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A kinematic model for continuous distributions of dislocations

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Abstract

In continuum theory of defects the notion of a flat connection is employed. This paper gives a characterisation of these connections via injective $\mathbb{R}^3$-valued differential forms. For material structures with continuous distributions of dislocations, a configuration space in the sense of global analysis is introduced and analysed. A kinematics for these dislocations is formulated which generalises from elasticity.

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1. Introduction

In continuum theory of defects the differential geometric description of crystals of Bravais type was first formulated by Kondo [9], Nye [13] and Bilby et al. [5]. Based on this theory, Kröner [10] as well as Noll [12] and Wang [17] developed different theories for characterising the interior structure of a material.

These theories have in common that the material structure of the *body manifold* M is characterised by flat connections on the tangent space TM of M. The torsion of a flat connection describes a continuous distribution of a certain type of defect of the material structure, called *dislocation density* or *material inhomogeneity*. Any flat connection implies

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the existence of three linear independent vector fields which may be interpreted as a basis of lattice vectors of a (continuised) crystal. Thus, the space of all flat connections becomes the starting point for non-linear continuum theory of dislocations, cf. [10].

On the other hand, configurations of a purely elastic material are given by the space of all embeddings, in classical terms called placements, of the body manifold M into $\mathbb{R}^3$, cf. [11]. Due to the translational symmetry, not the embedding itself but only the differential of the embedding, i.e. the deformation gradient, is crucial for the constitutive behaviour of the material. Mathematically, these gradients may be considered as exact $\mathbb{R}^3$-valued differential one-forms.

The main purpose of this paper is to show that the idea due to Taylor [16], that the discrepancy between the macroscopic deformation and the deformation of a crystallographic lattice is responsible for the evolution of defects, is encoded in the Helmholtz decomposition of differential forms. We assume the body manifold M to be a smooth three-dimensional compact oriented Riemannian manifold with boundary which is connected and embeddable into the physical space $\mathbb{R}^3$. After reviewing some facts about $\mathbb{R}^3$-valued differential forms in Section 2, flat connections on TM are characterised via the set of all fibrewise injective $\mathbb{R}^3$-valued differential one-forms $\mathcal{I}(M;\mathbb{R}^3)$ in Section 3. In Section 4 some basic ideas of continuum theory of dislocations, as can be found in [10], are reformulated in terms of $\mathbb{R}^3$-valued differential forms.

Section 5 links the theory of dislocations to elasticity. This is done by employing the Helmholtz decomposition theorem which claims that any differential form may uniquely be decomposed into an exact part, i.e. a gradient, and into a divergence-free part. A configuration space $\mathcal{V}(M;\mathbb{R}^3)$ which generalises from elasticity is constructed whose elements, called *generalised configurations*, are no pure deformation gradients anymore. Their divergence-free parts describe dislocation densities of a material. The Helmholtz decomposition allows to split any generalised configuration into an elastic (exact) part and into a plastic (divergence-free) part describing the kinematics of the dislocations (Section 6). Since $\mathcal{V}(M;\mathbb{R}^3)$ is a Fréchet manifold which contains the space of all deformation gradients as a submanifold, it appears to be an appropriate candidate for a configuration space for materials with dislocations in the sense of global analysis. The advantage of this approach seems to be that analytically, differential forms are much easier to handle than connections.

In Section 7, the approach presented in this paper is related to the works of other authors, e.g. [7,12,17]. The Ricci lemma is used in Section 8 to characterise dislocation densities as a quotient of a subspace of $\mathcal{I}(M;\mathbb{R}^3)$.

2. Hodge theory

Let M be a smooth connected three-dimensional compact oriented Riemannian manifold with boundary which is embeddable into the physical space $\mathbb{R}^3$. An $\mathbb{R}^3$-valued differential form $\omega \in \Omega^k(M;\mathbb{R}^3)$ of degree k is a smooth assignment of a skew-symmetric k-linear map ω_p on T_pM to each point $p \in M$, where

$$\omega_p : \underbrace{T_pM \times \cdots \times T_pM}_{k\ times} \longrightarrow \mathbb{R}^3 \quad \forall p \in M.$$

Differential forms may be considered as skew-symmetric two-point tensors of type $(1, k)$ on M which are well-known objects in continuum mechanics, cf. [11]. Let M represent the *body manifold* of the mechanical system in view. Then the deformation gradient and the first Piola–Kirchoff stress tensor are $\mathbb{R}^3$-valued one-forms on M, i.e. some $\omega \in \Omega^1(M; \mathbb{R}^3)$. Analogously, placements of M and force fields are elements in $\Omega^0(M; \mathbb{R}^3)$ which, by definition, is equal to $C^\infty(M; \mathbb{R}^3)$.

Each $\Omega^k(M; \mathbb{R}^3)$ may be equipped with a fibre metric by using the Riemannian metric g on M and the standard scalar product $\langle\cdot,\cdot\rangle_{\mathbb{R}^3}$ on $\mathbb{R}^3$. For our purposes, it suffices to consider the cases $k = 0, 1$. Let $E_1, E_2, E_3 \in \Gamma(TM)$ be a triple of vector fields orthonormal with respect to the metric g. A fibre metric on $\Omega^1(M; \mathbb{R}^3)$ is then defined by

$$\langle\omega, \eta\rangle := \sum_{l=1}^{3} \langle\omega(E_l), \eta(E_l)\rangle_{\mathbb{R}^3}, \quad \omega, \eta \in \Omega^1(M; \mathbb{R}^3). \tag{1}$$

The product (1) does only depend on the metric g but not on the chosen frame on M, cf. [1]. Notice that (1) corresponds to the contraction of skew-symmetric two-point tensors. If $e_1, e_2, e_3 \in \mathbb{R}^3$ denotes the standard basis in $\mathbb{R}^3$ and $\theta^1, \theta^2, \theta^3 \in \Omega^1(M)$ the dual frame corresponding to E_1, E_2, E_3, then, in coordinates, any one-forms ω and η may be written as $\omega = \sum_{L,l} \omega_l^L \theta^l e_L$ and $\eta = \sum_{L,l} \eta_l^L \theta^l e_L$. Thus (1) reads

$$\langle\omega, \eta\rangle = \sum_{L,l=1}^{3} \omega_l^L \eta_l^L.$$

With the help of the Riemannian volume element μ induced by g, the space $\Omega^1(M; \mathbb{R}^3)$ is now endowed with an L^2-product $\mathcal{G}$, given by

$$\mathcal{G}(\omega, \eta) := \int_M \langle\omega, \eta\rangle\mu, \quad \omega, \eta \in \Omega^1(M; \mathbb{R}^3). \tag{2}$$

