phi_V \in \mathcal{F}_0(V, \mathbb{R}^n)$.

An immediate consequence of the above proposition is a first description of the physical nature of $\mathcal{H}_V$ within our frame work:

Theorem 3.2

Let $F_V : \mathcal{F}_0(V, \mathbb{R}^n) \to \mathbb{R}$ be the linear functional of which $F_V(l)$ is the virtual work caused by the distortion $l \in \mathcal{F}_0(M, \mathbb{R}^n)$, assumed to vanish on the constant maps. Then there is a uniquely determined (internal) force density $\Phi_V \in \mathcal{F}_0(V, \mathbb{R}^n)$ such that

$$F_V(l) = \mathcal{G}_V(\Phi_V, l) . \tag{3.5}$$

This force density hence determines via the equation $\Delta_V \mathcal{H}_V = \Phi_V$ a unique map $\mathcal{H}_V \in \mathcal{F}_0(V, \mathbb{R}^n)$, called the constitutive map. Moreover any $\mathcal{H}_V \in \mathcal{F}_0(V, \mathbb{R}^n)$ determines uniquely the force density $\Phi_V(q)$ which evaluated at any $q \in V$ is

$$\Phi_V(q) = \Delta_V \mathcal{H}_V(q) = k(q)\mathcal{H}_V(q) - \sum_i \mathcal{H}_V(q_i) , \tag{3.6}$$

where $q_1, \ldots, q_{k(q)}$ are the nearest neighbours of q. Hence $\mathcal{H}_V$ is a potential for which $\mathcal{H}_V(q) - \mathcal{H}_V(q_i)$ is the interaction force density of the material particle at q_i with the one at q. Therefore $\Phi_V(q)$ is the resulting force density at q of the interaction force densities of all the nearest neighbours of q acting upon the particle at q. Let $\mathrm{ed}_q^i \in T_q M$ be such that $\exp \mathrm{ed}_q^i$ is the geodesic segment connecting q with q_i. The differential $dr^{-1}\mathcal{H}_V(q)\mathrm{ed}_q^i$ at q along the geodesic segment $\exp \mathrm{ed}_q^i$ approximates the interaction force density of the particle at q with the one at q_i.

Remark

A medium on V defined by a constitutive map $\mathcal{H}_V$ is called a **discrete** medium. Based on the observations just made $\mathcal{H}_V$ is called the **interaction potential** of a discrete medium on V.

In order to link $\Delta_V h$ with $\Delta(j_0)h$ for any $h \in C^\infty(M, \mathbb{R}^n)$ we introduce the following notion:
Let $C_0^\infty(M, \mathbb{R}^n)$ be the $\mathcal{G}(j_0)$-orthogonal of $\mathbb{R}^n$ in $C^\infty(M, \mathbb{R}^n)$. The map $r : C_0^\infty(M, \mathbb{R}^n) \to \mathcal{F}_0(V, \mathbb{R}^n)$ is surjective, too. Clearly $\mathcal{G}_V$ is a scalar product on $\mathcal{F}_0(V, \mathbb{R}^n)$ and $\dim \ker \Delta_V = 0$.

In order to work on M instead of V we will construct next a finite dimensional subspace $\mathcal{F}_0^\infty(M, \mathbb{R}^n)$ of $C_0^\infty(M, \mathbb{R}^n)$ stable under $\Delta(j_0)$ and such that

$$r : \mathcal{F}_0^\infty(M, \mathbb{R}^n) \longrightarrow \mathcal{F}_0(V, \mathbb{R}^n)$$

is an isomorphism. We do this as follows:
Let $\{e_i\}_{i=1,\ldots}$ be a $\mathcal{G}(j_0)$-orthonormal complete system of eigen vectors of $\Delta(j_0)$. Any $g \in C^\infty(M, \mathbb{R}^n)$ has thus the Fourier expansion

$$g = \sum \xi^i e_i \qquad \xi \in \mathbb{R} \text{ for all } i = 1, \ldots .$$

The right hand side converges uniformly. Equipping $C_0^\infty(M, \mathbb{R}^n)$ with the topology of uniform convergence yielding $C_0^\infty(M, \mathbb{R}^n)_{C_0}$ the restriction map

$$r : C_0^\infty(M, \mathbb{R}^n)_{C_0} \longrightarrow \mathcal{F}_0(V, \mathbb{R}^n)$$

is a continuous surjection. Thus $\{\, re_i \mid i = 1, \ldots \}$ generates $\mathcal{F}_0(V, \mathbb{R}^n)$. Out of this set we construct a basis of $\mathcal{F}_0(V, \mathbb{R}^n)$ as follows: We take the smallest i such that $re_i \neq 0$. Next we look for the smallest i' such that re_i and $re_{i'}$ are linearly independent. Continuing in this way we obtain a linearly independent system called $e_1^0, \ldots, e_{s_0}^0$ for which $re_1^0, \ldots, re_{s_0}^0$ is a basis of $\mathcal{F}_0(V, \mathbb{R}^n)$. The vectors $e_1^0, \ldots, e_{s_0}^0$, all eigen vectors of $\Delta(j_0)$, generate a subspace $\mathcal{F}_0^\infty(M, \mathbb{R}^n)$ of $C_0^\infty(M, \mathbb{R}^n)$.
By construction $\Delta(j_0)$ is a linear automorphism of $\mathcal{F}_0^\infty(M, \mathbb{R}^n)$ and $r : \mathcal{F}_0^\infty(M, \mathbb{R}^n) \to \mathcal{F}_0(V, \mathbb{R}^n)$ is an isomorphism. Since $\Delta(j_0)$ and Δ_V are invertible on $\mathcal{F}_0^\infty(M, \mathbb{R}^n)$ and $\mathcal{F}_0(V, \mathbb{R}^n)$, respectively, we immediately conclude the following technically convenient proposition:

Proposition 3.3

$\Delta(j_0)$ is a linear automorphism on $\mathcal{F}_0^\infty(M, \mathbb{R}^n)$. Moreover there is an unique linear map

$$\psi(j_0) : C_0^\infty(M, \mathbb{R}^n) \longrightarrow \mathcal{F}_0^\infty(M, \mathbb{R}^n)$$

such that

(i) $\ker \psi(j_0)$ *is* $\mathcal{G}(j_0)$*-orthogonal to* $\mathcal{F}_0^\infty(M, \mathbb{R}^n)$

(ii) $\psi(j_0)|_{\mathcal{F}_0^\infty(M, \mathbb{R}^n)}$ *is an isomorphism of* $\mathcal{F}_0^\infty(M, \mathbb{R}^n)$.

(iii) $\Delta_V = r\Delta(j_0)\psi(j_0)r^{-1}$ *with* $r : \mathcal{F}_0^\infty(M, \mathbb{R}^n) \to \mathcal{F}_0(V, \mathbb{R}^n)$ *the restriction map being an isomorphism. Hence* $\psi(j_0)|_{\mathcal{F}_0^\infty(M,\mathbb{R}^n)} = \Delta^{-1}(j_0)r^{-1}\Delta_V r$.

(iv) *For any* $\Phi_V \in \mathcal{F}_0(V, \mathbb{R}^n)$ *there is a unique solution* $\mathcal{H}_V \in \mathcal{F}_0(V, \mathbb{R}^n)$ *such that*

$$\Delta_V \mathcal{H}_V = \Phi_V = r\Delta(j_0)\psi(j_0)r^{-1}\mathcal{H}_V \ . \tag{3.7}$$

Remark

Given a sequence $e'_1, \dots, e'_k$ of eigen vectors of $\Delta(j_0)$. Then there is a graph V with enough vertices such that the $e_1, \dots, e_k$ are among the $e_1^0, \dots, e_{s_0}^0$.

