

Global Dynamics of Media with Microstructure

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1. INTRODUCTION

As is well-known, a differential geometric model of classical continuum mechanics is a medium \mathcal{B} , a m -dimensional differentiable manifold moving and deforming in the ambient space \mathcal{C} , a n -dimensional differentiable manifold ($m \leq n$). We note that the medium \mathcal{B} consists of material points without internal degrees of freedom. The corresponding configuration space is $\mathcal{E}(\mathcal{B}, \mathcal{C})$, i.e. the space of smooth embeddings from \mathcal{B} into \mathcal{C} ; the dynamics of the motion is given by the choice of an appropriate Lagrangian (cf. [10, 19, 20] and references therein).

However, there exists a large class of continua, whose constituting elements are material points with internal degrees of freedom, the so-called media with microstructure. For instance liquid crystals are fluids made up of particles which might be rodlike in shape and rather rigid in behaviour, so that locally a preferred direction is in evidence.

In order to understand the behaviour of a liquid crystal, let us consider at first a dumbbell-shaped particle, consisting of two masses m_1 and m_2 that are located near to each other (cf. [21]).

If the masses m_1 and m_2 are situated at \vec{x}_1 and \vec{x}_2 respectively then the linear momentum \vec{p} of the particle is given by

$$\vec{p} = m_1 \dot{\vec{x}}_1 + m_2 \dot{\vec{x}}_2 = m \dot{\vec{x}},$$

where $m = m_1 + m_2$ is the mass of the particle and \vec{x} is the center of mass.

Introducing a vector \vec{d}

$$\vec{d} = \frac{\sqrt{m_1 m_2}}{m} (\vec{x}_1 - \vec{x}_2),$$

we obtain

$$\vec{x}_1 = \vec{x} + \frac{m_2}{\sqrt{m_1 m_2}} \vec{d}, \quad \vec{x}_2 = \vec{x} - \frac{m_1}{\sqrt{m_1 m_2}} \vec{d}. \quad (1)$$

Hence the angular momentum \vec{k} and the kinetic energy \mathcal{T} of the particle are given respectively by

$$\begin{aligned} \vec{k} &= \vec{x}_1 \times m_1 \dot{\vec{x}}_1 + \vec{x}_2 \times m_2 \dot{\vec{x}}_2 = m(\vec{x} \times \dot{\vec{x}} + \vec{d} \times \dot{\vec{d}}), \\ \mathcal{T} &= \frac{1}{2}(m_1 \dot{\vec{x}}_1^2 + m_2 \dot{\vec{x}}_2^2) = \frac{1}{2}m(\dot{\vec{x}}^2 + \dot{\vec{d}}^2). \end{aligned}$$

Thus the dumbbell-shaped particle can be considered as a particle with microstructure, the microstructure being introduced by a preferred direction of the particle.

The above discrete model can be generalized to obtain a simple model of an anisotropic fluid, i.e. a fluid in which each particle has a preferred direction. The theory of anisotropic fluids (cf. [11]), is an outcome of an effort to explain the behaviour of liquid crystals, and, more generally, the behaviour of fluids with microstructure.

If we assume now that the medium \mathcal{B} has a microstructure, then the above mentioned differential geometric description is no longer valid. Indeed, a medium \mathcal{B} with microstructure as considered here is described by a principal bundle $\mathcal{P} \xrightarrow{\pi_{\mathcal{P}}} \mathcal{B}$ with a Lie group G as a structure group. Accordingly, the ambient space \mathcal{C} is a principal bundle $\mathcal{Q} \xrightarrow{\pi_{\mathcal{Q}}} \mathcal{C}$ with a Lie group K as structure group. The configuration space is then given by $\mathcal{E}(\mathcal{P}, \mathcal{Q})$, i.e. a space of smooth embeddings $\mathcal{P} \rightarrow \mathcal{Q}$ respecting the structure groups. In the following we shall characterize the geometric structure of $\mathcal{E}(\mathcal{P}, \mathcal{Q})$ and then we shall construct an appropriate Lagrangian.

2. THE GEOMETRIC STRUCTURE OF THE SPACE OF CONFIGURATIONS

For the sake of completeness let us remind at first that a homomorphism of a principal bundle $(\mathcal{P}, \mathcal{B}, G, \pi_{\mathcal{P}})$ into another one $(\mathcal{Q}, \mathcal{C}, K, \pi_{\mathcal{Q}})$ consists of:

- i) a differentiable, fibre preserving mapping $\tilde{\Phi} : \mathcal{P} \rightarrow \mathcal{Q}$ together with

- ii) a Lie group homomorphism $\lambda : G \longrightarrow K$ such that $\tilde{\Phi}$ satisfies the G -equivariance property

$$\tilde{\Phi}(p \cdot g) = \tilde{\Phi}(p) \cdot \lambda(g) \quad \forall p \in \mathcal{P}, g \in G.$$

Hence $\tilde{\Phi}$ maps fibres into fibres and thus induces a differentiable map $\Phi : \mathcal{B} \longrightarrow \mathcal{C}$ via $\Phi(b) := \pi_{\mathcal{Q}}(\tilde{\Phi}(p_b))$, where $p_b \in \mathcal{P}$ is an arbitrary point over $b \in \mathcal{B}$.

A homomorphism $\tilde{\Phi} : \mathcal{P} \longrightarrow \mathcal{Q}$ is called an embedding, if $\Phi : \mathcal{B} \longrightarrow \mathcal{C}$ is an embedding and $\lambda : G \longrightarrow K$ is an injection. In the following let $G \subset K$ and λ be the inclusion, for simplicity.

A map $\tilde{k} : \mathcal{P} \longrightarrow K$ is called a G -gauge transformation of \mathcal{P} , if it satisfies the relation

$$\tilde{k}(p \cdot g) = g^{-1} \cdot \tilde{k}(p) \cdot g \quad \forall p \in \mathcal{P}, g \in G.$$

We denote by $\mathcal{G}_{\mathcal{P}}^G$ the set of all G -gauge transformations of \mathcal{P} . As shown in [5] the geometric structure of the space of configurations $\mathcal{E}(\mathcal{P}, \mathcal{Q})$ is given by

THEOREM 2.1. *$\mathcal{E}(\mathcal{P}, \mathcal{Q})$ is a Fréchet manifold and $\mathcal{E}(\mathcal{P}, \mathcal{Q})$ is a $\mathcal{G}_{\mathcal{P}}^G$ -principal bundle over an open connected subspace O of the Fréchet manifold $\mathcal{E}(\mathcal{B}, \mathcal{C})$.*

3. THE DYNAMICS OF THE MEDIUM \mathcal{B} WITH MICROSTRUCTURE

Let $O = \mathcal{E}(\mathcal{P}, \mathcal{Q})$ for simplicity again. The next step is the construction of a Lagrangian \mathcal{L} , which is supposed to be $\mathcal{G}_{\mathcal{P}}^G$ -equivariant. We set $\mathcal{L} = \mathcal{T} - \mathcal{V}$, where the kinetic energy \mathcal{T} is determined by a metric on $\mathcal{E}(\mathcal{P}, \mathcal{Q})$, on which $\mathcal{G}_{\mathcal{P}}^G$ acts by isometries, and where the potential \mathcal{V} is equivariant, which hence can be considered as a function on $\mathcal{E}(\mathcal{B}, \mathcal{C})$. In order to construct the kinetic energy \mathcal{T} at $\tilde{\Phi} \in \mathcal{E}(\mathcal{P}, \mathcal{Q})$, we need at first a description of $T_{\tilde{\Phi}}\mathcal{E}(\mathcal{P}, \mathcal{Q})$ and a metric on it. Since the lift $L_{\tilde{\Phi}}$ is equivariant we get (cf. [5])

PROPOSITION 3.1.

$$T_{\tilde{\Phi}}\mathcal{E}(\mathcal{P}, \mathcal{Q}) = \{L_{\tilde{\Phi}} : \mathcal{P} \longrightarrow T\mathcal{Q} \mid L_{\tilde{\Phi}}R_g = TR_gL_{\tilde{\Phi}} \text{ and } \tau_{\mathcal{Q}}L_{\tilde{\Phi}} = \tilde{\Phi}\}$$

with $\tau_{\mathcal{Q}} : T\mathcal{Q} \longrightarrow \mathcal{Q}$ the canonical projection.

Here we denote by R_g the right action of G on \mathcal{P} . Next, we construct a metric on \mathcal{Q} . To this end we take a principal connection on the principal bundle $\mathcal{Q} \xrightarrow{\pi_{\mathcal{Q}}} \mathcal{C} \cong \mathcal{Q}/K$ with connection form $\alpha : T\mathcal{Q} \longrightarrow \mathcal{K}$, where \mathcal{K} is the Lie algebra of K . This means that α is a \mathcal{K} -valued one-form such that

- (i) $\alpha(Z_\xi(q)) = \xi \quad \forall \xi \in \mathcal{K}, q \in \mathcal{Q}$ and
- (ii) $\alpha(T_q R_k(v_q)) = \text{Ad}_{k^{-1}} \alpha(v_q) \quad \forall v_q \in T_q \mathcal{Q}, k \in K,$

where R_k denotes the right action of K on \mathcal{Q} , Ad denotes the adjoint action of K on \mathcal{K} and Z_ξ is the fundamental vector field defined by $\xi \in \mathcal{K}$. At each point $q \in \mathcal{Q}$ we have the decomposition $T_q \mathcal{Q} = \text{Hor}_q \oplus \text{Ver}_q$, where $\text{Hor}_q = \{v_q \in T_q \mathcal{Q} \mid \alpha(v_q) = 0\}$ and $\text{Ver}_q = \ker T_q \pi_{\mathcal{Q}}$ are respectively the horizontal space of the connection and the vertical space, i.e. the tangent space to the fibre q belongs to. Hence

$$v_q = Z_h(q) + \text{Hor}_q v_q,$$

where $v_q \in T_q \mathcal{Q}$ and Z_h is the fundamental vector field determined by $h \in \mathcal{K}$.