For $k = 0$ the corresponding L^2-product $\mathcal{G}$ is just the usual one. Let ∇ denote the Levi-Civita connection on M associated to g. Then ∇ induces a *covariant derivative* on $\Omega^1(M; \mathbb{R}^3)$, given by

$$(\nabla_Y\omega)(X) = D[\omega(X)](Y) - \omega(\nabla_Y X), \quad X, Y \in \Gamma(TM).$$

Here, the first term of the right-hand side means the directional derivative of the $\mathbb{R}^3$-valued function $\omega(X)$ in direction of the vector field Y. The covariant derivative allows to write the *exterior derivative* $\mathrm{d} : \Omega^1(M; \mathbb{R}^3) \longrightarrow \Omega^2(M; \mathbb{R}^3)$ as

$$\mathrm{d}\omega(X, Y) = (\nabla_X\omega)(Y) - (\nabla_Y\omega)(X), \quad X, Y \in \Gamma(TM).$$

For $k = 0$ the exterior derivative corresponds to the gradient. The *co-differential* $\delta : \Omega^1(M; \mathbb{R}^3) \longrightarrow C^\infty(M; \mathbb{R}^3)$ may be defined by

$$\delta\omega := -\sum_{l=1}^{3}(\nabla_{E_l}\omega)(E_l).$$

Notice that the co-differential δ, unlike the exterior derivative, depends on the chosen Riemannian metric g. In classical tensor notation, δ corresponds to the divergence of a tensor field.

Let $\mathcal{N}$ denote the outward pointing unit normal field on the boundary ∂M of M. A differential one-form ω is called *parallel* to ∂M iff its normal component vanishes, i.e. $\omega(\mathcal{N}) = 0$. Define the space of all divergence-free and parallel one-forms by

$$\mathcal{D}(M; \mathbb{R}^3) := \{\omega \in \Omega^1(M; \mathbb{R}^3) \mid \delta\omega = 0 \text{ and } \omega(\mathcal{N}) = 0\}.$$

We are now able to state the *Helmholtz decomposition* for the special case of $\mathbb{R}^3$-valued one-forms. For a general version and a proof see [14].

Theorem 2.1 (Helmholtz decomposition). *Let M be a compact oriented Riemannian manifold with boundary. Then for any $\omega \in \Omega^1(M; \mathbb{R}^3)$ there exist $u \in C^\infty(M; \mathbb{R}^3)$ and $\beta \in \mathcal{D}(M; \mathbb{R}^3)$ such that $\omega = \mathrm{d}u + \beta$. Moreover, $\mathrm{d}u$ and β are mutually L^2-orthogonal with respect to the inner product* (2), *i.e. is the decomposition*

$$\Omega^1(M; \mathbb{R}^3) = \mathrm{d}C^\infty(M; \mathbb{R}^3) \oplus \mathcal{D}(M; \mathbb{R}^3)$$

is direct and L^2-orthogonal.

3. Flat connections and differential forms

In order to ensure the existence of flat connections, we assume the tangent bundle TM of M to be trivialisable, i.e. the existence of a bundle isomorphism

$$\gamma : TM \stackrel{\cong}{\longrightarrow} M \times \mathbb{R}^3,$$

which on M induces the identity $id_M : M \longrightarrow M$. This *strong* bundle isomorphism γ is considered here as an $\mathbb{R}^3$-valued one-form in $\Omega^1(M; \mathbb{R}^3)$ which is fibrewise injective. The set of all fibrewise injective $\mathbb{R}^3$-valued one-forms is denoted by $\mathcal{I}(M; \mathbb{R}^3)$. Each one-form $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$ is a trivialisation of TM and vice versa TM is trivialisable iff $\mathcal{I}(M; \mathbb{R}^3) \neq \emptyset$. Obviously, $\mathcal{I}(M; \mathbb{R}^3)$ is an open subset of $\Omega^1(M; \mathbb{R}^3)$ when endowed with Whitney's C^∞-topology, cf. [2]. We identify sections $\Gamma(M \times \mathbb{R}^3)$ with $\mathbb{R}^3$-valued functions $C^\infty(M; \mathbb{R}^3)$ and interpret the standard scalar product $\langle\cdot,\cdot\rangle_{\mathbb{R}^3}$ on $\mathbb{R}^3$ as a metric on the trivial vector bundle $M \times \mathbb{R}^3$. Then, each $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$ defines a Riemannian metric on TM by pulling back the scalar product $\langle\cdot,\cdot\rangle_{\mathbb{R}^3}$:

$$m[\gamma](X, Y) := \langle\gamma X, \gamma Y\rangle_{\mathbb{R}^3}, \quad X, Y \in \Gamma(TM). \tag{3}$$

Let $\mathcal{M}(M)$ denote the Fréchet manifold of all Riemannian metrics on TM. The following lemma shows that each metric in $\mathcal{M}(M)$ may be induced by some $\gamma_0 \in \mathcal{I}(M; \mathbb{R}^3)$.

Lemma 3.1. *For each Riemannian metric* $m_0 \in \mathcal{M}(M)$, *there exists* $\gamma_0 \in \mathcal{I}(M; \mathbb{R}^3)$ *with* $m[\gamma] = m_0$.

Proof. Let $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$ be arbitrary. Then $m[\gamma] \in \mathcal{M}(M)$ and by the theorem of Fischer–Riesz, for each metric $m_0 \in \mathcal{M}(M)$ there is a strong bundle isomorphism $A_0 \in \mathrm{Aut}(TM)$ such that

$$m_0(X, Y) = m[\gamma](A_0 X, A_0 Y) \quad \forall X, Y \in \Gamma(TM).$$

Therefore, $m_0 = m[\gamma_0]$, where $\gamma_0 := \gamma A_0 \in \mathcal{I}(M; \mathbb{R}^3)$. □

Each $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$ induces a linear connection on TM by pulling back the trivial connection d on $M \times \mathbb{R}^3$, given by

$$\nabla[\gamma]_X Y := \gamma^{-1}\, \mathrm{d}(\gamma Y)(X) \quad \forall X, Y \in \Gamma(TM). \tag{4}$$

The set of all connections which are induced by some $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$ is denoted by

$$\mathcal{K} := \{\nabla[\gamma] \mid \gamma \in \mathcal{I}(M; \mathbb{R}^3)\}. \tag{5}$$

With the preceding identifications, d may also be considered as the exterior derivative of $\mathbb{R}^3$-valued differential forms. In particular,

$$\nabla[\gamma]_X Y = \gamma^{-1} \mathcal{L}_X(\gamma Y) \quad \forall X, Y \in \Gamma(TM), \tag{6}$$

where $\mathcal{L}_X(\gamma Y)$ denotes the Lie derivative of the $\mathbb{R}^3$-valued function γY in the direction of the vector field X.