On $\mathcal{F}_0^\infty(M, \mathbb{R}^n)$ the scalar products $r^*\mathcal{G}_V$ and $\mathcal{G}(j_0)$ are linked by a linear isomorphism $\varphi(j_0)$ of $\mathcal{F}_0^\infty(M, \mathbb{R}^n)$ meaning that

$$r^*\mathcal{G}_V(h,l) = \mathcal{G}(j_0)\big(\varphi(j_0)h, l\big) \qquad \forall h, l \in \mathcal{F}^\infty(M, \mathbb{R}^n) \ . \tag{3.8}$$

For any choice of $h, l \in \mathcal{F}_0^\infty(M, \mathbb{R}^n)$ the following equations hold:

$$\begin{aligned}\mathcal{G}_V\big(\Delta_V rh, rl\big) &= \mathcal{G}(j_0)\big(\varphi(j_0)\Delta(j_0)\psi(j_0)h, l\big)\\ \mathcal{G}_V\big(rh, \Delta_V rl\big) &= \mathcal{G}(j_0)\big(h, \psi(j_0)^*\Delta(j_0)\varphi(j_0)l\big)\end{aligned}$$

with $\psi(j_0)^*$ the $\mathcal{G}(j_0)$-adjoint of $\psi(j_0)$.

Each of the maps $\psi(j_0)$ and $\psi(j_0)^*$ link the discrete geometry on V with the Riemannian geometry on the continuum M.

For any eigen vector u of Δ_V the vector $\frac{r^{-1}u}{\|r^{-1}u\|_{\mathcal{G}(j)}}$ is also a $\mathcal{G}(j_0)$-orthonormed eigen vector of $\varphi(j_0)$. Thus $\varphi(j_0)$ commutes with $\Delta(j_0)\psi(j_0) = r^{-1}\Delta_V r$ and hence $\psi(j_0)^*\Delta(j_0) = (r^{-1}\Delta_V r)^*$. Therefore the following proposition holds:

Proposition 3.4

The following relations hold

(i) $\varphi(j_0)\Delta(j_0)\psi(j_0) = \Delta(j_0)\psi(j_0)\varphi(j_0)$ *on* $\mathcal{F}_0^\infty(M, \mathbb{R}^n)$.

(ii) $\Delta_V = r\psi(j_0)^*\Delta(j_0)r^{-1} = r\Delta(j_0)\psi(j_0)r^{-1}$ *on* $\mathcal{F}_0(V, \mathbb{R}^n)$.

As a consequence of 3.3 and 3.4 we obtain immediately a smooth description on M of a discrete medium specified on V:

Corollary 3.5

Any force density $\Phi_V \in \mathcal{F}_0(V, \mathbb{R}^n)$ *with* $\mathcal{H}_V$ *as its constitutive map satisfies*

$$r^{-1} \cdot \Phi_V = r^{-1}\Delta_V\mathcal{H}_V = \Delta(j_0)\psi(j_0)r^{-1}\mathcal{H}_V \ . \tag{3.9}$$

Hence $\mathcal{H}_V^M(j_0) := \psi(j_0)\varphi(j_0) \circ r^{-1}\mathcal{H}_V$ *is the constitutive map on* M *describing the medium on* V *as a smooth medium on* M, *for which*

$$F_V(l) = \mathcal{G}(j_0)\big(\Delta(j_0)\psi(j_0)\varphi(j_0)r^{-1}\mathcal{H}_V, l\big) = \mathcal{G}_V(\Delta_V\mathcal{H}_V, rl) = \mathcal{G}(j_0)\big(\varphi(j_0)r^{-1}\Phi_V, l\big) \tag{3.10}$$

holds for any $l \in \mathcal{F}_0^\infty(M, I\!R^n)$.

Remark

(i) Following the above theorem the quality of the physical model of a discrete medium is thus determined by the graph V and the specification of $\mathcal{H}_V$. Given a graph V any internal force density in $\mathcal{F}_0(V, I\!R^n)$ determines uniquely $\mathcal{H}_V \in \mathcal{F}_0(V, I\!R^n)$. What sorts of graphs V and constitutive maps $\mathcal{H}_V$ are useful has to be decided on physical grounds. A microscopic view point is thus needed to specify the physical meaningful $\mathcal{H}_V$.

(ii) However, given V any microscopic theory yielding a force density Φ_V on V determines some $\mathcal{H}_V$, i.e. yields a microscopic setting in a prescribed nearest neighbour geometry.

Based on the observations made so far, a **discretization procedure** in terms of V of a smooth medium is defined as follows: Suppose we have a force density $\Phi(j_0)$ on M causing a virtual work $F(j_0)$ in the sense of (2.10). The discretization of $\Phi(j_0)$ is by definition the map $r\varphi(j_0)r^{-1}r\Phi(j_0) : V \to I\!R^n$ with $r : C^\infty(M, I\!R^n) \to \mathcal{F}(V, I\!R^n)$ the restriction map and $r^{-1} : \mathcal{F}_0(V, I\!R^n) \to \mathcal{F}_0^\infty(M, I\!R^n)$ the inverse. The background of this definition is the requirement that the virtual work F on the continuum is identical with the virtual work F_V on the discrete medium: Let $l \in \mathcal{F}_0^\infty(M, I\!R^n)$. Assuming some $\Psi \in \mathcal{F}_0^\infty(M, I\!R^n)$ such that

$$F(j_0)(l) = \mathcal{G}(j_0)(\Phi(j_0), l) = \mathcal{G}(j_0)\big(\mathrm{Pr}\,\Phi(j_0), l\big) = \mathcal{G}_V(\Psi, l) = F_V(rl) \ , \tag{3.11}$$

where $\mathrm{Pr} : C_0^\infty(M, I\!R^n) \to \mathcal{F}^\infty(M, I\!R^n)$ is the $\mathcal{G}(j_0)$-orthogonal projection Hence $\Psi = r\varphi(j_0)^{-1}\mathrm{Pr}\,\Phi(j_0)$. Setting $\Phi'(j_0) := \Phi(j_0) - r^{-1}r\Phi(j_0)$ yields

$$\mathcal{G}(j_0)\big(\Phi'(j_0), l\big) = \mathcal{G}(j_0)\big(r^{-1}r\Phi'(j_0), r^{-1}rl\big) = 0 \qquad \forall l \in \mathcal{F}_0^\infty(M, I\!R^n)$$

showing $\mathrm{Pr} = r^{-1}r$. Transforming $\mathcal{G}_V$ into $\mathcal{G}(j_0)$,i.e. using (3.8), yields the desired expression for the discretization. The force density $\Phi(j_0)$ on M is described by a constitutive map $\mathcal{H}(j_0) \in C_0^\infty(M, I\!R^n)$ as

$$\Phi(j_0) = \Delta(j_0)\mathcal{H}(j_0) \ .$$

Using proposition 3.1 there is hence a unique map $\mathcal{H}(j_0)_V \in \mathcal{F}_0(V, I\!R^n)$ such that

$$r\varphi(j_0)^{-1}r^{-1}r\Phi(j_0) = \Delta_V\mathcal{H}(j_0)_V$$

implying

$$r\varphi(j_0)^{-1}r^{-1}r\Delta(j_0)\mathcal{H}(j_0) = \Delta_V\mathcal{H}(j_0)_V \ .$$