We define a metric on \mathcal{Q} via

$$m_{\mathcal{Q}}(v_q^1, v_q^2) = m_K(h_1, h_2) + m_{\mathcal{C}}(T_q \pi_{\mathcal{Q}}(v_q^1), T_q \pi_{\mathcal{Q}}(v_q^2)),$$

where m_K is a biinvariant metric on K and $m_{\mathcal{C}}$ is the Riemannian metric on \mathcal{C} . This yields the metric on $\mathcal{E}(\mathcal{P}, \mathcal{Q})$ given by

$$m_{\mathcal{E}}(\tilde{\Phi})(L_1, L_2) := \int_{\mathcal{B}} \varrho(\tilde{\Phi}) \cdot m_{\mathcal{Q}}(L_1, L_2) \Phi^* \mu.$$

Here $m_{\mathcal{Q}}(L_1, L_2)$ factors to \mathcal{B} , due to the $\mathcal{G}_{\mathcal{P}}^G$ -invariance, $\varrho(\tilde{\Phi})$ is a $\mathcal{G}_{\mathcal{P}}^G$ -invariant density, assumed to obey a continuity equation and μ is a volume form on \mathcal{C} .

To construct a dynamics for the medium \mathcal{B} with microstructure we choose a smooth potential $\mathcal{V} : \mathcal{E}(\mathcal{B}, \mathcal{C}) \rightarrow \mathbb{R}$. The Lagrangian \mathcal{L} has then the form $\mathcal{L} = \mathcal{T} - \mathcal{V}$, where $\mathcal{T}(L) = \frac{1}{2} \cdot m_{\mathcal{E}}(L, L)$ for every $L \in T\mathcal{E}(\mathcal{P}, \mathcal{Q})$.

4. EXAMPLES

A) COSSERAT MEDIA. By a Cosserat medium we mean a three-dimensional continuum of which to each point three linearly independent tangent vectors (the directors) are attached (cf. [8], [9], and [22]). The stored energy function W depends not only on the gradient deformation of the underlying body but also on how the directors are deformed. Therefore, a geometrical model for a Cosserat medium \mathcal{B} is just the linear frame bundle $\mathcal{F}\mathbb{R}^3$.

For simplicity, we take the Euclidean metric on \mathbb{R}^3 , and the induced metric on $\mathcal{F}\mathbb{R}^3$ defined by using the flat connection defined by the trivialization $\mathcal{F}\mathbb{R}^3 \cong \mathbb{R}^3 \times \text{Gl}(3, \mathbb{R})$.

If we take fibred coordinates $(\xi^\alpha, \Xi_\beta^\alpha)$ in \mathcal{FB} and (x^i, X_j^i) in \mathcal{FR}^3 , $1 \leq \alpha, \beta, i, j \leq 3$, we have $\mathcal{T} = \frac{1}{2} \cdot \varrho(\xi^\alpha) \dot{x}^2 + \frac{1}{2} \cdot \varrho(\Xi_\beta^\alpha) \dot{X}^2$ and $W = W(d_a^i, d_{a,\alpha}^i, \xi^\alpha)$, where $L_{\tilde{\Phi}} = \dot{x}^i \frac{\partial}{\partial x^i} + \dot{X}_j^i \frac{\partial}{\partial X_j^i}$ and d_1, d_2, d_3 are the directors obtained from the canonical basis of \mathbb{R}^3 by the isomorphism $\tilde{\Phi} : \mathcal{FB} \rightarrow \mathcal{FR}^3$. Here we assume that (x^i) are the Euclidean coordinates in \mathbb{R}^3 . The potential \mathcal{V} is assumed to be obtained from the stored energy W as follows:

$$\mathcal{V}(\tilde{\Phi}) = \int_{\mathcal{FB}} (W \circ j^1 \tilde{\Phi}) \Phi^* \mu.$$

The corresponding field equations are (cf. [22]):

$$\varrho(\xi) \ddot{x}^i = F_i + \frac{\partial}{\partial \xi^\alpha} \left(\frac{\partial W}{\partial x_{,\alpha}^i} \right) \quad \text{and} \quad \varrho(\Xi) \ddot{X}_a^i = G_i^a + \frac{\partial}{\partial \xi^\alpha} \left(\frac{\partial W}{\partial d_{a,\alpha}^i} \right) + \frac{\partial W}{\partial d_a^i},$$

where F_i and G_i^α are some external forces.

B) A GEOMETRICAL TYPE OF MICROSTRUCTURE. Here we will exhibit the presence of a geometric type of a microstructure associated with a stress form, naturally appearing in a global treatment of continuum mechanics (cf. [2] and references therein).

A stress form of a body \mathcal{B} is a smooth map

$$\alpha : \mathcal{E}(\mathcal{B}, \mathbb{R}^3) \longrightarrow A^1(\mathcal{B}, \mathbb{R}^3)$$

with values in the space of all smooth \mathbb{R}^3 -valued one-forms of the body \mathcal{B} .

Given an embedding $\Phi \in \mathcal{E}(\mathcal{B}, \mathbb{R}^3)$, any $\gamma \in A^1(\mathcal{B}, \mathbb{R}^3)$ can be splitted into

$$\gamma = c_\gamma \cdot d\Phi + d\Phi \cdot (C_\gamma + B_\gamma), \quad (2)$$

(cf. [2]), where $d\Phi : \mathcal{B} \rightarrow \mathbb{R}^3$ is the principal part of the tangent map $T\Phi : \mathcal{B} \rightarrow T\mathbb{R}^3$ and the coefficients c_γ, C_γ and B_γ are as follows:

- a) $c_\gamma : \mathcal{B} \rightarrow \text{End } \mathbb{R}^3$ assigns to each $b \in \mathcal{B}$ a skew map, mapping each $T_b \mathcal{B}$ into its normal space \mathcal{N}_b and vice versa, i.e. an infinitesimal Gauss map
- b) $C_\gamma \in \text{End } T\mathcal{B}$ is skew-adjoint with respect to $\Phi^* \langle, \rangle$,

and

- c) $B_\gamma \in \text{End } T\mathcal{B}$ is selfadjoint with respect to $\Phi^* \langle, \rangle$,

$\Phi^* \langle, \rangle$ being the pull back of \langle, \rangle . Thus (2) formulated pointwise reads for each tangent vector $v_b \in T_b \mathcal{B}$ at any $b \in \mathcal{B}$

$$\gamma(v_b) = c_\gamma(b)(d\Phi(v_b)) + d\Phi(C_\gamma(b)(v_b) + B_\gamma(v_b)).$$

Indeed, $c_\gamma(b)(d\Phi(v_b))$ is the normal part of $\gamma(v_b)$, and $C_\gamma(b)(v_b)$ and $B_\gamma(v_b)$ are its skew and symmetric parts, respectively.

Notice that $c_\gamma = 0$ provided $\dim \mathcal{B} = 3$. Moreover C_γ applied to $T_b \mathcal{B}$ is an infinitesimal rotation of it.

The virtual work $\mathcal{A}(\Phi)(dh)$ associated with a stress form $\alpha(\Phi)$ is defined by

$$\mathcal{A}(\Phi)(dh) = \int_{\mathcal{B}} \alpha(\Phi) \cdot dh \Phi^* \mu \quad \forall h \in C^\infty(\mathcal{B}, \mathbb{R}^3),$$

where the density $\alpha(\Phi) \cdot dh$ is given by

$$\alpha(\Phi) \cdot dh := -\frac{1}{2} \cdot \text{tr } c_{\alpha(\Phi)} \cdot c_{dh} - \text{tr } C_{\alpha(\Phi)} \cdot C_{dh} + \text{tr } B_{\alpha(\Phi)} \cdot B_{dh} \quad (3)$$

the trace being evaluated pointwise.

The term $\text{tr } B_{\alpha(\Phi)} \cdot B_{dh}$ in the virtual work density (3) can be interpreted as follows: $B_{dh} \in \text{End } T\mathcal{B}$ is the deformation tensor in operator form, i.e.

$$\langle d\Phi(v_b), d\Phi(B_{dh}(w_b)) \rangle = \langle d\Phi(v_b), dh(w_b) \rangle \quad \forall v_b, w_b \in T_b \mathcal{B} \text{ and } \forall b \in \mathcal{B}.$$

Notice that

$$\mathcal{W}^{sym}(\Phi, h) := \text{tr } \mathcal{B}_{\alpha(\Phi)} \cdot B_{dh}$$

is the work density the deformation tensor causes against the symmetric part of the constitutive entity $\alpha(\Phi)$. Clearly, $\mathcal{B}_{\alpha(\Phi)}$ is the symmetric stress tensor in operator form, here assumed to depend on the embedding Φ . Hence $\mathcal{W}^{sym}(\Phi, h)$ is usually called the stored energy density (cf. [21]) caused by the distortion dh .

The terms on the right hand side of (3) associated with the skew operators will be interpreted in terms of a special type of microstructure to be set up as follows.