Connections in $\mathcal{K}$ are flat, metric and, in general, will have non-vanishing torsion. This can be seen as follows: On one hand

$$\begin{aligned} \mathcal{L}_Z(m[\gamma](X, Y)) &= \langle \mathcal{L}_Z(\gamma X), \gamma Y\rangle_{\mathbb{R}^3} + \langle \gamma X, \mathcal{L}_Z(\gamma Y)\rangle_{\mathbb{R}^3} \\ &= m[\gamma](\nabla[\gamma]_Z X, Y) + m[\gamma](X, \nabla[\gamma]_Z Y) \end{aligned} \tag{7}$$

for all $X, Y, Z \in \Gamma(TM)$ and therefore $(\nabla[\gamma] m[\gamma]) = 0$, i.e. $\nabla[\gamma]$ *is metric with respect to* $m[\gamma]$. Using $\mathrm{d}^2 = 0$, a short calculation shows that the *curvature* $R[\gamma]$ of $\nabla[\gamma]$ is vanishing:

$$\begin{aligned} R[\gamma](X, Y)Z &:= \nabla[\gamma]_X \nabla[\gamma]_Y Z - \nabla[\gamma]_Y \nabla[\gamma]_X Z - \nabla[\gamma]_{[X,Y]} Z \\ &= \gamma^{-1}[\mathcal{L}_X \mathcal{L}_Y(\gamma Z) - \mathcal{L}_Y \mathcal{L}_X(\gamma Z) - \mathcal{L}_{[X,Y]}(\gamma Z)] \\ &= \gamma^{-1}[\mathrm{d}^2\gamma(X, Y, Z)] = 0 \end{aligned}$$

for all $X, Y, Z \in \Gamma(TM)$. Finally, observe that

$$\mathrm{d}\gamma(X, Y) = \mathcal{L}_X(\gamma Y) - \mathcal{L}_Y(\gamma X) - \gamma[X, Y] = \gamma T[\gamma](X, Y) \tag{8}$$

for all $X, Y \in \Gamma(TM)$, where the *torsion* $T[\gamma] \in \Omega^2(M; TM)$ of $\nabla[\gamma]$ is given by

$$T[\gamma](X, Y) := \nabla[\gamma]_X Y - \nabla[\gamma]_Y X - [X, Y] \quad \forall X, Y \in \Gamma(TM). \tag{9}$$

Since $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$ is fibrewise injective

$$d\gamma = 0 \iff T[\gamma] = 0, \tag{10}$$

which means that the torsion of $\nabla[\gamma]$ vanishes if and only if γ is closed, $d\gamma = 0$. Thus all torion-free connections, i.e. all Levi-Civita connections, in $\mathcal{K}$ are induced by closed one-forms in $\mathcal{I}(M; \mathbb{R}^3)$. In particular, $\mathcal{K}$ contains all flat Levi-Civita connections on TM. Summarising, we obtain the following.

Proposition 3.1. *Each $\nabla[\gamma] \in \mathcal{K}$, $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$ is metric with respect to $m[\gamma]$ and has vanishing curvature. Moreover, $\nabla[\gamma]$ is a Levi-Civita connection if and only if γ is closed.*

According to [10], the space of all flat metric connections $\mathcal{K}$ is the starting point for the non-linear theory of dislocations.

A vector field $X \in \Gamma(TM)$ is called *parallel* with respect to a connection ∇ iff $\nabla_Z X = 0$ for all $Z \in \Gamma(TM)$.

Lemma 3.2. *Let $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$. Then $X \in \Gamma(TM)$ is parallel with respect to $\nabla[\gamma]$ iff $\gamma(X)$ is a constant function in $C^\infty(M; \mathbb{R}^3)$.*

Proof. Identifying sections $\Gamma(M \times \mathbb{R}^3)$ with $\mathbb{R}^3$-valued functions $C^\infty(M; \mathbb{R}^3)$, (6) implies

$$\begin{aligned} &\nabla[\gamma]_Z X = 0 \quad \forall Z \in \Gamma(TM) \\ &\iff \quad \gamma(X)(p) = \gamma(p)X(p) \equiv v \in \mathbb{R}^3 \quad \forall p \in M. \end{aligned}$$

This completes the proof. □

Proposition 3.2. *A triple of vector fields $X_1, X_2, X_3 \in \Gamma(TM)$ is a globally defined frame iff there exists $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$ such that X_1, X_2, X_3 is $m[\gamma]$-orthonormal and parallel with respect to $\nabla[\gamma]$. γ is uniquely determined up to a choice of a basis in $\mathbb{R}^3$.*

Proof. Let $X_1, X_2, X_3 \in \Gamma(TM)$ be a globally defined frame. The parallelism P associated with this frame is then defined by setting

$$P(p,q) : T_pM \longrightarrow T_qM, \quad X_l(q) := P(p,q)X_l(p), \qquad p,q \in M, \quad l = 1,2,3.$$

Fixing $q = q_0$, this gives

$$P(p, q_0)X_l(p) \equiv \text{const.} \quad \forall p \in M, \quad l = 1,2,3. \tag{11}$$

Identifying $T_{q_0}M$ with $\mathbb{R}^3$ via a fixed isomorphism $c_0 : T_{q_0}M \xrightarrow{\cong} \mathbb{R}^3$, one obtains an injective $\mathbb{R}^3$-valued one-form $\gamma := c_0 \circ P(\cdot, q_0) \in \mathcal{I}(M; \mathbb{R}^3)$. By (11) $\gamma(X_l)$, $l = 1, 2, 3$, are constant functions which by Lemma 3.2 implies that X_1, X_2, X_3 is parallel with respect to $\nabla[\gamma]$. Clearly, c_0 may be chosen such that the frame is $m[\gamma]$-orthonormal.