Rewriting Δ_V with the help of 3.3 (iii) yields

$$\Delta_V\mathcal{H}(j_0)_V = r\Delta(j_0)\psi(j_0)r^{-1}\mathcal{H}(j_0)_V$$

and using 3.4 (i) implies

$$r\Delta(j_0)\mathcal{H}(j_0) = r\varphi(j_0)\Delta(j_0)\psi(j_0)r^{-1}\mathcal{H}(j_0)_V = r\Delta(j_0)\psi(j_0)\varphi(j_0)r^{-1}\mathcal{H}(j_0)_V \ .$$

Therefore
$$\mathcal{H}(j_0)_V = r\varphi(j_0)^{-1}\psi(j_0)^{-1}r^{-1}r\mathcal{H}(j_0)\ .$$
This yields the splitting
$$\mathcal{H}(j_0) = \psi(j_0)\varphi(j_0)r^{-1}\mathcal{H}(j_0)_V + \mathcal{H}(j_0)^\perp \tag{3.12}$$
with $\mathcal{H}(j_0)^\perp := \mathcal{H}(j_0) - \psi(j_0)\varphi(j_0)r^{-1}\mathcal{H}(j_0)_V$.

We call $\mathcal{H}(j_0)_V$ the **discretization** of $\mathcal{H}(j_0)$ on V and $\varphi(j_0)^{-1}\psi(j_0)^{-1}r^{-1}r\mathcal{H}(j_0)$ the **discretization** of $\mathcal{H}(j_0)$ on M.
In view of corollary 3.5 we thus state:

Theorem 3.6
Given the graph V and its geometry each constitutive map $\mathcal{H}(j_0)$ on M splits at j_0 uniquely into
$$\mathcal{H}(j_0) = \psi(j_0)\varphi(j_0)r^{-1}\mathcal{H}(j_0)_V + \mathcal{H}(j_0)^\perp \tag{3.13}$$
with $\mathcal{H}_V(j_0) \in \mathcal{F}_0(V, I\!R^n)$ being defined by
$$\Delta_V\mathcal{H}_V(j_0) = r\psi(j_0)r^{-1}\Delta(j_0)\mathcal{H}(j_0) \tag{3.14}$$
and hence being of the form
$$\mathcal{H}(j_0)_V = r\varphi(j_0)^{-1}\psi(j_0)^{-1}r^{-1}r\mathcal{H}(j_0)\ . \tag{3.15}$$
Moreover $\mathcal{H}(j_0)_V^M := \psi(j_0)\varphi(j_0)\mathcal{H}(j_0)_V$ is in $\mathcal{F}^\infty(M, I\!R^n)$ while as $\mathcal{H}(j_0)^\perp$ is in the orthogonal complement $\mathcal{F}_0(M, I\!R^n)^\perp$ of $\mathcal{F}_0(M, I\!R^n)$ in $C_0^\infty(M, I\!R^n)$. Therefore $\psi(j_0)\varphi(j_0)\mathcal{H}(j_0)_V$ is the smooth description of the discretization of the medium on M.

Remark
We call a smooth medium on M to be of **discrete nature** if $\mathcal{H}(j_0) = \psi(j_0)\varphi(j_0)r^{-1}r\mathcal{H}(j_0)_V$, i.e. if $\mathcal{H}(j_0)^\perp = 0$. Clearly the discretization of $\mathcal{H}_V^M(j_0) : M \to I\!R^n$ in corollary 3.5 is $\mathcal{H}_V$ again.

As **example** of a discretization let us consider the volume map $\mathcal{V} : E(M, I\!R^n) \to I\!R$ given by $\mathcal{V}(j) := \int_M \mu(j)$. Then for $j_0 \in E(M, I\!R^n) \cap C_0^\infty(M, I\!R^n)$
$$d\mathcal{V}(j_0)(l) = \int \langle \Delta(j_0)j_0, l\rangle\, \mu(j_0)\ .$$
Our one form F is thus $d\mathcal{V}(j_0)$. Hence $\mathcal{H}(j_0) = j_0$ and
$$\mathcal{H}(j_0)_V = j_{0V} = r\varphi(j_0)^{-1}\psi(j_0)^{-1}r^{-1}rj_0\ .$$
If $\mathcal{F}_0^\infty(M, I\!R^n)$ and $\mathcal{F}_0(V, I\!R^n)$ are identified by r, then
$$\mathcal{H}(j_0)_V = j_{0V} = \varphi(j_0)^{-1}\psi(j_0)^{-1}j_0|_V\ . \tag{3.16}$$

Due to (3.7) the derivative $\mathbb{d}\mathcal{V}(j_0)$ at j_0 of the volume map $\mathcal{V}$ rewrites hence as

$$\mathbb{d}\mathcal{V}(j_0)_V(l) = \mathcal{G}_V(\Delta_V \varphi(j_0)^{-1}\psi(j_0)^{-1} {j_0}_V, l) \; .$$

As we introduced capillarity in [Bi2] we proceed accordingly in the discrete case: We omit the identification by r. Given $\mathcal{H}_V$, a constitutive map for a discrete medium on V, we take the $\mathcal{g}$-orthogonal component of $d(\psi(j_0)\varphi(j_0)r^{-1}\mathcal{H}_V)$ along $d(\psi(j_0)\varphi(j_0)r^{-1}{j_0}_V)$. This component is a multiple $a_V \cdot d(\psi(j_0)\varphi(j_0)r^{-1}{j_0}_V)$ of $d(\psi(j_0)\varphi(j_0)r^{-1}{j_0}_V)$. Hence

$$\mathcal{H}_V = a_V {j_0}_V + \mathcal{H}'_V \tag{3.17}$$

with $\mathcal{H}'_V := \mathcal{H}_V - a_V {j_0}_V$. The real number a_V is called the **capillarity** of the discrete medium.

The interpretation of $\mathcal{H}_V$ as presented in theorem 3.2 is obviously supplemented by the following interpretation of the force density at locations of material particles:

Proposition 3.7

Let $v^r_{q_s} \in \mathcal{F}(V, \mathbb{R}^n)$ be the map assigning to q the r^{th} basis vector in $\mathbb{R}^n$ and zero otherwise then $\{ v^r_{q_s} \mid r = 1, \ldots, n; \; s = 1, \ldots, s_0 \} \subset \mathcal{F}(V, \mathbb{R}^n)$ is a basis. Representing $\Delta_V \mathcal{H}_V$ in this basis reads as

$$\Delta_V \mathcal{H}_V = \sum_{r,s} w^r_s v^r_s \; . \tag{3.18}$$

Thus $w^r_{q_s}$ is the work against the resulting interaction force densities of all its nearest neighbours needed to lift up the particle at q_s by one unit length in the direction of $v^r_{q_s}$.

Clearly a physically more real picture would be obtained by starting with a graph and then pass to a good fitting smooth surface through it (characterized by special kinds of $\psi(j_0)$ and $\phi(j_0)$). We will study this much more difficult situation elsewhere.

4. Deformation of the graph

Let $j_0 \in E_0(M, \mathbb{R}^n)$ be fixed. We call j_0 a **reference configuration**. Here we study the deformations of the medium of which the material particles are at the vertices of $V \subset M$. We describe these deformations with respect to a reference configuration in order to involve a fixed Laplacian, namely Δ_V. The first goal is to give a definition of what is meant by the medium on V at the configuration $j \in E_0(M, \mathbb{R}^n)$ near j_0.