First of all let $\Phi_0 \in E(\mathcal{B}, \mathbb{R}^3)$ be fixed. The principal bundle $Q \rightarrow \mathcal{B}$ shall be the \langle, \rangle -orthonormal frame bundle and $\mathcal{P} \rightarrow \mathcal{B}$ the bundle of $\Phi_0^* \langle, \rangle$ -orthogonal frames of \mathcal{B} , an $SO(2)$ or an $SO(3)$ principal bundle according as to whether $\dim \mathcal{B} = 2$ or $\dim \mathcal{B} = 3$. Given $\Phi \in \mathcal{E}(\mathcal{B}, \mathbb{R}^3)$ we will construct $\tilde{\Phi} : \mathcal{P} \rightarrow Q$, next. At first, we observe that

$$d\Phi = \Psi \cdot d\Phi_0 \cdot f, \quad (4)$$

where $\Psi \in C^\infty(\mathcal{B}, \text{SO}(3))$ and $f \in \text{End } TM$ being an isomorphism, positive definite with respect to $\Phi_0^* \langle, \rangle$. Equation (4) reads for each $v_b \in T_b \mathcal{B}$ as

$$d\Phi(v_b) = \Psi(b) \left(d\Phi_0(f(v_b)) \right) \quad \forall b \in \mathcal{B}.$$

Then $\tilde{\Phi}$ is defined by

$$\tilde{\Phi}(p_b) = \left(\Psi(b) \left(d\Phi_0(f^{-1}(p_b)) \right), \Psi(b)(\tilde{\mathcal{N}}_{\Phi(b)}) \right) \quad \forall p_b \in \mathcal{P}_b \text{ and } \forall b \in \mathcal{B}. \quad (5)$$

Here $\tilde{\mathcal{N}}_{\Phi(b)}$ is the outward directed unit normal to $T_b \Phi_0(T_b \mathcal{B})$ in case $\dim \mathcal{B} = 2$; it is the axis of rotations in $T_b \Phi(T_b \mathcal{B})$. Since $Q = \mathbb{R}^3 \times \text{SO}(3)$ we may identify the right hand side of (5) with $\Psi : \mathcal{B} \rightarrow \text{SO}(3)$.

Thus a tangent vector to $\tilde{\Phi}$ is given by a tangent vector h to Ψ and hence is of the form

$$\tilde{h} : \mathcal{B} \rightarrow \text{so}(3)$$

with

$$\tilde{h}(b) = \frac{1}{\sqrt{2}} \cdot c_h(b) + C_h(b) \quad \forall b \in \mathcal{B}.$$

(c_h describes the infinitesimal change of the rotation axis of tangent planes if $\dim \mathcal{B} = 2$).

Hence

$$\mathcal{A}_{sk}(\tilde{\Phi})(\tilde{h}) = - \int_{\mathcal{B}} \left(\text{tr} \frac{1}{\sqrt{2}} \cdot c_{\alpha(\Phi)} \cdot \frac{1}{\sqrt{2}} \cdot c_{dh} + \text{tr} C_{\alpha(\Phi)} \cdot C_{dh} \right) \Phi^* \mu,$$

extended $\mathcal{G}_{\mathcal{P}}^{SO(2)}$ -equivariantly coincides with $\mathcal{A}_{sk}(\tilde{\Phi})(\tilde{h})$. Moreover, $\mathcal{A}_{sk}(\tilde{\Phi})(\tilde{h})$ added to $\int_{\mathcal{B}} \mathcal{W}^{sym}(\Phi, h) \Phi^* \mu$ is $\mathcal{A}(\Phi)(dh)$.

In case $\dim \mathcal{B} = 3$, only $C_{\alpha(\Phi)}$ is present in the decomposition of $\alpha(\Phi)$. This means that the symmetric stress tensor $B_{\alpha(\Phi)}$ (written in operator form) has to be complemented by $C_{\alpha(\Phi)}$ to take care of the microstructure $\mathcal{P} \rightarrow \mathcal{B}$. The energy density $\mathcal{W}^{sk}(\Phi, dh)$ produced by the distortion dh is thus

$$\mathcal{W}^{sk}(\Phi, dh) = - \left(\frac{1}{2} \cdot \text{tr} c_{\alpha(\Phi)} \cdot c_{dh} + \text{tr} C_{\alpha(\Phi)} \cdot C_{dh} \right)$$

Notice that in case of $\dim \mathcal{B} = 3$ the stress tensor $B_{\alpha(\Phi)} + C_{\alpha(\Phi)}$ (in operator form) of the medium describing both elasticity and the geometric microstructure is not symmetric.

The Lagrangian is hence

$$L = \mathcal{T} - (\mathcal{W}^{sym} + \mathcal{W}^{sk}).$$

APPENDIX A: INFINITE DIMENSIONAL LAGRANGIAN SYSTEMS
WITH NONHOLONOMIC CONSTRAINTS

In this appendix we first recall the Lagrangian formalism for mechanical systems in the context of infinite dimensional manifolds. A symplectic framework for nonholonomic dynamics is also given. As we will show the presence of nonholonomic constraints is very frequent in continuum mechanics.

A.1. INFINITE DIMENSIONAL LAGRANGIAN SYSTEMS. Let Q be a C^∞ Banach manifold modelled on a Banach space \mathbb{E} . We denote by TQ and T^*Q the tangent and cotangent bundles of Q , respectively, with canonical projections $\tau_Q : TQ \rightarrow Q$ and $\pi_Q : T^*Q \rightarrow Q$.

If U is an open set of Q and $\phi : U \rightarrow \phi(U)$ is a chart for Q , then

$$T\phi : \tau_Q^{-1}(U) \rightarrow \phi(U) \times \mathbb{E}, \quad T^*\phi : \pi_Q^{-1}(U) \rightarrow \phi(U) \times \mathbb{E}^*$$

are local trivializations for TQ and T^*Q . Thus, a point $x \in Q$ admits a local representation as q with $q \in \mathbb{E}$, and a tangent vector X (resp. covector α) at x admits a representation (q, v) (resp. (q, p)) where $q, v \in \mathbb{E}$ and $p \in \mathbb{E}^*$.

We also can induce local trivializations for TTQ and T^*TQ as follows:

$$TT\phi : \tau_{TQ}^{-1}(TU) \rightarrow \phi(U) \times \mathbb{E} \times \mathbb{E} \times \mathbb{E},$$

$$T^*T\phi : \pi_{T^*Q}^{-1}(TU) \rightarrow \phi(U) \times \mathbb{E} \times \mathbb{E}^* \times \mathbb{E}^*,$$

such that we obtain the following local representations:

$$\tilde{X} = (q, v, a, b) \in T_X(TQ), \quad \tilde{\alpha} = (q, v, \tilde{a}, \tilde{b}) \in T_X^*(TQ).$$

There are two geometrical ingredients which characterize the tangent bundle TQ (cf. [16] and [18]):

- the Liouville vector field $\Delta : TQ \rightarrow TTQ$; and
- the canonical vertical endomorphism $S : TTQ \rightarrow TTQ$ (also called canonical almost tangent structure).

The Liouville vector field Δ is the infinitesimal generator of the global 1-parameter group of dilations in TQ , say, $\Phi_t(X) = e^t X$, $\forall X \in TQ$, $\forall t \in \mathbb{R}$.

The canonical vertical endomorphism S is defined by $S(\tilde{X}) = (T\tau_Q(\tilde{X}))^v$, where $\tilde{X} \in T_X(TQ)$, and $(T\tau_Q(\tilde{X}))^v$ is the vertical lift of $T\tau_Q(\tilde{X})$ to $T_X(TQ)$.

In local trivializations, we have

$$\Delta(q, v) = (q, v, 0, v), \quad S(q, v, a, b) = (q, v, 0, a).$$

We will denote by S^* the adjoint operator of S , that is, $S^*(\tilde{\alpha})(\tilde{X}_1, \dots, \tilde{X}_r) = \tilde{\alpha}(S(\tilde{X}_1), \dots, S(\tilde{X}_r))$, for any r -form $\tilde{\alpha}$ on TQ . In local trivializations we have $S^*(q, v, \tilde{a}, \tilde{b}) = (q, v, \tilde{b}, 0)$.

The vector fields appearing in Lagrangian mechanics are second order differential equations.

DEFINITION 4.1. A vector field Γ on TQ is said to be a second order differential equation (SODE for brevity) if $S(\Gamma) = \Delta$.

Therefore, a SODE Γ admits a local representation as follows: $\Gamma(q, v) = (q, v, v, \gamma(q, v))$. A curve $\sigma : \mathbb{R} \rightarrow Q$ is called a solution of Γ if its tangent curve $\dot{\sigma} : \mathbb{R} \rightarrow TQ$ is an integral curve of Γ . If $\sigma(t) = (q(t))$, we have that σ is a solution of Γ if and only if

$$\left. \begin{aligned} \dot{q}(t) &= v \\ \ddot{q}(t) &= \gamma(q, \dot{q}) \end{aligned} \right\}$$

In addition, all the integral curves of Γ are of this form.

Let $\mathcal{L} : TQ \rightarrow \mathbb{R}$ be a Lagrangian function. We construct:

- the energy $E_{\mathcal{L}} = \Delta(\mathcal{L}) - \mathcal{L}$;
- the Poincaré-Cartan 1-form $\alpha_{\mathcal{L}} = S^*(d\mathcal{L})$, and
- the Poincaré-Cartan 2-form $\omega_{\mathcal{L}} = -d\alpha_{\mathcal{L}}$.

A direct computation shows that $\omega_{\mathcal{L}}$ is locally given by (cf. [1] and [12])

$$\begin{aligned} \omega_{\mathcal{L}}(q, v)((a, b), (\bar{a}, \bar{b})) &= D_1 D_2 \mathcal{L}(q, v) \cdot \bar{a} \cdot a - D_1 D_2 \mathcal{L}(q, v) \cdot a \cdot \bar{a} \\ &\quad + D_2 D_2 \mathcal{L}(q, v) \cdot \bar{b} \cdot a - D_2 D_2 \mathcal{L}(q, v) \cdot b \cdot \bar{a}, \end{aligned} \tag{6}$$

where D_1 (resp. D_2) denotes the derivative on the base (resp. along the fibre).

In general, $\omega_{\mathcal{L}}$ is only a weak symplectic form. Therefore, we introduce the following definition, which coincides with the usual one in the finite dimensional setting.

DEFINITION 4.2. A Lagrangian function $\mathcal{L} : TQ \rightarrow \mathbb{R}$ is said to be regular if ω_L is a strong symplectic form on TQ .