Now let $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$ be given. Choose an orthonormal basis v_1, v_2, v_3 in $\mathbb{R}^3$ and set $X_k := \gamma^{-1}v_k$, $k = 1, 2, 3$. Then $X_1, X_2, X_3 \in \Gamma(TM)$ is $m[\gamma]$-orthonormal by (3) and parallel with respect to $\nabla[\gamma]$ by Lemma 3.2. □

When M is simply connected each flat connection ∇ has a unique parallelism P, cf. [8]. Since any parallelism P may be written as $P(p, q) = \gamma_0^{-1}(q) \circ \gamma_0(p)$, $p, q \in M$, for some $\gamma_0 \in \mathcal{I}(M; \mathbb{R}^3)$, for each flat connection ∇ on TM, there exists a $\gamma_0 \in \mathcal{I}(M; \mathbb{R}^3)$ with $\nabla = \nabla[\gamma_0]$.

4. The geometry of dislocations

In this approach a crystal of Bravais type is considered to be a continuum in the shape of a smooth manifold M on which a crystallographic lattice is impressed whose points are also called atoms. The lattice spacings are assumed to be zero as compared to all other lengths of interest. Thus, the lattice vectors of the crystal constitute a frame $X_1, X_2, X_3 \in \Gamma(TM)$ of the manifold M as proposed by Kröner [10].

By Proposition 3.2, the existence of a globally defined frame $X_1, X_2, X_3 \in \Gamma(TM)$ on M is equivalent to the existence of an injective one-form $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$ such that the frame becomes $m[\gamma]$-orthonormal and parallel with respect to $\nabla[\gamma]$. Hence, from the mathematical point of view, there is no difference between a continuised crystal in the sense of Kröner and a material whose interior structure is characterised by some $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$. In order to obtain a geometric intuition for dislocations, we go along the crystallographic lines.

Since M is compact, each vector field X_k has a flow ψ_k, $k = 1, 2, 3$. Assuming $X_1, X_2, X_3 \in \Gamma(TM)$ to be the frame of lattice vectors of a crystal, the flows ψ_k, $k = 1, 2, 3$, describe a crystallographic lattice on M whose spacing is infinitesimally small. In other words, these flows constitute a crystallographic coordinate system in the original sense of continuum theory of crystals, cf. [6,10].

The crystallographic coordinate system will be a coordinate system on M in the sense of differential geometry if and only if all flows commute, i.e.

$$\psi_l(t, \psi_k(s, p)) = \psi_k(s, \psi_l(t, p)), \quad p \in M, \quad t, s \in \mathbb{R}, \quad l, k = 1, 2, 3.$$

In general, this will not be the case. It is well known that the flows ψ_1, ψ_2, ψ_3 are a coordinate system on M if and only if the Lie bracket of its corresponding vector fields vanishes:

$$[X_l, X_k] \equiv 0, \quad l, k = 1, 2, 3,$$

cf. [15]. If the Lie bracket does not vanish, the resulting 'non-closing' of the flows of X_1, X_2, X_3 becomes a continuous analogue of the so-called *Burgers circuit* in classical crystallography, see Fig. 1. Continuous distributions of dislocations are thus completely characterised by the Lie bracket.

Let $T[\gamma]$ be the torsion of the connection $\nabla[\gamma]$ associated with the frame $X_1, X_2, X_3 \in \Gamma(TM)$. Since $\nabla[\gamma]$ is flat, (9) yields

$$T[\gamma](X_l, X_k) = -[X_l, X_k], \quad l, k = 1, 2, 3. \tag{12}$$

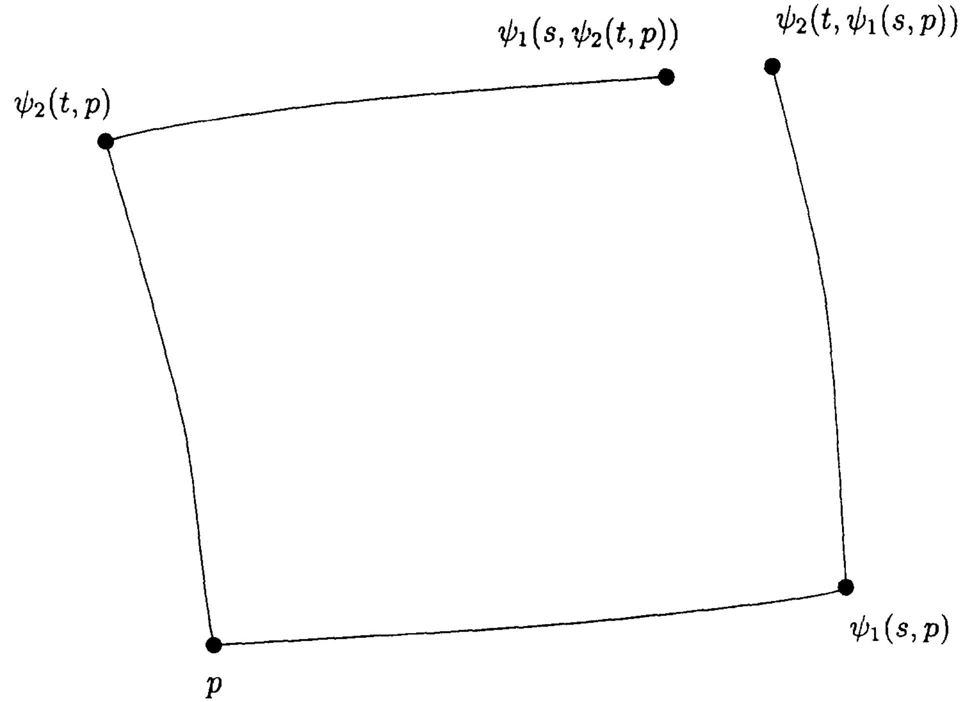

Fig. 1. Non-closing integral curves.