We study the analogous situation for a continuum first: Suppose we are given a medium on M characterized at the configuration j by a constitutive map $\mathcal{H}(j)$. We will describe the medium at the configuration $j \in E(M, \mathbb{R}^n)$ with respect to the reference configuration j_0. Since we use the Laplacian at a fixed reference configuration j_0 we need to pull back $\mathcal{H}(j)$ to j_0. This pull back $\widehat{\mathcal{H}}(j)$ is defined as the solution of the following equation

$$\det f(j)\Delta(j)\mathcal{H}(j) \;=\; \Delta(j_0)\widehat{\mathcal{H}}(j) \qquad \forall j \in E_0(M, \mathbb{R}^n) \tag{4.1}$$

where $\mu(j) = \det f(j)\mu(j_0)$ and $m(j)(X,Y) = m(j_0)(f^2(j)X,Y)$ holding for each pair $X,Y \in \Gamma(TM)$ (cf. sec.1). Hence we verify immediately

$$F(j)(l) = \int_M \langle \det f(j)\Delta(j)\mathcal{H}(j), l\rangle\, \mu(j_0) = \int_M \langle \Delta(j_0)\widehat{\mathcal{H}}(j), l\rangle\, \mu(j_0) \,.$$

The medium on M at the configuration j is hence characterized by $\widehat{\mathcal{H}}(j)$ with respect to the geometry of the reference configuration j_0. In the analogous way we treat the discrete situation.

To do so we need the following notions: Let $E_0(V,\mathbb{R}^n) := \{\, rj \mid j \in E_0(M,\mathbb{R}^n)\,\}$. Clearly $E_0(V,\mathbb{R}^n)$ is open in $\mathcal{F}_0(V,\mathbb{R}^n)$ and $r\big(E(M,\mathbb{R}^n) \cap C_0^\infty(M,\mathbb{R}^n)\big) = E_0(V,\mathbb{R}^n)$.
A physical remark is necessary here: Stretching a physical configuration of material particles with prescribed nearest neighbours interactions may change this interaction completely. If the type of the graph has to be preserved then only embeddings very close to $j_0 \in E_0(V,\mathbb{R}^n)$ ought to be considered, i.e. we vary j in an open neighbourhood $W(j_0)$ of $j_0 \in E_0(V,\mathbb{R}^n)$.

Assuming a given virtual work $F_V(j)$ characterizing the discrete medium on V at the configuration $j \in W(j_0)$, then

$$F_V(j) = \mathcal{G}_V\big(\Phi_V(j), l\big) \qquad \forall l \in \mathcal{F}(V,\mathbb{R}^n) \tag{4.2}$$

for some well defined force density $\Phi_V(j)$ in $\mathcal{F}_0(V,\mathbb{R}^n)$. Hence by proposition 3.1

$$\Phi_V(j) = \Delta_V \widehat{\mathcal{H}}_V(j) \tag{4.3}$$

for some well defined $\widehat{\mathcal{H}}_V(j) \in \mathcal{F}_0(V,\mathbb{R}^n)$. This map $\widehat{\mathcal{H}}_V$ describes the medium on V at the configuration $j \in W(j_0) \subset E_0(V,\mathbb{R}^n)$. The description of the force density (4.3) on V is expressed on M (again with the help of proposition 3.2) as

$$r^{-1}\Phi_V(j) = \Delta(j_0)\psi(j_0)r^{-1}\widehat{\mathcal{H}}_V(j) \,.$$

To describe the work caused by Φ_V on V in a continuous fashion on M and hence with the metric $\mathcal{G}(j_0)$ we need to modify $r^{-1}\Phi_V(j)$ by applying $\varphi(j_0)$ to it:

$$\begin{aligned}\varphi(j_0)r^{-1}\Phi_V(j) &= \varphi(j_0)\Delta(j_0)\psi(j_0)r^{-1}\widehat{\mathcal{H}}_V(j)\\ &= \Delta(j_0)\psi(j_0)\varphi(j_0)r^{-1}\widehat{\mathcal{H}}_V\end{aligned}$$

showing

$$F_V(j)(l) = \mathcal{G}(j_0)\big(\Delta(j_0)\psi(j_0)\varphi(j_0)r^{-1}\widehat{\mathcal{H}}_V(j), r^{-1}l\big) \,.$$

Let $j' \in E(M,\mathbb{R}^n) \cap C_0^\infty(M,\mathbb{R}^n)$ be such that $r(j') = j$ and $\mathcal{H}_V^M(j)$ be the solution on M of

$$\det f^{-1}(j')\Delta(j_0)\psi(j_0)\varphi(j_0)r^{-1}\widehat{\mathcal{H}}(j')_V = \Delta(j')\widehat{\mathcal{H}}_V^M(j') \tag{4.4}$$

which is assumed to be $\mathcal{G}(j)$-orthogonal to the constants $\mathbb{R}^n$. Then

$$\Delta(j_0)\psi(j_0)\varphi(j_0)r^{-1}\widehat{\mathcal{H}}(j')_V^M = \det f(j') \cdot \Delta(j')\widehat{\mathcal{H}}_V^M(j') \,.$$

Thus $\det f(j')\Delta(j')\mathcal{H}_V^M(j')$ is the force density $\Phi_V^M(j')$ on M at the configuration j' of the medium on V described on M with respect to the reference configuration j_0. It causes the same virtual work as Φ_V does. Moreover $\Delta(j')\mathcal{H}_V^M(j')$ is the force density on M of the medium on V at the configuration j' described with respect to j_0'.

The basic equation of the virtual work F_V at any configuration $j \in r^{-1}\big(W(j_0)\big)$ caused by a distortion $r^{-1}l \in \mathcal{F}_0^\infty(M, I\!R^n)$with $l \in \mathcal{F}_0(V, I\!R^n)$ is

$$F_V(j)(l) := \mathcal{G}_V\big(\Delta_V\widehat{\mathcal{H}}_V(j), l\big) = \mathcal{G}(j')\big(\Delta(j')\widehat{\mathcal{H}}_V^M(j'), r^{-1}l\big)$$

for any $j' \in E(M, I\!R^n)$.

We therefore have

Lemma 4.1

The discrete medium on V at the configuration $j \in W(j_0) \subset E_0(V, I\!R^n)$ is characterized by a map $\widehat{\mathcal{H}}_V(j)$, smoothly depending on j. The same medium is characterized on M by $\widehat{\mathcal{H}}(j')_V^M$, smoothly depending on $j' \in r^{-1}(W(j_0)) \subset E(M, I\!R^n)$ too. Its force density on M with respect to $\mathcal{G}(j_0)$ is

$$\Phi_V^M(j') = \det f(j')\Delta(j')\widehat{\mathcal{H}}(j')_V^M \ ,$$

while as the force density on V is $\Phi_V(j) = \Delta_V\widehat{\mathcal{H}}(j)$. The virtual work of the medium on V at the configuration j is expressed either on M or V by

$$F_V(j)(l) = \mathcal{G}_V\big(\Delta_V\widehat{\mathcal{H}}(j)_V, l\big) = \mathcal{G}(j')\big(\Delta(j')\widehat{\mathcal{H}}(j')_V^M, r^{-1}l\big) \qquad \forall l \in \mathcal{F}_0(V, I\!R^n)\ . \tag{4.5}$$

To get a more physical approach we need to answer the following question: Given F_V on $\mathcal{F}_0(V, I\!R^n)$ can we determine a collection of irredundant configurational variables near j_0? This question will be relevant with respect to a thermodynamical description as well as with respect to determine the spectrum of the medium.