If \mathcal{L} is regular we have the symplectic isomorphisms $\flat_{\mathcal{L}} : TTQ \longrightarrow T^*TQ$ and $\sharp_{\mathcal{L}} : T^*TQ \longrightarrow TTQ$ defined by

$$\flat_{\mathcal{L}}(\tilde{Y}) = i_{\tilde{Y}} \omega_{\mathcal{L}}, \text{ respectively, } \sharp_{\mathcal{L}} = \flat_{\mathcal{L}}^{-1}.$$

Remark 4.3. In most of cases, $\mathcal{L} = \mathcal{T} - \mathcal{V}$, where \mathcal{T} is the kinetic energy of a Riemannian metric g on Q , and $\mathcal{V} : Q \longrightarrow \mathbb{R}$ is the potential energy. If g is a strong Riemannian metric, then $\omega_{\mathcal{L}}$ is a strong symplectic form on TQ . In such a case $\mathcal{L} = \mathcal{T} - \mathcal{V}$ is regular, and (6) can be notably simplified (cf. [12] and [13]):

$$\begin{aligned} \omega_{\mathcal{L}}(q, v)((a, b), (\bar{a}, \bar{b})) &= D_1g(v, a)(q) \cdot \bar{a} - D_1g(v, \bar{a})(q) \\ &\quad + g(\bar{b}, a)(q) - g(b, \bar{a})(q). \end{aligned} \quad (7)$$

Therefore, if \mathcal{L} is a regular Lagrangian, the equation

$$i_X \omega_{\mathcal{L}} = dE_{\mathcal{L}} \quad (8)$$

has a unique solution $\Gamma_{\mathcal{L}}$ which will be called the Euler-Lagrange vector field for \mathcal{L} . Indeed, $\Gamma_{\mathcal{L}}$ is the Hamiltonian vector field for $dE_{\mathcal{L}}$. A direct computation shows that

- $\Gamma_{\mathcal{L}}$ is a SODE, and
- the solutions of $\Gamma_{\mathcal{L}}$ are the ones of the Euler-Lagrange equations for \mathcal{L} .

If $\mathcal{L} = \mathcal{T} - \mathcal{V}$, we have

$$\Gamma_{\mathcal{L}} = \Gamma_{\mathcal{T}} - (\text{grad } \mathcal{V})^v,$$

where $\Gamma_{\mathcal{T}}$ is the geodesic spray of the Riemannian metric g with kinetic energy \mathcal{T} , and $(\text{grad } \mathcal{V})^v$ is the vertical lift to TQ of the gradient of the potential energy \mathcal{V} , say $i_{\text{grad } \mathcal{V}} g = d\mathcal{V}$. Therefore, the equations of motion become

$$\nabla_{\dot{q}(t)} \dot{q}(t) = -\text{grad } \mathcal{V}(q(t)).$$

Let f and g be two functions defined on TQ , and assume that \mathcal{L} is regular. In such a case, we define the Poisson bracket of f and g as (cf. [1] and [6])

$$\{f, g\}_{\mathcal{L}} = \omega_{\mathcal{L}}(X_f, X_g)$$

where X_f and X_g are the Hamiltonian vector fields for f and g , respectively. A direct computation shows that

$$\dot{f} = \{f, E_{\mathcal{L}}\}_{\mathcal{L}}$$

which means that the evolution of any observable f is given by the Poisson bracket of f with the energy $E_{\mathcal{L}}$.

Remark 4.4. If \mathcal{L} is not regular, then the Poisson bracket $\{f, g\}_{\mathcal{L}}$ is defined on the overlapping of the domains of X_f and X_g (cf. [19]).

A.2. NONHOLONOMIC LAGRANGIAN SYSTEMS. In this section, we will treat with a mechanical system determined by a regular Lagrangian function $\mathcal{L} : TQ \rightarrow \mathbb{R}$ subjected to nonholonomic constraints given by a submanifold M of TQ . We will assume that $(\tau_Q)_M : M \rightarrow Q$ is a vector subbundle of $\tau_Q : TQ \rightarrow Q$, that is, the constraints are linear in the velocities.

As we have proved in [14] and [15], the dynamics of this mechanical system are just the solutions of the following equations:

$$i_X \omega_{\mathcal{L}} - dE_{\mathcal{L}} \in S^*(TM^o), \tag{9}$$

$$X \in TM, \tag{10}$$

where TM^0 stands for the annihilator of TM .

Of course, since \mathcal{L} is regular, Eq. (9) has always a solution, say X , but, in addition, X has to be tangent to the constraint submanifold M . In order to go further, we will assume some compatibility condition.

DEFINITION 4.5. The nonholonomic system (\mathcal{L}, M) is said to be regular if \mathcal{L} is a regular Lagrangian on TQ and in addition we have

$$T(TQ)|_M = TM \oplus \mathcal{R},$$

where \mathcal{R} is the vector subbundle over M which corresponds to $S^*(TM^o)$ via the isomorphism $\flat_{\mathcal{L}}$, that is, $\mathcal{R} = \flat_{\mathcal{L}}(S^*(TM^o))$.

In such a case, the nonholonomic system is compatible. Indeed, let $\Gamma_{\mathcal{L}}$ be the solution of the unconstrained system, and denote by $\pi_1 : T(TQ)|_M \rightarrow TM$, $\pi_2 : T(TQ)|_M \rightarrow \mathcal{R}$ the complementary projectors associated to the above decomposition. Therefore, the vector field $\Gamma_{\mathcal{L},M} = \pi_1(\Gamma_{\mathcal{L}})$ is the solution for the constrained dynamics. $\Gamma_{\mathcal{L},M}$ is a SODE which can be written as $\Gamma_{\mathcal{L},M} = \Gamma_{\mathcal{L}} + \Lambda$, where $\Lambda \in \mathcal{R}$. We shall show how to obtain Λ in an explicit way.

Remark 4.6. The above conditions are very strong, however we will show that they are fulfilled in many interesting cases, as the next result proves.

THEOREM 4.7. Let Q be a Hilbert manifold with a (positive or negative) definite Riemannian metric g , and define $\mathcal{L} = \mathcal{T} - \mathcal{V}$ where \mathcal{T} is the kinetic energy given by g . Then the nonholonomic system (\mathcal{L}, M) is regular.

Proof. Clearly \mathcal{L} is regular. Since $M \rightarrow Q$ is vector subbundle of $TQ \rightarrow Q$, then it is modelled on a vector subspace \mathbb{E}_1 of \mathbb{E} such that \mathbb{E} splits into: $\mathbb{E} = \mathbb{E}_1 \oplus \mathbb{E}_2$. In addition, we can assume that the above decomposition is orthogonal with respect to the metric g . More precisely, each tangent space $T_x Q$ admits an orthogonal decomposition $T_x Q = M_x \oplus M_x^\perp$, where M_x (resp. M_x^\perp) denotes the fibre over x of M (resp. of its orthogonal complement M^\perp with respect to g). So, the local expression of a point X in M is: $(q_1, q_2, v_1, 0)$, where $q_1, v_1 \in \mathbb{E}_1$, and $q_2 \in \mathbb{E}_2$. Thus, the local expressions of $T_X(TQ)$ and $T_X^*(TQ)$ at a point $X \in TQ$ are the following: $(q_1, q_2, v_1, v_2, a_1, a_2, b_1, b_2)$ and $(q_1, q_2, v_1, v_2, A_1, A_2, B_1, B_2)$, where $q_1, v_1, a_1, b_1 \in \mathbb{E}_1$, $q_2, v_2, a_2, b_2 \in \mathbb{E}_2$, $A_1, B_1 \in (\mathbb{E}_1)^*$, and $A_2, B_2 \in (\mathbb{E}_2)^*$.

Consequently, we have

$$TM = \{(q_1, q_2, v_1, 0, a_1, a_2, b_1, 0)\}, \quad TM^o = \{(q_1, q_2, v_1, 0, 0, 0, 0, B_2)\},$$

$$S^*(TM^o) = \{(q_1, q_2, v_1, 0, 0, B_2, 0, 0)\}.$$

Therefore, since $D_2 D_2 \mathcal{L}(q, v)$ is definite (indeed, it coincides with g along the fibre) and using (7) we deduce that $\mathcal{R} = \{(q_1, q_2, v_1, 0, 0, 0, 0, b_2)\}$, and the result follows. ■

(It should be noticed that the same result was recently obtained by A.D. Lewis [17]).

Under the above hypotheses, we have complementary projectors

$$\pi_1 : T(TQ)|_M = TM \oplus \mathcal{R} \rightarrow TM, \quad \pi_2 : T(TQ)|_M = TM \oplus \mathcal{R} \rightarrow \mathcal{R}$$

such that the constrained dynamics is given by the SODE $\Gamma_{\mathcal{L}, M} = \pi_1(\Gamma_{\mathcal{L}})$. In this case the "Lagrange multiplier" can be explicitly computed. Indeed, we have $\Gamma_{\mathcal{L}, M} = (v_1, 0, \gamma_1 + \lambda_1, \gamma_2 + \lambda_2)$, where $\Gamma_{\mathcal{L}} = (v_1, v_2, \gamma_1, \gamma_2)$ and $\Lambda = (0, 0, \lambda_1, \lambda_2) \in \mathcal{R}$. But applying π_1 we obtain

$$\Gamma_{\mathcal{L}, M} = (v_1, 0, \gamma_1, 0),$$

which implies that $\lambda_1 = 0$ and $\lambda_2 = -\gamma_2$.

There is an alternative way to obtain the constrained dynamics by projecting the unconstrained one. Indeed, define a new vector subbundle: $H = \mathcal{R}^\perp \cap TM$, where \mathcal{R}^\perp is the symplectic complement of \mathcal{R} with respect to $\omega_{\mathcal{L}}$.

THEOREM 4.8. *Under the same hypotheses as in Theorem 4.7 we have*

$$T(TQ)|_M = H \oplus H^\perp,$$

that is, H is a symplectic vector subbundle of $(T(TQ)|_M, \omega_{\mathcal{L}})$.