Therefore, the torsion $T[\gamma]$ is a measure for the non-closing of the integral curves of X_1, X_2, X_3. In other words, a crystallographic coordinate system is a coordinate system in the sense of differential geometry iff the torsion $T[\gamma]$ vanishes. Using (8), we obtain

$$\mathrm{d}\gamma(X,Y) = \gamma T[\gamma](X,Y), \quad X,Y \in \Gamma(TM). \tag{13}$$

Since γ is fibrewise injective, the exact two-form $\mathrm{d}\gamma \in \Omega^2(M;\mathbb{R}^3)$ describes the dislocation density (or the material inhomogeneity) $T[\gamma]$ as well.[2] For this reason, in this set-up each $\mathrm{d}\gamma$, $\gamma \in \mathcal{I}(M;\mathbb{R}^3)$, is called dislocation density. The *Burgers vector* $b \in \mathbb{R}^3$ then has a particular simple form. It computes as the integral

$$b = \int_S \mathrm{d}\gamma, \tag{14}$$

where $S \subset M$ is some arbitrary surface,[3] i.e. b is the flux of the dislocation density $\mathrm{d}\gamma$ through the surface S. By (13), a material characterised by γ has no dislocations if and only if γ is closed, $\mathrm{d}\gamma = 0$. The discussion shows that the state of the crystallographic lattice on M is completely determined by specifying γ. Summarising, we have the following.

[2] See Theorem 8.1 for another characterisation.

[3] The Burgers vector is usually defined by the integral of the torsion T over a surface S. Such an integral depends heavily on the chosen trivialisation of TM, cf. [18]. By (13), the Burgers vector (14) is measured in the trivialisation given by γ, i.e. it is just the usual one.

Theorem 4.1. *Any configuration of the interior structure of M is completely determined by some $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$. The corresponding Burgers vector b of an arbitrary surface $S \subset M$ is given by the integral*

$$b = \int_S \mathrm{d}\gamma,$$

where $\mathrm{d}\gamma$ describes the dislocation density on M.

By Theorem A.1, Appendix A, for each $\mathrm{d}\xi \in \Omega^2(M; \mathbb{R}^3)$ there exists an injective one-form $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$ with $\mathrm{d}\xi = \mathrm{d}\gamma$. Hence, each exact $\mathbb{R}^3$-valued two-form $\mathrm{d}\xi$ describes a dislocation density on M.

Notice that there are three equivalent characterisations of a dislocated material: It can be characterised by frames $X_1, X_2, X_3 \in \Gamma(TM)$, by flat connections $\nabla[\gamma] \in \mathcal{K}$, and by injective one-forms $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$. The defect structure is then specified by either the application of the Lie bracket $[\cdot, \cdot]$ on TM, the torsion $T[\gamma]$ or the two-form $\mathrm{d}\gamma$. For a purely intrinsic description, the spaces $\mathcal{K}$ and $\mathcal{I}(M; \mathbb{R}^3)$ serve equally well as configuration spaces, see Section 7. However, being interested how the defect structure affects the embedding (placement) of M into the physical space $\mathbb{R}^3$, it is very natural to take $\mathcal{I}(M; \mathbb{R}^3)$, see Section 5.

The invariance of this set-up under diffeomorphisms can easily be seen as follows. Let $j : M \longrightarrow \mathbb{R}^3$ be an embedding of M into the physical space $\mathbb{R}^3$. Then the push-forward $j_*\gamma$ is an injective one-form $j_*\gamma \in \mathcal{I}(j(M); \mathbb{R}^3)$ which determines a defect structure on the embedded body $j(M)$. Since the exterior differential d commutes with push-forwards, the respective dislocation densities satisfy $j_*\,\mathrm{d}\gamma = \mathrm{d}(j_*\gamma)$. This implies

$$b = \int_S \mathrm{d}\gamma = \int_{j(S)} \mathrm{d}(j_*\gamma) \tag{15}$$

for the Burgers vector, that is the Burgers vector is invariant under diffeomorphisms.[4]

5. The configuration space $\mathcal{V}(M; \mathbb{R}^3)$

Let $E(M; \mathbb{R}^3)$ denote the space of all smooth embeddings of the body manifold M into the physical space $\mathbb{R}^3$. A placement of M in the sense of elasticity is then given by a smooth embedding $j \in E(M; \mathbb{R}^3)$. Since the tangent bundle of $\mathbb{R}^3$ is trivial $T\mathbb{R}^3 \equiv \mathbb{R}^3 \times \mathbb{R}^3$, the tangent map $Tj : TM \longrightarrow T\mathbb{R}^3$ splits $Tj = (j, \mathrm{d}j)$. As a consequence, $\mathrm{d}j$ is an exact $\mathbb{R}^3$-valued differential form in $\mathcal{I}(M; \mathbb{R}^3)$.

Consider a material M whose interior structure is given by some frame $X_1, X_2, X_3 \in \Gamma(TM)$ describing a non-dislocated reference lattice on M. Since the push-forward j_* of any embedding j commutes with the Lie bracket, one has $j_*[X_k, X_l] = [j_*X_k, j_*X_l]$,

[4] It is not hard to prove that the non-exact component of $j_*\gamma$ is given by $j_*\beta \in \mathcal{D}_{j_*g}(j(M); \mathbb{R}^3)$. Thus, the defect structure on $j(M)$ is determined by $j_*\beta$, whereas j_*g is the metric pushed forward by j, cf. [18].

$k, l = 1, 2, 3$ and j induces a frame j_*X_1, j_*X_2, j_*X_3 on $j(M)$ describing a non-dislocated lattice on $j(M)$. Notice that this observation (as well as (15)) allows us to view any change in j as a deformation which is *compatible* with the reference lattice.

By Proposition 3.2, there exists a Levi-Civita connection $\nabla[\mathrm{d}j_0]$ which is assumed here to be induced by some *reference embedding*[5] $j_0 \in E(M; \mathbb{R}^3)$ such that X_1, X_2, X_3 is $m[\mathrm{d}j_0]$-orthonormal and parallel with respect to $\nabla[\mathrm{d}j_0]$. Using Lemma 3.2, one may assume that

$$j_{0*}X_l = \mathrm{d}j_0 X_l \equiv e_l, \quad l = 1, 2, 3, \tag{16}$$

where e_1, e_2, e_3 denotes the standard basis of $\mathbb{R}^3$. Here, we identified vector fields with their principal parts.

In view of the Helmholtz decomposition, let an arbitrary but fixed divergence-free component $\beta_0 \in \mathcal{D}(M; \mathbb{R}^3)$ be the quantity by which the frame X_1, X_2, X_3 is deformed. Identifying $\mathrm{d}j_0 + \beta_0$ with $(j_0, \mathrm{d}j_0 + \beta_0) \in \Omega^1(M; \mathbb{R}^3 \times \mathbb{R}^3)$, one obtains three vector fields $(\mathrm{d}j_0 + \beta_0)X_1, (\mathrm{d}j_0 + \beta_0)X_2, (\mathrm{d}j_0 + \beta_0)X_3$, which constitute a frame on $j_0(M)$ if and only if $\mathrm{d}j_0 + \beta_0$ is injective. In Appendix A we will give a criterion for $\mathrm{d}j_0 + \beta_0$ lying in $\mathcal{I}(M; \mathbb{R}^3)$. For $\beta_0 \neq 0$ this frame represents a dislocated lattice on $j_0(M)$. In this sense, the original frame X_1, X_2, X_3 is deformed *incompatibly* with the original non-dislocated reference lattice.