We study this problem as follows: Decomposing $\widehat{\mathcal{H}}_V$ with respect to the eigen basis $u_1, \ldots, u_n$ of Δ_V yields

$$\widehat{\mathcal{H}}_V(j) = \sum_{i=1}^{s_0} \kappa^i(j)u_i \qquad \forall j \in W(j_0) \subset E_0\big(V, I\!R^n\big)\ . \tag{4.6}$$

The Fourier coefficients $\kappa^i(j)$ are called the coefficients of F_V. Let $\kappa_1^i, \ldots, \kappa_K^i$ be those coefficients which do not identically vanish on $W(j_0)$. Then $u_1^i, \ldots, u_K^i$ span $I\!R^K \subset \mathcal{F}_0(V, I\!R^n)$. We assume moreover that $\mathcal{H}_V(j_0) \in I\!R^K$ is a regular value of $\mathcal{H}_V$. Hence there is a neighbourhood $W_1(j_0) \subset W(j_0) \subset \mathcal{F}_0(V, I\!R^n)$ of j_0 such that

$$W_1(j_0) = \mathcal{M} \times \mathbf{F}$$

with $\mathcal{M} = \mathcal{H}_V^{-1}\big(\mathcal{H}_V(j_0)\big)$. Thus $\mathbf{F}$ is spanned by the elements in $\{u_1, \ldots, u_{s_0}\}\backslash\{u_1^i, \ldots, u_K^i\}$. In studying F_V we may therefore restrict us to $\mathcal{M}$. Since the one-forms $\mathcal{G}_V(u_i, \cdot)$ with

$i = 1, \ldots, K$ are exact on $\mathcal{M}$ and hence are of the form $\mathrm{d}x_1, \ldots, \mathrm{d}x_K$ (after a renumbering), the coordinates $x_1, \ldots, x_K$ form a collection of irredundant variables. In terms of these variables F_V is represented by

$$F_V(j) = \sum_{i=1}^{K} \nu^i \kappa^i(j) \mathrm{d}x_i \qquad \forall j \in \mathcal{M} \tag{4.7}$$

with ν^i the eigen value associated with u^i. These eigen values are all positive. If all but one of the κ^i vanish identically the corresponding F_V is called an **elementary constitutive law**.

To simplify the notation let us assume $K = s_0$ and $W_1(j_0) = W(j_0)$.

If the distortions are very small then F_V can be linearized at j_0. To do so we introduce the linearization of F_V: Differentiating F_V at j_0 yields for all $h, l \in \mathcal{F}(V, I\!R^n)$

$$F_V(j_0 + h)(l) = F_V(j_0)(l) + \mathrm{d}F_V(j_0)(h)(l) + \text{ higher order terms } .$$

We write $\mathrm{d}F_V(j)(h, l)$ instead of $\mathrm{d}F_V(j)(h)(l)$.

Clearly $\mathrm{d}F_V$ splits into a symmetric and skew symmetric part $\mathrm{d}_s F_V$ and $\mathrm{d}_a F_V$, respectively. Evidently $2 \cdot \mathrm{d}_a F_V(h, l)$ is identical with the exterior differential of F_V at j.

Representing $\mathrm{d}_s F_V(j)$ via $\mathcal{G}_V$ yields the endomorphisms $\mathbf{b}(j)$ of $\mathcal{F}(V, I\!R^n)$. The eigen values of $\mathbf{b}(j)$ are called the **modes** of F_V or the modes of the medium. The totality of the modes is called the spectrum of the medium. If $F_V = \mathrm{d}L$ for some smooth map $L : W(j_0) \to I\!R$ then the modes are the eigen values of the Hessian $\mathrm{d}^2 L$ of L.

F_V at $j \in W(j_0)$ is said to satisfy **Hook's law** if

$$F_V(j + h)(h) = F_V(j)(h) + \mathrm{d}_s F_V(j)(h, h) \tag{4.8}$$

for all small distortions $h \in \mathcal{F}_0(V, I\!R^n)$ (cf. [L,L], [C,St]).
If $F_V(j) = 0$ for some $j \in \mathcal{M}$ we call j an **equilibrium configuration of the internal force density** or just an equilibrium configuration. If F_V satisfies Hook's law at this kind of configurations then

$$F_V(j + h)(h) = \mathrm{d}_s F_V(j)(h, h) \tag{4.9}$$

and $\mathrm{d}_a F_V = 0$. Not any virtual work admits equilibrium configurations of the above sort; e.g. $\mathrm{d}\mathcal{V}$, where $\mathcal{V}$ is the volume function on $E(M, I\!R^n)$ does not.
The following is now obvious:

Proposition 4.2

Let j_0 be an equilibrium configuration of internal force densities of a linearized constitutive law F_V satisfying a Hook law on $W(j_0)$. The force density $\Phi(j_0 + h)$ causing the work $F_V(j_0 + h)(h)$ for any small distortion $h \in \mathcal{F}(V, I\!R^n)$ satisfies

$$\Phi(j_0 + h) = \sum_{i=1}^{s_0} \nu^i \frac{\partial \kappa^i(j_0)}{\partial x_i} \cdot h_i \quad \textit{with } h_i = \mathcal{G}_V(h, u_i) \; . \tag{4.10}$$

$\frac{\partial \kappa^i(j_0)}{\partial \mathrm{x}_i}$ *are hence the "spring constants" with respect to the coordinate axis given by* $u_1, \ldots, u_K$ *on* $\mathcal{W}(j_0)$.

Let us pause the general discussion of the coefficients κ^i made so far and illustrate it at a special type of situation. At first we point out that these spring constants mentioned in proposition 4.2 have nothing to do with the spring constants along edges of the graph used in some models in solid state physics (cf. [C,St]).
Hook's law used to describe bond stretching is as follows: Let $F_V(j_0) = 0$. To each distortion h there is associated a potential energy, called pot (cf. [C,St]). Its quadratic approximation (cf. [C,St]) reads as

$$\mathrm{pot}(j_0 + h) = \frac{1}{2} \sum_{q,q_i} w_{\overline{q,q_i}} \left\langle \frac{j_0(q) - j_0(q_i)}{|j_0(q) - j_0(q_i)|_{\mathbb{R}^n}}, h(q) - h(q_i) \right\rangle^2 |\sigma(q)| \ .$$

$w_{\overline{q,q_i}}$ are the **spring constants** in the direction of the edge $\overline{q,q_i}$. The work $F_V(j+h)(h)$ caused by the distortion h is then

$$F_V(j+h)(h) = \mathrm{d}\mathrm{pot}(j_0 + h)(h) \tag{4.11}$$

and hence

$$F(j_0 + h)(h) = \sum_q \sum_{q_i} w_{\overline{q,q_i}} \left\langle \frac{j_0(q) - j_0(q_i)}{|j_0(q) - j_0(q_i)|_{\mathbb{R}^n}}, h(q) - h(q_i) \right\rangle^2 |\sigma_q| \ . \tag{4.12}$$