Proof. Using (7) and the orthogonality of E_1 and E_2 we first deduce that the elements in \mathcal{R}^\perp have the following local representation: $(a_1, 0, b_1, b_2)$. Therefore, an element in H is locally represented as $(a_1, 0, b_1, 0)$. Next, by similar arguments as before using again (7) we deduce that the local representation of an arbitrary element in H^\perp is as follows: $(0, a_2, 0, b_2)$ from which we deduce the result. ■

We then obtain two complementary projectors

$$\tilde{\pi}_1 : T(TQ)|_M \longrightarrow H, \quad \tilde{\pi}_2 : T(TQ)|_M \longrightarrow H^\perp.$$

A direct computation shows that $\Gamma_{\mathcal{L},M} = \tilde{\pi}_1(\Gamma_{\mathcal{L}})$.

Furthermore, this second decomposition leads us to define a nonholonomic bracket as follows:

$$\{f, g\}_{nh} = \omega_{\mathcal{L}}(\tilde{\pi}_1(X_{\tilde{f}}), \tilde{\pi}_1(X_{\tilde{g}})),$$

for any two functions f and g on M , where \tilde{f} and \tilde{g} are two arbitrary extensions to TQ of f and g , respectively, and the Hamiltonian vector fields are obtained with respect to $\omega_{\mathcal{L}}$. The nonholonomic bracket is well-defined and satisfies the following properties:

- If $\phi \in C^\infty(TQ)$ vanishes on M , then $\{f, \phi\}_{nh} = 0$.
- Any observable $f \in C^\infty(TQ)$ evolves according to $\dot{f} = \{f, E_{\mathcal{L}}\}_{nh}$.

A.3. AN APPLICATION. As it was shown in [7] there is a large class of continua with perfect internal constraints. These materials are described as continua with microstructure, the complete placements of the velocities of which are restricted. One of the most typical examples occurs when we constraint the micromotion to depend on the choice of an arbitrary vector field on the macromedium through a rigid rotation. In geometrical terms, we are assuming that a connection is given in the ambient principal bundle, and the horizontal distribution is deforming according the deformations of the medium with microstructure, in such a way that the micromotion remains horizontal with respect to the actual connection.

Let us assume that a medium with microstructure is geometrically represented as a principal bundle $\pi_{\mathcal{P}} : \mathcal{P} \longrightarrow \mathcal{B}$ with structure group G ; \mathcal{P} can be deformed into another principal bundle (the ambient physical space) $\pi_{\mathcal{Q}} : \mathcal{Q} \longrightarrow \mathcal{C}$ with structure group K , G being a Lie subgroup of K . We

assume that \mathcal{Q} is endowed with a principal connection given by a horizontal distribution $\mathbb{H}^{\mathcal{Q}}$.

The configuration manifold is the space of equivariant embeddings $\mathcal{E}(\mathcal{P}, \mathcal{Q})$ which becomes a principal bundle over the space of embeddings $\mathcal{E}(\mathcal{B}, \mathcal{C})$ with structure group the gauge group $\mathcal{G}_{\mathcal{P}}^G$. Next, we define a connection in $\mathcal{E}(\mathcal{P}, \mathcal{Q})$ as follows. A tangent vector $L \in T_{\tilde{\Phi}}\mathcal{E}(\mathcal{P}, \mathcal{Q})$ is a mapping $L : \mathcal{P} \rightarrow T\mathcal{Q}$ covering the embedding $\tilde{\Phi} : \mathcal{P} \rightarrow \mathcal{Q}$. Therefore, we define the horizontal subspace $\mathbb{H}_{\tilde{\Phi}}^{\mathcal{E}(\mathcal{P}, \mathcal{Q})}$ consisting of the tangent vectors of the form $\mathbb{H}_{\mathcal{Q}}(L)$, where $\mathbb{H}_{\mathcal{Q}}(L)$ denotes the horizontal projection of L with respect to the given connection in \mathcal{Q} . A straightforward computation shows that $\mathbb{H}^{\mathcal{E}(\mathcal{P}, \mathcal{Q})}$ is in fact $\mathcal{G}_{\mathcal{P}}^G$ -invariant and complementary to the vertical bundle.

So, the constrained equations of motion are:

$$\left. \begin{array}{l} i_X \omega_{\mathcal{L}} - dE_{\mathcal{L}} \in S^*(T(\mathbb{H}^{\mathcal{E}(\mathcal{P}, \mathcal{Q})})^o) \\ X \in T(\mathbb{H}^{\mathcal{E}(\mathcal{P}, \mathcal{Q})}) \end{array} \right\}$$

A direct application of Theorems (4.7) and (4.8) permits to obtain the constrained dynamics $\Gamma_{\mathcal{L}, \mathbb{H}}$ by projecting the unconstrained one.

If, in addition, the potential $\mathcal{V} : \mathcal{E}(\mathcal{P}, \mathcal{Q}) \rightarrow \mathbb{R}$ is invariant, then \mathcal{L} is also invariant, and we can define a projected Lagrangian function $\mathcal{L}^* : T\mathcal{E}(\mathcal{B}, \mathcal{C}) \rightarrow \mathbb{R}$ as follows: $\mathcal{L}^*(L_{\Phi}) = \mathcal{L}((L_{\Phi})_{\tilde{\Phi}}^h)$, where $(L_{\Phi})_{\tilde{\Phi}}^h$ denotes the horizontal lift of L_{Φ} with respect to $\mathbb{H}^{\mathcal{E}(\mathcal{P}, \mathcal{Q})}$, and $\tilde{\Phi}$ is an arbitrary embedding covering Φ . Moreover, we can define a 1-form along $\mathbb{H}^{\mathcal{E}(\mathcal{P}, \mathcal{Q})}$ by

$$\tilde{\alpha} = i_{\Gamma_{\mathcal{L}, \mathbb{H}}} (h^* d(j^* \alpha_{\mathcal{L}}) - d h^*(j^* \alpha_{\mathcal{L}})),$$

where $j : \mathbb{H}^{\mathcal{E}(\mathcal{P}, \mathcal{Q})} \rightarrow T\mathcal{E}(\mathcal{P}, \mathcal{Q})$ is the inclusion map, and h^* is the transpose operator defined by the horizontal projector. $\tilde{\alpha}$ is also invariant and horizontal, so that it projects onto a 1-form α on $T\mathcal{E}(\mathcal{B}, \mathcal{C})$. A direct computation shows that the constrained equations of motion are equivalent to the following unconstrained equation

$$i_Y \omega_{\mathcal{L}^*} = dE_{\mathcal{L}^*} + \alpha,$$

which has a non-exact term α satisfying $i_Y \alpha = 0$.

APPENDIX B: DISCRETE SYSTEMS WITH MICROSTRUCTURE (E. BINZ)

In this appendix we show how the notion of a microstructure dealt with above can be introduced over a finite collection of interacting particles.

We do this without going too much into the physical details, it will be done elsewhere. Examples can be deduced from the continuum approach given above.

The main motivation for considering the discrete case are the relations between the continuum approach and the discrete one. These relations can be used to implement the physics from the small scale to the discrete setting and then to apply the link to the continuum to show how the small scale structure influences the large scale structure of the continuum. Clearly, this approach is hindered by the approximative character the discrete mechanism inherits from continuum approach (cf. [3] and [4]).

B.1. DISCRETE SYSTEMS OF INTERACTING PARTICLES. Let L be a finite connected graph, i.e. a finite collection S^0L of vertices, some of them connected by one edge (only). The collection of all edges shall be denoted by S^1L . The graph is supposed to be oriented, i.e. every edge $e \in S^1L$ is directed, with e^- as initial vertex and e^+ as final vertex.

A configuration of the graph is an embedding $j : L \rightarrow \mathbb{R}^n$. The map j is defined as follows: j is injective on S^0L ; if q and $q' \in S^0L$ are joined by an edge e , then $j(e)$ shall be the edge joining $j(q)$ with $j(q')$. (Neither e nor $j(e)$ need to be parameterized). Let $F(L, \mathbb{R}^n) := \{h : S^0L \rightarrow \mathbb{R}^n\}$, an \mathbb{R} -linear space under pointwise defined operations. The collection of all configurations is denoted by $E(L, \mathbb{R}^n)$. Clearly, $E(L, \mathbb{R}^n) \subset F(L, \mathbb{R}^n)$ is an open subset.

Physical reasons may require to consider a submanifold *conf* of $E(L, \mathbb{R}^n)$, the configuration space.

The interpretation of $j(L)$ for a configuration j is as follows: The vertices $j(q) \in \mathbb{R}^n$ with $q \in S^0L$ are the mean locations of material particles. If any two of them interact with each other the respective vertices are connected by an edge $j(e)$ with $e \in S^1L$ visualizing the interaction. Hence L describes geometrically the interaction scheme.

We therefore call L a discrete system of interacting material particles.

B.2. GEOMETRY OF DISCRETE SYSTEMS OF INTERACTING PARTICLES. An \mathbb{R}^n -valued one-form on L is a map $\gamma : S^1L \rightarrow \mathbb{R}^n$; the collection of all these one-forms on L is denoted by $A^1(L, \mathbb{R}^n)$, an \mathbb{R} -linear space under edge-wise defined operations.

A one-form $\alpha \in A^1(L, \mathbb{R}^n)$ is exact if $\alpha = dh$, where $h : S^0L \rightarrow \mathbb{R}^n$ is a map and dh is defined by

$$dh(e) = h(e^+) - h(e^-) \quad \forall e \in S^1L.$$

Let $dF(L, \mathbb{R}^n) \subset A^1(L, \mathbb{R}^n)$ denote the linear subspace of all \mathbb{R}^n -valued exact one-forms on L .

Next, we present natural bases of $F(L, \mathbb{R}^n)$ and $A^1(L, \mathbb{R}^n)$. Given any $z \in \mathbb{R}^n$ and a fixed $q \in S^0L$, then $a_q^z \in F(L, \mathbb{R}^n)$ is given by

$$a_q^z(q') = \begin{cases} z & \text{if } q = q', \\ 0 & \text{otherwise.} \end{cases} \quad (11)$$

On the other hand, given $e \in S^1L$, let $\gamma_e^z \in A^1(L, \mathbb{R}^n)$ be defined by

$$\gamma_e^z(e') = \begin{cases} z & \text{if } e = e', \\ 0 & \text{otherwise.} \end{cases}$$

γ_e^z is in general not exact. Given a base $z_1, \dots, z_m \in \mathbb{R}^n$, then

$$\{a_q^{z_i} \mid q \in S^0L, i = 1, \dots, m\} \subset F(L, \mathbb{R}^n)$$

and

$$\{\gamma_e^{z_i} \mid e \in S^1L, i = 1, \dots, m\} \subset A^1(L, \mathbb{R}^n)$$

are the natural bases mentioned above.