This, of course, is nothing else but the idea that the evolution of defects is responsible for the discrepancy between the macroscopic displacement and the deformation of the lattice of the material, cf. Taylor [16]. The commutative diagram

$$\begin{array}{ccc} TM & \xrightarrow{(j_0,\, \mathrm{d}j_0+\beta_0)} & j_0(M) \times \mathbb{R}^3 \\ \downarrow{\scriptstyle \tau_M} & & \downarrow{\scriptstyle pr_1} \\ M & \xrightarrow{j_0} & j_0(M) \end{array}$$

attempts to reflect this fact to some extent. Using $\mathrm{d}^2 = 0$, for each $\gamma = \mathrm{d}j + \beta \in \mathcal{I}(M; \mathbb{R}^3)$ with $j \in E(M; \mathbb{R}^3)$, $\beta \in \mathcal{D}(M; \mathbb{R}^3)$, we have $\mathrm{d}\gamma = \mathrm{d}\beta$. Dislocations, i.e. the material structure on M, are thus encoded in the *non-exact* part β of a configuration γ. The sum $\gamma = \mathrm{d}j + \beta$ is a decomposition which is orthogonal with respect to the L^2-product $\mathcal{G}$ induced by g, i.e. it is the Helmholtz decomposition with respect to g. This gives rise to the following definition.

Definition 5.1. *The configuration space of a material M whose interior structure is specified by some $\beta \in \mathcal{D}(M; \mathbb{R}^3)$ is defined by*

$$\mathcal{V}(M; \mathbb{R}^3) := \{\gamma \in \mathcal{I}(M; \mathbb{R}^3) \mid \gamma = \mathrm{d}j + \beta, \;\; j \in E(M; \mathbb{R}^3), \;\; \beta \in \mathcal{D}(M; \mathbb{R}^3)\}. \tag{17}$$

[5] By Proposition 3.1, Levi-Civita connections are induced by closed forms $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$. If M is contractible, by the Poincaré lemma closed forms are exact $\gamma = \mathrm{d}i$, where the injectivity means that i must be an immersion. Since $E(M; \mathbb{R}^3)$ is dense in the space of all immersions, this assumption is not too restrictive. In general, closed forms in $\mathcal{I}(M; \mathbb{R}^3)$ differ from immersions essentially by a finite-dimensional subspace, cf. [18].

Clearly, $\mathcal{V}(M;\mathbb{R}^3)$ contains the space of all differentials of embeddings

$$\mathrm{d}E(M;\mathbb{R}^3) := \{\mathrm{d}j \in \Omega^1(M;\mathbb{R}^3) \mid j \in E(M;\mathbb{R}^3)\} \tag{18}$$

as a subset. Since it can be shown that the crucial kinematic quantity in elasticity is the deformation gradient, i.e. the differential $\mathrm{d}j$ of an embedding j, the classical configuration space of elasticity $E(M;\mathbb{R}^3)$ is replaced here by $\mathrm{d}E(M;\mathbb{R}^3)$, cf. [3,11]. By Proposition A.2 below, $\mathrm{d}E(M;\mathbb{R}^3)$ is a Fréchet submanifold of $\mathcal{V}(M;\mathbb{R}^3)$. Thus, $\mathcal{V}(M;\mathbb{R}^3)$ becomes a natural generalisation of the configuration space $\mathrm{d}E(M;\mathbb{R}^3)$ of defect-free continuum mechanics. Configurations in $\mathcal{V}(M;\mathbb{R}^3)$ will be referred to as *generalised configurations*. Due to Theorem A.1 and the remark made at the end of Section 4, generalised configurations are capable of describing any possible dislocation density.

A priori, one is free in choosing a reference metric g. The only metrics relevant are those with Helmholtz decompositions $\gamma = \mathrm{d}j + \beta$ such that the exact part $\mathrm{d}j$ stems from an embedding $j \in E(M;\mathbb{R}^3)$. This is reflected in our definition of $\mathcal{V}(M;\mathbb{R}^3)$. In general, this need not be the case. A canonical choice is the pull-back metric $g = m[\mathrm{d}j_0]$ induced by some reference embedding $j_0 \in E(M;\mathbb{R}^3)$ according to (3). The corresponding Fréchet space $\mathcal{D}(M,\mathbb{R}^3)$ is then interpreted as follows: Let $\mu[\gamma] = \mu_{m[\gamma]}$ be the Riemannian volume form on M induced by $m[\gamma]$ and define the volume function by

$$\mathbf{Vol} : \mathcal{V}(M;\mathbb{R}^3) \longrightarrow \mathbb{R}, \qquad \gamma \longmapsto \mathbf{Vol}[\gamma] := \int_M \mu[\gamma].$$

We differentiate $\mathbf{Vol}$ at $\mathrm{d}j_0 \in \mathrm{d}E(M;\mathbb{R}^3) \subset \mathcal{V}(M;\mathbb{R}^3)$ in direction of an arbitrary $\beta \in \Omega^1(M;\mathbb{R}^3)$ and obtain

$$D\mathbf{Vol}[\mathrm{d}j_0](\beta) = \int_M D\mu[\mathrm{d}j_0](\beta) = \int_M \operatorname{tr} B[\mathrm{d}j_0]\mu[\mathrm{d}j_0],$$

where $B[\mathrm{d}j_0] \in \mathrm{End}(TM)$ is given by $\beta = \mathrm{d}j_0 \circ B[\mathrm{d}j_0]$. From the definition of the L^2-product $\mathcal{G}$ on $\Omega^1(M;\mathbb{R}^3)$ corresponding to $m[\mathrm{d}j_0]$ it follows that

$$\int_M \operatorname{tr} B[\mathrm{d}j_0]\, \mu[\mathrm{d}j_0] = \mathcal{G}(\mathrm{d}j_0|\beta) = 0 \quad \forall \beta \in \mathcal{D}(M;\mathbb{R}^3).$$

Therefore, $\mathcal{D}(M;\mathbb{R}^3) \subset T_{\mathrm{d}j_0}\mathcal{V}(M;\mathbb{R}^3)$ is a subspace tangent to the level set of $\mathbf{Vol}$ through $\mathrm{d}j_0 \in \mathcal{V}(M;\mathbb{R}^3)$.