On the other hand

$$F_V(j+h)(h) = \mathcal{G}_V\big(\mathrm{d}\mathcal{H}_V(j_0)(h), h\big) \ .$$

In particular we have for each $r = 1, \ldots, s_0$

$$F_V(j + u_r)(u_r) = \frac{\partial \kappa^r(j_0)}{\partial \mathrm{x}_r} \tag{4.13}$$

and therefore

$$\frac{\partial \kappa^r(j_0)}{\partial \mathrm{x}_r} = \sum_q \sum_{q_i} w_{\overline{q,q_i}} \left\langle \frac{j_0(q) - j_0(q_i)}{|j_0(q) - j_0(q_i)|_{\mathbb{R}^n}}, u_r(q) - u_r(q_i) \right\rangle^2$$

or

$$\frac{\partial \kappa^r(j_0)}{\partial \mathrm{x}_r} = \sum_q \sum_{q_i} w_{\overline{q,q_i}} \cdot \iota_r^2 \ , \tag{4.14}$$

where

$$\iota_r := \left\langle \frac{j_0(q) - j_0(q_i)}{|j_0(q) - j_0(q_i)|_{\mathbb{R}^n}}, u_r(q) - u_r(q_i) \right\rangle \ .$$

5. Thermodynamical interpretation of the coefficients and the modes of F_V

As we learned in the last section any discrete medium on V is given by the collection $\{\kappa^i \mid i = 1, \ldots, s_0\}$ of the coefficients. These can be expressed in any thermodynamical equilibrium as follows:
The collection of equilibrium states in thermodynamics is given by $\mathcal{W}(j_0) \times I\!R$ (cf. [Str] and [B,St]). Call the projection of $\mathcal{W}(j_0) \times I\!R$ to $\mathcal{W}(j_0)$ by π. Then the following decomposition is supposed to hold:

$$\pi^* F_V = -dU + TdS \tag{5.1}$$

with $U, S, T : \mathcal{W}(j_0) \times I\!R \to I\!R$ the internal energy, the entropy and the absolute temperature, respectively. $x_1, \ldots, x_{s_0}, U$ are the coordinates on $W(j_0) \times I\!R$. The differentiation in (5.1) takes place on $W(j_0) \times I\!R$. Only the partial differentiation along $W(j_0)$ influences F_V, however. We omit π^* in (5.1) therefore if no confusion arises.
The free energy Fr is defined to be

$$\mathrm{Fr} := -U + TS\ . \tag{5.2}$$

This thermodynamical function will provide us below with a simple interpretation of our constitutive map $\mathcal{H}$ at constant temperature.

Suppose F_V admits in addition a splitting of the form (5.1) near $j \in W(j_0)$. The following equations are obvious

$$F_V = d\mathrm{Fr} - SdT = \sum_{i=1}^{s_0} \nu^i \kappa^i dx_i \tag{5.3}$$

$$d_s F_V = -d^2 U + \frac{1}{2} dT \vee dS + T \cdot d^2 S = \frac{1}{2} \sum_{i=1}^{s_0} \nu^i d\kappa^i \vee dx_i \tag{5.4}$$

as well as

$$d_a F_V = \frac{1}{2} dT \wedge dS = \frac{1}{2} \sum \nu^i d\kappa^i \wedge dx_i \tag{5.5}$$

and in particular

$$F_V(j) = d\mathrm{Fr}(j) \quad \text{if } dT(j) = 0\ . \tag{5.6}$$

Equation (5.1), (5.2), (5.3), (5.4), (4.6) and (4.7) yield a thermodynamic interpretation of the coefficients and the modes of F_V, stated in the following:

Theorem 5.1

On $W(j_0) \times I\!R$ the coefficients κ^i for $i = 1, \ldots, s_0$ of any constitutive law F_V are thermodynamically expressed by

$$\kappa^i = \frac{T}{\nu^i} \cdot \frac{\partial S}{\partial x_i} = \frac{T}{\nu^i} dS(u_i)\ , \tag{5.7}$$

where ∂ denotes the partial derivatives on $\mathcal{M} \times I\!R$. Moreover

$$\frac{1}{T} = \frac{\partial S}{\partial U} \tag{5.8}$$

holds as well. The functions Fr, S, T *and* $\mathbf{div}\, F$ *are related on* $W(j_0) \times I\!R$ *by*

$$2 \cdot \mathbf{div}\, F_V = \mathbf{\Delta}\mathrm{Fr} + (T\mathbf{\Delta}S - S\mathbf{\Delta}T) \,. \tag{5.9}$$

Here $\mathbf{div}$ *and* $\mathbf{\Delta}$ *are the divergence and Laplace operators formed with respect to* $\mathcal{G}_V$ *on* $\mathcal{F}_0(V, I\!R^n)$. *If* $\mathrm{d}T(j) = 0$ *then*

$$\kappa^i = \frac{1}{\nu^i}\frac{\partial \mathrm{Fr}\,(j)}{\partial \mathrm{x}_i} = \frac{1}{\nu_i}\mathrm{d}\mathrm{Fr}\,(j)(u_i) \qquad i = 1, \ldots, s_0 \tag{5.10}$$

and thus the constitutive map evaluated at j *reads as*

$$\widehat{\mathcal{H}}_V(j) = \sum_{i=1}^{s_0} \frac{1}{\nu^i}\frac{\partial \mathrm{Fr}\,(j)}{\partial \mathrm{x}_i} u_i \,; \tag{5.11}$$

the force density is hence

$$\Delta(j_0)\widehat{\mathcal{H}}_V(j) = \sum_{i=1}^{K} \frac{\partial \mathrm{Fr}\,(j)}{\partial \mathrm{x}_i} = \mathrm{Grad}_{\mathcal{G}_V} \mathrm{Fr}\,(j) \tag{5.12}$$

with $\mathrm{Grad\,Fr}$ *being the gradient of* Fr *with respect to* $\mathcal{G}_V$.

Proof: We only verify (5.9) for arbitrary $j \in W(j_0)$ since the other claims are immediate. Equation (5.2) implies

$$F_V(j)(u_i) = \mathrm{d}\mathrm{Fr}\,(j)(u_i) - S(j)\mathrm{d}T(j)(u_i)$$

and in turn

$$\mathrm{d}F_V(j)(u_i)(u_r) = \mathrm{d}^2\mathrm{Fr}\,(j)(u_i, u_r) - \mathrm{d}S(j)(u_i) \cdot \mathrm{d}T(j)(u_r) - S(j)\mathrm{d}^2T(j)(u_i, u_r) \,.$$

(5.7) on the other hand yields

$$\sum_{s=1}^{s_0} \nu^s \mathrm{d}\kappa^s(j)(u_r)\mathrm{d}\mathrm{x}_s(u_i) = \nu^r \cdot \mathrm{d}\kappa^r(j)(u_r) = \mathrm{d}T(j)(u_r)\mathrm{d}S(j)(u_i) + T(j)\mathrm{d}^2S(j)(u_r, u_i)$$

and thus

$$2 \cdot d_s F(j)(u_i)(u_r) = \mathrm{d}^2\mathrm{Fr}\,(j)(u_r)(u_i) + T(j)\mathrm{d}^2S(j)(u_r, u_i) - S(j)\mathrm{d}^2T(j)(u_r, u_i) \,.$$

Taking traces we find

$$2 \cdot \mathbf{div}\, F_V = \mathbf{\Delta}\mathrm{Fr} + (T\mathbf{\Delta}S - S\mathbf{\Delta}T) \,.$$