Given a scalar product \langle, \rangle on \mathbb{R}^n , we define the scalar products \mathcal{G}_L^0 and \mathcal{G}_L^1 on $F(L, \mathbb{R}^n)$ respectively on $A^1(L, \mathbb{R}^n)$ by

$$\mathcal{G}^0(h_1, h_2) := \sum_{q \in S^0L} \langle h_1(q), h_2(q) \rangle \quad \forall h_1, h_2 \in F(L, \mathbb{R}^n)$$

and

$$\mathcal{G}^1(\gamma_1, \gamma_2) := \sum_{e \in S^1L} \langle \gamma_1(e), \gamma_2(e) \rangle \quad \forall \gamma_1, \gamma_2 \in A^1(L, \mathbb{R}^n).$$

The differential d yields the divergence operator defined by

$$\mathcal{G}^1(dh, \gamma) = \mathcal{G}^1(h, \delta\gamma) \quad \forall h \in F(L, \mathbb{R}^n) \text{ and } \forall \gamma \in A^1(L, \mathbb{R}^n).$$

The Laplacian on $F(L, \mathbb{R}^n)$ is defined by

$$\Delta_L := \delta \circ d.$$

This geometry is the basis for the description of the interacting force and the virtual work caused by it, as we shall see in the next section.

B.3. THE INTERACTION FORM AND ITS VIRTUAL WORK. The quality of the discrete medium is given by the interaction form

$$\alpha(j) \in A^1(L, \mathbb{R}^n)$$

for every j in the configuration space $conf \subset E(L, \mathbb{R}^n)$. This interaction form assigns to each edge $e \in S^1L$ the vector $\alpha(j)(e) \in \mathbb{R}^n$, which has the direction of $j(e) \subset \mathbb{R}^n$ if the particles at e^+ and e^- attract each other and the opposite one in case of repulsion. Thus $\alpha(j)(e)$ is the force by which the particles at e^+ and e^- attract or repulse each other. We hence write

$$\alpha(j)(e) = b(j)(e) \cdot d(j)(e) \quad \forall e \in S^1L$$

with $b(j)(e) \in \mathbb{R}$. Clearly, $b(j)(e)$ characterizes the strength of the interaction force.

The interaction form is the analogon of the stress form in the discrete case and hence replaces the first Piola Kirchhoff stress tensor from continuum mechanics (cf. [3]).

As shown in [3] the following holds true:

PROPOSITION 4.9. *The interaction form $\alpha(j)$ splits uniquely and \mathcal{G}^1 -orthogonally into*

$$\alpha(j) = dh(j) + \beta(j) \quad \forall j \in conf$$

with $\delta\beta(j) = 0$ and $\delta\alpha(j) = \Delta h(j)$, $\forall j \in conf$.

The interpretation of the divergence of interaction form is as follows (cf. [3]): Given a vertex $q \in S^1L$, the mean location of a particle,

$$\delta\alpha(j)(q) = \sum_i^{n(q)} \Phi(j)_{q,q_i} = \Phi(j)(q)$$

is the total force by which the collection of particles act up on the one at q . Here $\Phi(j)_{q,q_i}$ is the force by which the i^{th} neighbour at q_i acts up on the one at q . The total number of neighbours of q is $n(q)$.

As shown in [3], the interaction form $\alpha(j)$ for any $j \in conf$ is in general not exact.

B.4. THE VIRTUAL WORK FOR INTERACTING PARTICLES. Given an interaction form $\alpha(j)$ for some $j \in \text{conf}$, the virtual work $\mathcal{A}(j)$ caused by any distortion $\gamma \in A^1(L, \mathbb{R}^n)$ is defined by

$$\mathcal{A}(j)(\gamma) := \mathcal{G}^1(\alpha(j), \gamma) = \sum_{e \in S^1 L} \langle \alpha(j)(e), \gamma(e) \rangle. \quad (12)$$

This definition is motivated by the fact that $\alpha(j)$ is not exact, in general. In case $\gamma = dk$, then $\mathcal{A}(j)(dk) = G^1(\alpha(j), dk)$ or by using the divergence operator δ and Proposition (4.9)

$$\mathcal{A}(j)(dk) = G^0(\delta\alpha(j), k) = G^0(\Delta h(j), k).$$

Hence $\mathcal{A}|_{T\text{conf}}$ is a one-form on conf , while \mathcal{A} as defined in (12) is not. However, general distortions in $A^1(L, \mathbb{R}^n)$ are of particular interest.

Let a_q^z be as in (11) then $\mathcal{A}(j)(da_q^z)$ is the work caused by only distorting the particle at $j(q)$ in the direction of z ; the force at q is $\delta\alpha(j)(q)$ as mentioned in Proposition 4.9.

Remark 4.10. \mathcal{A} is in general not exact on conf , even for exact distortions. However, if \mathcal{A} is determined by a potential, then it is exact on conf .

B.5. MICROSTRUCTURES OVER THE GRAPH L . Let G be a Lie group with Lie algebra \mathfrak{g} . For simplicity we assume G to be compact.

A principal bundle with structure group G over a topological space X is a topological space \mathcal{P} with a projection $\pi_{\mathcal{P}} : \mathcal{P} \rightarrow X$ and a right action

$$\mathcal{P} \times G \xrightarrow{\Psi} \mathcal{P}$$

such that the following holds:

- i) Ψ commutes with $\pi_{\mathcal{P}}$ and the action of G on the fibre of $\pi_{\mathcal{P}}^{-1}(q)$ for any $q \in X$ is transitive and without fixed points.
- ii) For any $q \in X$ the fibre $\pi_{\mathcal{P}}^{-1}(q)$ is a smooth manifold such that the map

$$\Psi_{p'} : G \rightarrow \pi_{\mathcal{P}}^{-1}(\pi_{\mathcal{P}}(p))$$

defined by $\Psi_{p'}(g) = p' \cdot g$ for any $g \in G$ and any $p' \in \pi_{\mathcal{P}}^{-1}(\pi_{\mathcal{P}}(p))$ is a diffeomorphism.

A principal bundle over $X = S^0L$ is called a microstructure over S^0L .

Since $\#S^0L$, the number of vertices in L is finite, the bundle \mathcal{P} is trivial. This means that there is a G -equivariant bijection from \mathcal{P} to $S^0L \times G$.

The graph L , i.e. the collection of edges, is not yet reflected in the microstructure, as just introduced. To link S^1L with \mathcal{P} we may proceed as follows:

A connection ζ on \mathcal{P} is a family of G -equivariant smooth maps

$$\zeta_e : \pi_{\mathcal{P}}^{-1}(e^-) \longrightarrow \pi_{\mathcal{P}}^{-1}(e^+) \quad \forall e \in S^1L.$$

We call \mathcal{P} together with a connection ζ a microstructure with interaction scheme over the graph L . Clearly, $T\zeta_e : T\pi_{\mathcal{P}}^{-1}(e^-) \longrightarrow T\pi_{\mathcal{P}}^{-1}(e^+)$ is equivariant as well. Using the group action Ψ we can link $T\pi_{\mathcal{P}}^{-1}(e^+)$ with the Lie algebra \mathfrak{g} of G . For edges $e \in S^1L$ we use $\Psi_{e^+} := \Psi|_{\pi_{\mathcal{P}}^{-1}(e^+)} \times G$ and form $T\Psi_{e^+}^{-1} \circ T\zeta_e : T\pi_{\mathcal{P}}^{-1}(e^+) \longrightarrow \mathfrak{g}$ which is a (fibrewise) \mathfrak{g} -valued one-form, the connection form of ζ .

Let $\mathcal{Q} \xrightarrow{\pi_{\mathcal{Q}}} \mathbb{R}^n$ be a principal bundle with structure group $K \supset G$ and Lie algebra \mathcal{K} . This principal bundle is trivial, i.e. it is of the form $\mathbb{R}^n \times K$. The configuration space $Conf$ is a subset of the collection of fibre preserving maps

$$j_{\mathcal{P}} : \mathcal{P} \longrightarrow \mathcal{Q}$$

such that $j_{\mathcal{P}}|_{\pi_{\mathcal{P}}^{-1}(p)} : \pi_{\mathcal{P}}^{-1}(p) \longrightarrow \pi_{\mathcal{Q}}^{-1}(\pi_{\mathcal{Q}}(j_{\mathcal{P}}(p)))$ is a G -equivariant smooth embedding for any $p \in \mathcal{P}$. Since \mathcal{Q} is trivial, we can identify $j_{\mathcal{P}}$ with a tuple (j, j_G) where $j \in conf$ and $j_G : G \longrightarrow K$ is an injective Lie group homomorphism. Clearly $j(q) = \pi_{\mathcal{Q}}j_{\mathcal{P}}(p)$ for any $p \in \pi_{\mathcal{P}}(q)$ and any $q \in S^0L$.

Let us assume that $\pi_{Conf}(Conf) =: conf$, where π_{conf} assigns to each configuration $j_{\mathcal{P}}$ (which maps fibres of \mathcal{P} into fibres of \mathcal{Q}) the induced embedding $j : L \longrightarrow \mathbb{R}^n$, defined as above.

Each configuration $j_{\mathcal{P}} \in Conf$ yields a connection $j_{\mathcal{P}}(\zeta)$ on $j_{\mathcal{P}}(\mathcal{P})$, by $j_{\mathcal{P}}(\zeta)_{j(e)}(j(e^-)) := j_{\mathcal{P}}(\zeta_e(e^-))$ for any edge e ; the G -equivariance of $\zeta(j_{\mathcal{P}})$ is obviously satisfied.