It is shown in [19] that the Helmholtz decomposition depends smoothly on the metric g. For any metric g' close enough to g, the Helmholtz decomposition of γ with respect to g' yields

$$\gamma = \mathrm{d}j' + \beta' \quad \text{with } \mathrm{d}j' \in \mathrm{d}E(M;\mathbb{R}^3), \quad \beta' \in \mathcal{D}'(M;\mathbb{R}^3).$$

Then $\mathrm{d}\gamma = \mathrm{d}\beta = \mathrm{d}\beta'$ such that the defect structure on M remains invariant. However, in general, $\mathrm{d}j \neq \mathrm{d}j'$ and $\beta \neq \beta'$. In particular, the embedding j of the material will change.

6. The kinematics of dislocations

A deformation of the material is now given by a smooth curve

$$\gamma : \mathbb{R} \longrightarrow \mathcal{V}(M; \mathbb{R}^3) \tag{19}$$

in the configuration space $\mathcal{V}(M; \mathbb{R}^3)$. For each t, we decompose $\gamma(t)$ according to Helmholtz with respect to a fixed reference metric g and obtain

$$\gamma(t) = \mathrm{d}j(t) + \beta(t), \quad t \in \mathbb{R}.$$

Then the smooth curve of differentials of embeddings

$$\mathrm{d}j : \mathbb{R} \longrightarrow \mathrm{d}E(M; \mathbb{R}^3) \tag{20}$$

represents the motion of the *exact*, i.e. *elastic* or *integrable* parts of the deformation. The smooth curve

$$\beta : \mathbb{R} \longrightarrow \mathcal{D}(M; \mathbb{R}^3) \tag{21}$$

represents the motion of the *non-integrable* or *plastic* parts of the deformation. By assumption, only the integrable parts of $\gamma(t)$ will manifest themselves in the physical space $\mathbb{R}^3$ as deformations. If $\beta(t) \equiv 0\ \forall t \in \mathbb{R}$, then the deformation is purely *elastic* and we are within the realm of elasticity. However, in the presence of a constant dislocation density, i.e. $\beta(t) \equiv \beta_0 \neq 0\ \forall t \in \mathbb{R}$, the evolution of the exact components $\mathrm{d}j(t)$ of $\gamma(t)$ encounter a geometric obstruction given by β_0, see Corollary A.1, Appendix A.

One may visualise the deformation (19) of the dislocated material M as a motion in the physical space $\mathbb{R}^3$ in the sense of *Euler*'s description in fluid dynamics. For simplicity assume that at $t = 0$ the deformation $\gamma(t)$ satisfies

$$\gamma(0) = \mathrm{d}j_0 \quad \text{with } j_0 \in E(M; \mathbb{R}^3). \tag{22}$$

Then, according to (16), the frame $X_1, \ldots, X_3$ defined by $\gamma(0)$ represents the undeformed lattice structure on M. This frame induces a crystallographic coordinate system on $j_0(M)$ which by construction coincides with the geometric coordinate system of straight lines inherited from $\mathbb{R}^3$.

The crystallographic coordinate system will be dragged along by the curve of embeddings (20) which describes how M will be embedded into $\mathbb{R}^3$ at any instant of time. The crystallographic lattice is incompatibly deformed by the curve (21) of non-integrable parts, such that $\gamma(t)X_1, \gamma(t)X_2, \gamma(t)X_3$ describes a dislocated lattice on $j(t)(M)$, unless $\beta(t) = 0$ for all t. The crystallographic coordinate system on $j(t)(M)$ is curvilinear and will, in general, deviate from the initial coordinate system dragged along by the embeddings (20) alone.

We now introduce the concept of an internal and an external observer in the sense of Kröner [10]. The internal observer lives on M and uses either $\mathcal{K}$ or $\mathcal{I}(M; \mathbb{R}^3)$ for a configuration space. He is thus able to measure the dislocation density on M. The external observer lives in the physical space $\mathbb{R}^3$ and uses $\mathcal{V}(M; \mathbb{R}^3)$ as a configuration space. He can do anything the internal observer can. However, in contrast to the internal observer, the external observer knows how the material is embedded in the physical space $\mathbb{R}^3$ by using the Helmholtz decomposition.

Since in elasticity one likes to compare configurations of a material by means of a deformation tensor, we finish the section by discussing the deformation tensor of *Green–Lagrange* $\boldsymbol{E}$. In this approach, the Green–Lagrange deformation tensor between two configurations $\gamma, \bar{\gamma} \in \mathcal{V}(M; \mathbb{R}^3)$ is given by

$$\boldsymbol{E}(X, Y) := \tfrac{1}{2}(m[\gamma](X, Y) - m[\bar{\gamma}](X, Y)) \quad \forall X, Y \in \Gamma(TM). \tag{23}$$

Clearly, $\boldsymbol{E}$ is a symmetric two-tensor. Notice that in the presence of dislocations, one cannot associate a pure displacement field $u \in C^\infty(M; \mathbb{R}^3)$ with the deformation tensor $\boldsymbol{E}$. The Helmholtz decompositions $\gamma = \mathrm{d}j + \beta$ and $\bar{\gamma} = \mathrm{d}\bar{j} + \bar{\beta}$, respectively, yield

$$\chi = \bar{\gamma} - \gamma = \mathrm{d}u - \chi, \quad \text{where } \mathrm{d}u = \mathrm{d}\bar{j} - \mathrm{d}j, \quad \chi = \bar{\beta} - \beta$$

and $\mathrm{d}u \in \mathrm{d}\Omega^0(M; \mathbb{R}^3)$, $\chi \in \mathcal{D}(M; \mathbb{R}^3)$. Then $u \in C^\infty(M; \mathbb{R}^3)$ is the *displacement field* associated with $\boldsymbol{E}$, which is uniquely determined up to translations, and the non-integrable χ is the 'displacement' of the dislocations. We define the *elastic* component $\boldsymbol{E}^{(\mathrm{e})}$ of $\boldsymbol{E}$ by

$$\boldsymbol{E}^{(\mathrm{e})}(X, Y) := \tfrac{1}{2}(m[\mathrm{d}\bar{j}](X, Y) - m[\mathrm{d}j](X, Y)) \quad \forall X, Y \in \Gamma(TM)$$

and the *plastic* component $\boldsymbol{E}^{(\mathrm{p})}$ by $\boldsymbol{E}^{(\mathrm{p})} := \boldsymbol{E} - \boldsymbol{E}^{(\mathrm{e})}$. $\boldsymbol{E}^{(\mathrm{e})}$ and $\boldsymbol{E}^{(\mathrm{p})}$ both are symmetric tensors of second order. If $\boldsymbol{E}^{(\mathrm{p})} \equiv 0$, then $\boldsymbol{E} = \boldsymbol{E}^{(\mathrm{e})}$ is the just deformation tensor of classical elasticity induced by a displacement field $u = \bar{j} - j$.