□

To understand $\mathrm{d}_s F_V$ and $\mathrm{d}\mathrm{Fr}$ from the point of view of Hodge theory we decompose $\widehat{\mathcal{H}}_V$ on a closed ball $K_{j_0} \subset W(j_0)$ centered about $j_0 \in E_0(V, I\!R^n)$ as follows:

$$\Phi_V(j) = \Delta_V\widehat{\mathcal{H}}_V = \mathrm{Grad}_{\mathcal{G}_V} L + \Phi_V^0(j) \qquad \forall j \in K_{j_0} \tag{5.13}$$

with the boundary condition

$$\mathrm{d}L(j)(n_{j_0}) = F_V(j)(n_{j_0}) \qquad \text{and} \qquad \langle Y(j)|\partial K_{j_0}, n_{j_0}\rangle = 0 \tag{5.14}$$

where $L : K_{j_0} \to \mathbb{R}^n$ is a smooth map and where n_{j_0} is the outward directed $\mathcal{G}_V$-unit normal of the sphere ∂K_{j_0}. This is done by solving the elliptic boundary problem

$$\operatorname{tr}_{\mathcal{G}_V} \mathrm{d}_s F = \mathbf{\Delta} L \tag{5.15}$$

with the boundary conditions mentioned in (5.14). Clearly L pulled back onto $W(j_0) \times \mathbb{R}$ is not independent of the variables in $W(j_0)$ as e.g. the coordinate U is. Solving

$$\Delta_V \widehat{\mathcal{H}} = \operatorname{Grad}_{\mathcal{G}_V} L \tag{5.16}$$

yields a constitutive map for $\mathrm{d}L$. We have shown:

Proposition 5.2

F_V on K_{j_0} splits uniquely into

$$F_V = \mathrm{d}L + \mathcal{G}_V(\Phi_V^0, \ldots) , \tag{5.17}$$

where $\mathrm{d}L$ and Φ_V^0 satisfy the boundary (5.14). Both $\mathrm{d}L$ and $\mathcal{G}_V(\Phi_V^0, \ldots)$ admit constitutive maps $\widehat{\mathcal{H}}_L$ and $\widehat{\mathcal{H}}_V^0$, respectively. If j_0 is an equilibrium configuration of internal force densities and F_V satisfies a Hook law on $W(j_0)$ then $F_V = \mathrm{d}L$ and hence $\mathrm{d}_s F_V = \mathrm{d}^2 L$ showing

$$F_V(j+h)(h) = \sum_{\nu}^{i} \frac{\partial \kappa^i(j)}{\partial \mathrm{x}_i} (\xi^i)^2$$

with $h \in \mathcal{F}_0^\infty(M, \mathbb{R}^n)$ and $h = \sum \xi^i \cdot u_i$.

The relation between the thermodynamic decomposition (5.1) and the Hodge one (5.16) is immediate: The equations (5.9) and (5.15) combined together yield immediately:

Corollary 5.3

The smooth real valued functions L, Fr, T and S on $W(j_0) \times \mathbb{R}^n$ are related by

$$\mathbf{\Delta}(\mathrm{Fr} - 2L) = (T\mathbf{\Delta}S - S\mathbf{\Delta}T) . \tag{5.18}$$

If T is kept constant near j then we can interpret the map L in (5.17) in proposition 5.2 via (5.6) and the system consisting of (5.13) and (5.14) immediately as follows.

Corollary 5.4

If T is constant on a closed ball centered about j_0 then

$$\mathrm{Fr} = L \tag{5.19}$$

on K_{j_0} up to an additive constant.

The above corollary motivates us to interpret L for a fixed $j \in K_{j_0}$ by means of statistical mechanics. The formalism we adopt here is the one presented by [B,St]. We will make constant use of the identification of $\mathcal{F}_0^\infty(M, \mathbb{R}^n)$ and $\mathcal{F}_0(V, \mathbb{R}^n)$, and this in fact not only for $\mathbb{R}^n$ being the ambient space of our embeddings, but also for any $\mathbb{R}^m$ with $m \geq 1$.

We quickly repeat this formalism adopted to our situation. At first we specify some $\mathbb{R}^m$ and a functional $\gamma \in (\mathbb{R}^m)^*$. (The formalism works also if $\mathbb{R}^n$ is replaced by an infinite dimensional vector space.) Let $J \in \mathcal{F}_0^\infty(K_{j_0} \times M, \mathbb{R}^m)$ be any observable. K_{j_0} is the set of auxiliary variables. The partition function $Z(\gamma, J)$ associated with γ and Z is defined by

$$Z(\gamma, J) := \int_M e^{-\gamma \cdot J} \mu(j_0) . \tag{5.20}$$

An equilibrium state is then

$$\rho_\gamma := \frac{1}{Z(\gamma, J)} e^{-\gamma \cdot J} . \tag{5.21}$$

The expectation value $E(J, \rho_\gamma)$ for J with respect to ρ_γ abbreviated by $\overline{J}$ is

$$\overline{J} := \int_M J \rho_\gamma^* \mu(j_0) . \tag{5.22}$$

The entropy $S(J, \rho_\gamma)$ reads as

$$S(J, \rho_\gamma) := -\int_M \rho_\gamma \log \rho_\gamma \, \mu(j_0) \tag{5.23}$$

and hence is expressed as

$$S(J, \rho_\gamma) = \log Z(J, \gamma) + \gamma \cdot \overline{J} . \tag{5.24}$$

All maps $J, \rho_\gamma, S(J, \rho_\gamma)$ and $Z(J, \gamma)$ depend smoothly on $j \in K_{j_0}$. (Any mass density ρ with mass $\mathbf{m}$ (cf. (1.13)) can be regarded as an equilibrium state, with $\gamma = \mathrm{tr}$ and $J = \log f$. The continuity equation follows from (5.24) above from the fact that the entropy of an equilibrium state has to be maximal.)

If now $\gamma := \frac{1}{T}$ with T the absolute temperature (which is a fixed parameter), $m = 1$ and $J = H$, an energy, then

$$T \log Z(J, \frac{1}{T}) = -U + TS = \mathrm{Fr} \tag{5.25}$$

with $U := E(H, \frac{1}{T})$. Let H depend smoothly on j. Hence U is smooth on K_{j_0}. We now vary j in a very small neighbourhood $\mathcal{W}'$ of j and observe that T, being a constant, does not depend on j. Therefore we have at j

$$T \mathrm{d} \log Z(J, \frac{1}{T})(j) = -\mathrm{d}U(j) + T \mathrm{d}S(j) . \tag{5.26}$$

Now we apply these considerations to our map Fr in (5.6). For simplicity we omit the variables J, γ and ρ_γ in Z and S if no confusion will arise. Since J depends on $j \in K_{j_0}$ it can be expressed by the coordinates $\mathrm{x}_1, \ldots, \mathrm{x}_{s_0}$.

Looking at (5.1), (5.6) and (5.19) we therefore obtain for our fixed j and constant T the description of the coefficients κ_L^i of $F_V = \mathrm{d}L$ where $i = 1, \ldots, s_0$ of the constitutive map $\widehat{\mathcal{H}}_{\mathrm{Fr}} = \widehat{\mathcal{H}}_L$:

Theorem 5.5

Let $j \in K_{j_0}$ be fixed and T kept constant in a small neighbourhood of j. Then with respect to the state $\rho_\gamma = \frac{1}{Z}e^{-\frac{1}{T}H}$ the virtual work $F_V(j)$ can be expressed as

$$F_V(j) = \mathrm{d}L = \sum_{i=1}^{s_0} \nu^i \kappa_L^i \mathrm{d}\mathrm{x}_i = T\mathrm{d}\log Z(j)\ , \tag{5.27}$$

with H an energy. At a fixed temperature T the coefficients $\kappa_L^i(j)$ for $i = 1, \ldots, s_0$ satisfy the equations

$$\kappa_L^i(j) = \frac{T}{\nu^i}\mathrm{d}\log Z(j)(u_i) = \frac{T}{\nu_i}\frac{\partial \log Z(j)}{\partial \mathrm{x}_i} = \frac{1}{\nu^i}\frac{\partial \mathrm{Fr}\,(j)}{\partial \mathrm{x}_i} \tag{5.28}$$

with Fr *the free energy. More explicitly and differently written the above formula may be stated as*

$$\kappa_L^i(j) = -\frac{T}{\nu^i}E(\frac{\partial H(j)}{\partial \mathrm{x}_i}, \rho_{\frac{1}{T}}) \tag{5.29}$$

with

$$E(\frac{\partial H}{\partial \mathrm{x}_i}, \rho_{\frac{1}{T}}) = \frac{\int_M \frac{\partial H}{\partial \mathrm{x}_i} e^{-\frac{1}{T}H}\, \mu(j_0)}{\int_M e^{-\frac{1}{T}H}\, \mu(j_0)} \qquad \forall i = 1, \ldots, s_0\ . \tag{5.30}$$