We will show next that $Conf \xrightarrow{\pi_{Conf}} conf$ is a principal bundle. To do so we need again the notion of a gauge transformation $\tilde{k} : \mathcal{P} \longrightarrow \mathcal{Q}$, a fibre preserving map satisfying

$$\tilde{k}(p \cdot g) = g^{-1} \cdot k(p) \cdot g \quad \forall p \in \mathcal{P} \text{ and } \forall g \in G.$$

Given two configurations $j_{\mathcal{P}}^1, j_{\mathcal{P}}^2 \in Conf$ with $\pi_{Conf}(j_{\mathcal{P}}^1) = \pi_{Conf}(j_{\mathcal{P}}^2)$ then there is a unique gauge transformation \tilde{k} such that

$$j_{\mathcal{P}}^1 \cdot \tilde{k} = j_{\mathcal{P}}^2.$$

One easily verifies that

$$\mathcal{G}_{\mathcal{P}}^G := \{ \tilde{k} : \mathcal{P} \longrightarrow \mathcal{Q} \mid \tilde{k} \text{ gauge transformation} \}$$

is a group. We will show that $\mathcal{G}_{\mathcal{P}}^G$ is in fact a (finite dimensional) Lie group, next.

To this end let G operate on a smooth manifold F from the left. We thus have the joint action

$$\begin{aligned} G \times (\mathcal{P} \times F) &\longrightarrow \mathcal{P} \times F \\ (g, (p, f)) &\longrightarrow (p \cdot g^{-1}, g \cdot f) \end{aligned}$$

The orbit space, i.e the quotient is denoted by $\mathcal{P} \times_G F$ or just by \mathbb{F} , if no confusion arises. \mathbb{F} is a bundle over S^0L ; it is a vector or a group bundle according as to whether F is a vector space or a group. $\mathcal{P} \times_G F$ is called the associated bundle to \mathcal{P} with typical fibre F .

Let $\Gamma\mathbb{F}$ be the space of all sections of S^0L to \mathbb{F} , a finite dimensional manifold. Any section $s \in \Gamma\mathbb{F}$ defines a map $\tilde{k}_s : \mathcal{P} \longrightarrow F$ determined by

$$s(q) = \overline{(p \cdot g^{-1}, g \cdot \tilde{k}_s(p))} \quad \forall q \in S^0L.$$

The bar denotes the equivalence class. Hence

$$g \cdot \tilde{k}_s(p) = \tilde{k}_s(p \cdot g^{-1}) \quad \forall p \in \mathcal{P} \text{ and } \forall g \in G. \quad (13)$$

\tilde{k}_s is called an F -valued gauge transformation. On the other hand any such gauge transformation defines a section. The assignment $s \mapsto \tilde{k}_s$ yields a (well-known) bijection

$$\Gamma\mathbb{F} \xrightarrow{\varphi} \text{gauge}_G\mathbb{F}.$$

Hence $\text{gauge}_G\mathbb{F}$ is a vector space or a group according as to whether F is a linear space or a group. It is a Lie group if F is a Lie group.

For the purpose under consideration we consider the action of G on K by inner automorphisms

$$\begin{aligned} G \times K &\longrightarrow K \\ (g, f) &\mapsto g^{-1} \cdot f \cdot g, \quad \forall g \in G \text{ and } \forall f \in K, \end{aligned}$$

i.e. G acts by inner automorphisms on K . The associated bundle $\mathcal{P} \times_G K$ is the quotient of $G \times K$ with respect to the action of G on K just introduced. Thus, by the above remark

$$\Gamma\mathbb{K} \longrightarrow \mathcal{G}_{\mathcal{P}}^G$$

is a bijection. Since $\Gamma\mathcal{K}$ is a finite dimensional Lie group, $\mathcal{G}_{\mathcal{P}}^G$ is one too.

Now it is a matter of routine to show

THEOREM 4.11. *Conf is a principal bundle over conf with $\mathcal{G}_{\mathcal{P}}^G$ as structure group. The Lie algebra $\mathfrak{g}_{\mathcal{P}}^G$ of $G_{\mathcal{P}}^G$ is*

$$\mathfrak{g}_{\mathcal{P}}^G = \Gamma(\mathcal{P} \times_G \mathcal{K}),$$

where G acts on \mathcal{K} via the adjoint representation.

Next, we generalize the concept of a principal bundle over S^0L to a principal bundle over the graph L itself. The reason is that the graph may encode a non-trivial topology (as in case of a C_{60} -molecule) which is not reflected on S^0L , of course. The principal bundle \mathcal{P} over S^0L (being trivial) as introduced above is hence not sensitive to this global structure. We will overcome this deficit partly in the next section.

B.6. MICROSTRUCTURES WITH INTERACTION SCHEME. To implement the interaction between elements in the microstructure \mathcal{P} we will extend the concept of a microstructure as follows:

At first we introduce a metric structure on our oriented graph L . This is to say that each edge e is linearly parameterized; the parameter grows in the direction of the orientation. For simplicity the length of unity shall be the same on all edges in S^0L . The graph is hence equipped with a topology, inherited by this parameterization of the edges.

A microstructure with an interaction scheme is a principal bundle \mathcal{P}_L over the topological space L . Its projection is called $\pi_{\mathcal{P}_L}$. The reason the edges of L are parameterized is that the principal bundle \mathcal{P}_L over L needs not to be trivial and hence reflects topological features of the interaction scheme L .

Let the structure group be G again. In addition we assume that $\pi_{\mathcal{P}_L}^{-1}(e) \subset \mathcal{P}_L$ is diffeomorphic to the cartesian product $e \times G$ for each edge $e \in S^1L$. This does not imply that \mathcal{P}_L is trivial over L .

Clearly, $\mathcal{P}_L|_{S^0L}$, (the restriction of \mathcal{P}_L to the discrete subspace $S^0L \subset L$), is a microstructure in the sense of Section B.5. We call it \mathcal{P} again.

This microstructure $\mathcal{P}_L|_{S^0L}$ is supposed to carry a connection ζ . This connection turns \mathcal{P}_L into a graph. Given any edge e , then any $p \in \pi_{\mathcal{P}_L}^{-1}(e^-)$ shall be connected with $\zeta_e(p) \in \pi_{\mathcal{P}_L}^{-1}(e^+)$ by an edge $e_{\mathcal{P}_L}$ in \mathcal{P}_L . This edge is assumed to be a parameterized straight line segment contained in \mathcal{P}_L such that the projection of this segment to e is an isometry. $e_{\mathcal{P}_L}$ has the same direction as e has. Hence \mathcal{P}_L is oriented.

Next, let us introduce the notion of a configuration of the metric graph L . An embedding

$$j : L \longrightarrow \mathbb{R}^n ,$$

called a configuration of L , is supposed to be injective on S^0L and isometric on each edge of L . This implies, of course, that j is determined by the values on its vertices since it is linear on each edge. This is the reason for introducing a linear parametrization on each edge. Thus any configuration of the metric graph is a configuration of L without its metric and vice versa. $conf$ refers therefore to both, the collection of all configuration of L with or without its metric.

A configuration $j_{\mathcal{P}_L}$ of \mathcal{P}_L is an equivariant embedding of \mathcal{P}_L into \mathcal{Q} which is linear on each edge of \mathcal{P}_L ; the induced embedding $j : L \longrightarrow \mathbb{R}^n$ is a configuration of the metric graph.

Let $Conf_L$ be a collection of all the configurations of \mathcal{P}_L . The map associating with each $j_{\mathcal{P}_L} \in Conf_L$ the induced configuration j of L is called $\Pi_{\mathcal{P}_L}$. Let $conf_L \subset conf$ be such that $\Pi_{\mathcal{P}_L} : Conf_L \longrightarrow conf_L$ is surjective.

Both $Conf_L$ and $conf_L$ are assumed to be smooth manifolds. They are finite dimensional due to the linearity of the parametrization of the edges, one essential feature of having finitely many particles.

The key idea implemented in this construction is that not only the particles at $j(e^-)$ and $j(e^+)$ for a given edge e interact with each other, but also that the objects at $j_{\mathcal{P}_L}^1(p^1)$ and $j_{\mathcal{P}_L}^2(p^2)$ do so, provided $p^2 = \zeta(p^1)$ for $p^1 \in \pi_L^{-1}(e^-)$. The following is shown accordingly as in Theorem 4.11:

THEOREM 4.12. *$Conf_L$ is a principal bundle over $conf_L$ with $\mathcal{G}_{\mathcal{P}_L}^G$ as structure group; the structure group $\mathcal{G}_{\mathcal{P}_L}^G = \Gamma(\mathcal{P}_L \times_G K)$ is a finite dimensional Lie group.*

Let $S^0\mathcal{P}_L$ and $S^1\mathcal{P}_L$ denote the collection of all vertices, respectively, edges of \mathcal{P}_L . Clearly, $S^0\mathcal{P}_L = \mathcal{P}_L|S^0L$, which is a principal bundle over S^0L with structure group G as mentioned above.

In fact, $S^1\mathcal{P}_L$ can be given the structure of a principal bundle as well. Given $e \in S^1L$, the manifold $\pi_{\mathcal{P}_L}^{-1}(e)$ is diffeomorphic to $e \times G$ and is, due to connection given, foliated into a collection of one-dimensional leaves, the edges over $e \in S^1L$. Clearly, the group G operates transitively and without fixed points on this collection of leaves. We can consider the quotient space S of \mathcal{P}_L with respect to this foliation. This quotient space is clearly identical

with S^1L as a set. On each fibre over $e \in S^1L$ in $S^1\mathcal{P}_L$ the group operates transitively.

Let $\pi_{S^1\mathcal{P}_L} : S^1\mathcal{P}_L \rightarrow S^1L$ denote the projection, it is obviously related to $\pi_{\mathcal{P}_L}$. Clearly, $S^1\mathcal{P}_L$ is a principal bundle over S^1L with structure group G .

By a function on \mathcal{P}_L , we mean a smooth fibre preserving G -equivariant map on $S^0\mathcal{P}_L$ and by a one-form, (with respect to the graph structure) a fibrewise smooth G -equivariant map over $S^1\mathcal{P}_L$. Here we assume that G operates on the range as well. Let us denote the collection of \mathbb{R}^n - and \mathcal{K} -valued functions and forms by $F(\mathcal{P}_L, \mathbb{R}^n)$ and $A^1(\mathcal{P}_L, \mathbb{R}^n)$ respectively $F(\mathcal{P}_L, \mathcal{K})$ and $A^1(\mathcal{P}_L, \mathcal{K})$. Here G operates on \mathcal{K} by inner automorphisms.

Associated with the graph structure on \mathcal{P} , reflected by \mathcal{P}_L , we have the concept of G -equivariant forms and hence the respective generalizations of d, δ and Δ introduced in Section B.2.

B.7. THE GEOMETRY OF THE PRINCIPAL BUNDLE $Conf_L$. Let \mathcal{P}_L be as above. $Conf_L$ is a finite dimensional manifold. The tangent space $T_{j_{\mathcal{P}_L}} Conf_L$ at $j_{\mathcal{P}_L} \in Conf_L$ consists of all G -equivariant maps $\xi : \mathcal{P}_L \rightarrow T(\mathbb{R}^n \times K) = (\mathbb{R}^n \times K) \times (\mathbb{R}^n \times \mathcal{K})$ with $\tau_{TQ} \circ \xi = j_{\mathcal{P}_L}$. Here $\tau_{TQ} : T(\mathbb{R}^n \times K) \rightarrow \mathbb{R}^n \times K$ is the natural projection. Due to the triviality of Q , any $\xi \in T_{j_{\mathcal{P}_L}} Conf_L$ can naturally be identified with

$$\xi = (l_{\mathbb{R}^n}, l_{\mathcal{K}})$$

where $l_{\mathbb{R}^n} : L \rightarrow \mathbb{R}^n$ and $l_{\mathcal{K}} : \mathcal{P}_L \rightarrow \mathcal{K}$ since the fibre preservation is encoded in $j_{\mathcal{P}}$. Here $l_{\mathbb{R}^n}$ is invariant since G acts on \mathbb{R}^n trivially and $l_{\mathcal{K}}$ is G -equivariant ($G \subset K$ as a subgroup acting on \mathcal{K} by the adjoint representation). Hence

$$T Conf_L = T conf_L \times \Gamma(\mathcal{P}_L \times_G \mathcal{K}).$$

Any left invariant metric $(,)_K$ on K yields the following metric $\mathcal{G}_{\mathcal{P}_L}^l(,)$ on the linear space $T_{j_{\mathcal{P}}} Conf$ defined by

$$\mathcal{G}_{\mathcal{P}_L}^0(\xi_1, \xi_2) = \mathcal{G}_L^0(l_{\mathbb{R}^n}^1, l_{\mathbb{R}^n}^2) + \mathcal{G}_K^0(l_{\mathcal{K}}^1, l_{\mathcal{K}}^2) \tag{14}$$

where

$$\xi_1 = (l_{\mathbb{R}^n}^1, l_{\mathcal{K}}^1) \text{ and } \xi_2 = (l_{\mathbb{R}^n}^2, l_{\mathcal{K}}^2)$$

are splitted in the above sense. The terms on the right hand side of (14) are respectively defined by

$$\mathcal{G}_L^0(l_{\mathbb{R}^n}^1, l_{\mathbb{R}^n}^2) = \sum_{q \in S^0L} \langle l_{\mathbb{R}^n}^1(q), l_{\mathbb{R}^n}^2(q) \rangle$$

and

$$\mathcal{G}_K^0(l_K^1, l_K^2) = \sum_{\pi_{\mathcal{P}_L}(p) \in S^0 L} \left(l_K^1(p), l_K^2(p) \right)_K.$$

Here we have to observe that $\left(l_K^1(p), l_K^2(p) \right)$ is G -invariant and hence depends only on $\pi_{\mathcal{P}}(p) \in S^0 L$. Let us point out moreover that the compactness of neither G nor K is needed to define $\mathcal{G}_{\mathcal{P}_L}^0$.

Let $A_G^1(\mathcal{P}_L, \mathbb{R}^n \times \mathcal{K})$ denote the collection of all G -equivariant one-forms of the graph \mathcal{P}_L into $\mathbb{R}^n \times \mathcal{K}$ (G acts on \mathcal{K} by the adjoint representation). Hence the one-form $\Theta \in A_G^1(\mathcal{P}_L, \mathbb{R}^n \times \mathcal{K})$ can be written as

$$\Theta = (\gamma, \varphi_L)$$

where $\gamma \in A_G^1(L, \mathbb{R}^n)$ and

$$\varphi_L : S^1(\mathcal{P}_L) \longrightarrow \mathcal{K}$$

is a G -equivariant fibrewise smooth map (here $S^1(\mathcal{P}_L)$ denotes the collection of all edges of \mathcal{P}_L).

The metric \mathcal{G}^1 on L extends to \mathcal{P}_L as follows:

$$\mathcal{G}^1(\Theta^1, \Theta^2) = \mathcal{G}^1(\gamma_1, \gamma_2) + \mathcal{G}_K^1(\varphi_L^1, \varphi_L^2)$$

where

$$\mathcal{G}_K^1(\varphi_L^1, \varphi_L^2) = \sum_{\pi_{\mathcal{P}_L}(e_{\mathcal{P}_L}) \in S^1 L} (\varphi_L^1(e_{\mathcal{P}_L}), \varphi_L^2(e_{\mathcal{P}_L})).$$

B.8. THE VIRTUAL WORK ON $Conf_L$. In this section we will generalize the virtual work \mathcal{A} on $conf$, introduced in Section B.3 to $Conf_L$. The virtual work \mathcal{A} on $conf$ is based on the graph structure of L . This is the reason why we endowed \mathcal{P} with such a type of structure.

As mentioned, $S^0 L$ and $S^1 \mathcal{P}_L$ are defined accordingly as $S^0 L$ and $S^1 L$. The respective projections from $S^0 \mathcal{P}_L$ and $S^1 \mathcal{P}_L$ onto $S^0 L$ and $S^1 L$ are called $\pi_{\mathcal{P}_L}$, too. $S^0 \mathcal{P}_L$ and $S^1 \mathcal{P}_L$ are principal bundles over $S^0 L$ and $S^1 L$ with structure group G .

Let us remind that $F(\mathcal{P}_L, \mathbb{R}^n)$ and $A^1(\mathcal{P}_L, \mathbb{R}^n)$ are the \mathbb{R} -linear spaces of all \mathbb{R}^n -valued smooth maps defined on the principal bundles $S^0 \mathcal{P}_L$, respectively $S^1 \mathcal{P}_L$. In order to generalize the virtual work from $conf$ to $Conf_L$ we have to deal with $\mathbb{R}^n \times \mathcal{K}$ -valued one-forms.

We begin the construction of the generalization mentioned with $j_L \in \text{Conf}_L$ and an element s_L in $T_{j_L} \text{Conf}_L$. This map is naturally identified with a pair

$$s_L = (\gamma, \gamma_{\mathcal{K}})$$

where $\gamma \in A^1(L, \mathbb{R}^n)$ and $\gamma_{\mathcal{K}} \in \Gamma(\mathcal{P}_L \times_G \mathcal{K}) = \mathcal{G}_{\mathcal{P}_L}^G$, a smooth section defined on L . Clearly, $s_L \in A^1(\mathcal{P}_L, \mathbb{R}^n \times \mathcal{K})$ is a G -equivariant section.

An interaction form of a microstructure is a smooth map

$$\alpha_{\mathcal{P}_L} : \text{Conf}_L \longrightarrow A^1(L, \mathbb{R}^n) \times \mathcal{G}_{\mathcal{P}_L}^G$$

where

$$\alpha_{\mathcal{P}_L} = (\alpha, \alpha_{\mathcal{K}}) \tag{15}$$

maps each $j_{\mathcal{P}} \in \text{Conf}_L$ into $\alpha_{\mathcal{P}_L}(j_{\mathcal{P}}) = (\alpha(j), \alpha_{\mathcal{K}}(j_{\mathcal{P}_L}))$ where $j = \pi_{\text{Conf}_L}(j_{\mathcal{P}})$ and $\alpha_{\mathcal{K}}(j_{\mathcal{P}_L})(p) \in \mathcal{K}$ for all $p \in \mathcal{P}_L$.

Notice that α in (15) has no relation to the interaction form on the graph, a priori. However, we assume that α coincides with the interaction form on L (provided L is equipped with one).

To define α_L we needed the graph structure of \mathcal{P}_L , since interaction forms are defined in collection of edges. The virtual work is then defined by

$$\mathcal{A}_{\mathcal{P}_L}(j_{\mathcal{P}})(\gamma, \gamma_{\mathcal{K}}) = \mathcal{G}^1(\alpha(j), \gamma) + \mathcal{G}_{\mathcal{K}}^1(\alpha_{\mathcal{K}}(j_{\mathcal{P}_L}), \gamma_{\mathcal{K}})$$

for each $s_L = (\gamma, \gamma_{\mathcal{K}}) \in A^1(L, \mathbb{R}^n) \times \mathcal{G}_{\mathcal{P}_L}^G$. Here we let $\alpha(j)$ be the interaction form on $j(L)$, as introduced in Section B.3. The new quality comes into the setting of microstructures by the $\mathcal{G}_{\mathcal{P}_L}^G$ -valued form $\alpha_{\mathcal{K}}$.

The dynamics of discrete microstructure with interaction scheme is set up as in Section 3 with the only change that the differential of \mathcal{V} appearing in the formula for the differential of the energy is replaced by $\mathcal{A}_{\mathcal{P}_L}$.

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