The constitutive map $\widehat{\mathcal{H}}_{\mathrm{Fr}} = \widehat{\mathcal{H}}_L$ in $\mathcal{F}_0(V, I\!R^n)$ of $\mathrm{dFr} = \mathrm{d}L = F_V$ evaluated at j is hence

$$\widehat{\mathcal{H}}_L(j) = \widehat{\mathcal{H}}_{\mathrm{Fr}}(j) = \sum_{i=1}^{s_0} \frac{T}{\nu^i}\frac{\partial \log Z(j)}{\partial \mathrm{x}_i} \cdot u_i\ . \tag{5.31}$$

The Hessian of the free energy is the sum of all

$$\nu^i \frac{\partial \kappa_L^i(j)}{\partial \mathrm{x}_i} = TE(\frac{\partial^2 H(j)}{\partial^2 \mathrm{x}_i}, \rho_{\frac{1}{T}}) = T\frac{\partial^2 \mathrm{Fr}\,(j)}{\partial^2 \mathrm{x}_i} = T\frac{\partial^2 \log Z}{\partial \mathrm{x}_i} \qquad i = 1, \ldots, s_0\ . \tag{5.32}$$

If j is an equilibrium configuration of internal force densities the coefficients $\kappa_L^i(j)$ vanish for all $i = 1, \ldots, s_0$.

Next we describe the modes of F at a constant temperature T in the light of corollary 5.4. Since $\mathrm{d}^2 L = \mathrm{d}_s F$ (cf. (5.6)) in a neighbourhood K_{j_0} we have

$$\begin{aligned} \mathrm{d}_s F(j)(h,k) &= \mathcal{G}_V\big(\mathrm{d}\Delta_V \widehat{\mathcal{H}}_L(j)(h), k\big) \\ &= \mathcal{G}_V\big(\Delta_V \mathrm{d}\widehat{\mathcal{H}}_L(j)(h), k\big)\ . \end{aligned} \tag{5.33}$$

On $\mathcal{F}_0^\infty(M, I\!R^n)$ the quadratic form $\mathcal{G}_V(\Delta_V \ldots, \ldots)$ is a scalar product called $\mathcal{G}_V^{\Delta_V}$. (The eigen values of Δ_V are all positive on this space.) We hence find a $\mathcal{G}_V^{\Delta_V}$-orthonormed basis

$v_1, \ldots, v_{s_0}$ in which the endomorphism $\mathrm{d}\widehat{\mathcal{H}}_L(j)$ of $\mathcal{F}_0^\infty(M, I\!R^n)$ diagonalizes. Let us call the respective eigen values by $\sigma_1, \ldots, \sigma_{s_0}$. then

$$\mathcal{G}_V^{\Delta_V}\left(\mathrm{d}\widehat{\mathcal{H}}_L(j)(v_j), v_r\right) = \sigma_i \delta_{i,r} = \sigma_i \mathcal{G}_V\left(\Delta_V v_i, v_r\right) . \tag{5.34}$$

If hence $\sigma_i \neq 0$ then v_i is an eigen vector of Δ_V of $\mathcal{G}_V$-length $(\nu^r)^{-\frac{1}{2}}$. With the help of (5.10) and theorem 5.6 we then may immediately formulate the description of the modes of F_V at constant temperature as follows:

Theorem 5.6

Let j be an equilibrium configuration of an internal force density. The modes of $\mathrm{d}_s F(j)$ at constant temperature are the eigen values $\sigma_1, \ldots, \sigma_{s_0}$ of $\mathrm{d}^2 L(j) = \mathrm{d}^2 \mathrm{Fr}$. If $\sigma_i \neq 0$ then the eigen vector of σ_i is an eigenvector u_r of Δ_V. Hence

$$\sigma_i = \mathcal{G}_V\left(\Delta_V \mathrm{d}\widehat{\mathcal{H}}_L(j)(u_r) u_r, u_r\right) = \frac{1}{\nu^r} \frac{\partial \kappa_L^r(j)}{\partial \mathrm{x}_r} \tag{5.35}$$

and hence

$$\sigma_i = \frac{1}{\nu^i} \frac{\partial \kappa_L^i(j)}{\partial \mathrm{x}_i} = \frac{T}{(\nu^i)^2} \frac{\partial^2 \log Z}{\partial^2 \mathrm{x}_i} \tag{5.36}$$

after a renumbering of the eigen values of $\mathrm{d}^2 L$.
If $\boldsymbol{\Delta}$ denotes the Laplacian on K_{j_0} then

$$\sum_{i=1}^{s_0} \frac{\nu^i}{T} \frac{\partial \kappa_L^i}{\partial \mathrm{x}_i} = \sum_{i=1}^{s_0} \frac{(\nu^i)^2}{T} \sigma^i = (\boldsymbol{\Delta} \log Z)(j) . \tag{5.37}$$

Given the graph V and its geometry the theorem above allows to construct (mathematically) out of the spectrum $\sigma_1, \ldots, \sigma_{s_0}$ a linear nearest neighbour interaction model (i.e. satisfying Hook's law) at constant temperature causing the same spectrum $\sigma_1, \ldots, \sigma_{s_0}$. This is done as follows:
Let the configuration of the medium in $I\!R^n$ be called by j_0. We then are in then realm of sec.3. Moreover we assume that j_0 is an equilibrium configuration of internal force densities. We set in accordance with (4.1) in proposition 4.2 for any $h \in \mathcal{F}(V, I\!R^n)$ the virtual work it causes as

$$F_V(h) = \mathcal{G}_V\left(\Phi(j_0 + h), h\right) = \sum (\nu^i)^2 \sigma^i h_i^2 ,$$

where $h = \sum h_i u_i$. The medium hence can be characterized by the constitutive map

$$\mathcal{H}_V = \sum_{i=1}^{s_0} (\nu^i)^2 \sigma^i u_i h_i .$$

Clearly $F_V(u_i) = (\nu^i)^2 \sigma_i$.

Combining corollary 5.4 with theorem 5.6, we immediately obtain

Theorem 5.7

At constant temperature the spectrum of a discrete medium at an equilibrium configuration of internal force densities is entirely determined by $\mathbb{d}^2 L$, the derivative of the exact part (with Neumann datum e.g.) $\mathbb{d}L$ of the virtual work.

Finally let j be an equilibrium configuration of internal force densities and assume moreover that F_V is linear and satisfies a Hook law on K_{j_0}. In treating this situation we may need to generalize the setting of statistical mechanics somewhat. The variables on which the energy H shall depend are j, a tangential vector to it, q and the edges, geodesic segments connecting q with any of its neighbours q_i. Obviously this generalization is carried out in a straight forward manner.

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