7. The geometric structure of $\mathcal{I}(M; \mathbb{R}^3)$

To indicate how the formulation presented in the preceding sections relates to the works of other authors, see e.g. [7,12,17], we identify $\mathcal{I}(M; \mathbb{R}^3)$ with the global sections of the frame bundle of TM. From there on, how $\pi_{\mathcal{K}} : \mathcal{I}(M; \mathbb{R}^3) \longrightarrow \mathcal{K}$ becomes a trivial principal $Gl(3)$-bundle is outlined. If $\mathrm{Is}(\mathbb{R}^3, T_pM)$ denotes the set of all linear isomorphisms $\mathbb{R}^3 \xrightarrow{\cong} T_pM$, the frame bundle of TM is defined by

$$\mathbb{P} := \bigcup_{p \in M} \mathrm{Is}(\mathbb{R}^3, T_pM).$$

$\mathbb{P}$ is a principal $Gl(3)$-bundle. Consider the 'inverted frame bundle' $\hat{\mathbb{P}}$ given by

$$\hat{\mathbb{P}} := \bigcup_{p \in M} \mathrm{Is}(T_pM, \mathbb{R}^3),$$

where $\mathrm{Is}(T_pM, \mathbb{R}^3)$ is defined analogously. On $\hat{\mathbb{P}}$ there is the natural free right action

$$\hat{R} : \hat{\mathbb{P}} \times Gl(3) \longrightarrow \hat{\mathbb{P}}, \quad (\hat{z}, g) \longmapsto g^{-1} \cdot \hat{z}\,. \tag{24}$$

Then, fibrewise inversion $\Psi : \mathbb{P} \longrightarrow \hat{\mathbb{P}}$, pointwise given by

$$\Psi_p : z_p \in \mathrm{Is}(\mathbb{R}^3, T_pM) \longmapsto \hat{z}_p := z_p^{-1} \in \mathrm{Is}(T_pM, \mathbb{R}^3) \quad \forall p \in M,$$

is an equivariant, strong bundle isomorphism between $\mathbb{P}$ and $\hat{\mathbb{P}}$. Therefore, we endow $\hat{\mathbb{P}}$ with the structure of a principal $Gl(3)$-bundle via Ψ such that Ψ becomes a strong isomorphism of principal bundles. Notice that $\mathcal{I}(M;\mathbb{R}^3) = \Gamma(\hat{\mathbb{P}})$. Since TM trivialisable, the set $\mathcal{I}(M;\mathbb{R}^3)$ is not empty, cf. Section 3. On the other hand, the existence of a global section is equivalent to the triviality of a principal bundle, cf. [8]. Therefore, both bundles $\mathbb{P}$ and $\hat{\mathbb{P}}$ are trivial, i.e. $\mathbb{P} \cong M \times Gl(3)$ and $\hat{\mathbb{P}} \cong M \times Gl(3)$. Using Ψ, this yields the following.

Proposition 7.1. *Let TM be trivialisable. Then the fibrewise injective one-forms $\mathcal{I}(M;\mathbb{R}^3)$ are isomorphic with the global sections $\Gamma(\mathbb{P})$ of the frame bundle of TM:*

$$\mathcal{I}(M;\mathbb{R}^3) \cong \Gamma(\mathbb{P}) \cong C^\infty(M; Gl(3)).$$

Next, we establish the relationship between the more classical space $\mathcal{K}$ and the space of all injective one-forms $\mathcal{I}(M;\mathbb{R}^3)$.

Proposition 7.2. *Let $\gamma, \beta \in \mathcal{I}(M;\mathbb{R}^3)$. Then $\nabla[\gamma] = \nabla[\beta]$ iff $\beta = a\gamma$, where $a \in Gl(3)$. Consequently, the natural surjection*

$$\pi_{\mathcal{K}} : \mathcal{I}(M;\mathbb{R}^3) \longrightarrow \mathcal{K}, \quad \gamma \longmapsto \nabla[\gamma]$$

satisfies $\pi_{\mathcal{K}}^{-1}(\nabla) \cong Gl(3)$ for each $\nabla \in \mathcal{K}$.

Proof. For given $\gamma, \beta \in \mathcal{I}(M;\mathbb{R}^3)$, there exists $a \in C^\infty(M; Gl(3))$ such that $\beta = a\gamma$. Thus

$$\beta\nabla[\beta]_X Y = \mathcal{L}_X(a\gamma Y) = (\mathcal{L}_X a)(\gamma Y) + \beta\nabla[\gamma]_X Y, \quad X, Y \in \Gamma(TM).$$

Since β is fibrewise injective, this implies

$$\nabla[\gamma] \equiv \nabla[\beta] \iff \beta = a\gamma \quad \text{with } a \in Gl(3),$$

where constant functions in $C^\infty(M; Gl(3))$ are identified with $Gl(3)$. □

Consider the free right action of $Gl(3)$ on $\mathcal{I}(M;\mathbb{R}^3)$

$$\Phi : \mathcal{I}(M;\mathbb{R}^3) \times Gl(3) \longrightarrow \mathcal{I}(M;\mathbb{R}^3), \quad (\gamma, g) \longmapsto g^{-1} \cdot \gamma \tag{25}$$

and denote the set of all right cosets of (25) by

$$\mathcal{I}(M;\mathbb{R}^3)_{/Gl(3)} := \{[\gamma] \mid \gamma \in \mathcal{I}(M;\mathbb{R}^3)\}, \tag{26}$$

where $\beta \in [\gamma] \iff \exists g \in Gl(3)$ with $\beta = g^{-1} \cdot \gamma$. Now the following becomes obvious.

Theorem 7.1. *The space of all flat metric connections $\mathcal{K}$ is isomorphic with the quotient $\mathcal{I}(M;\mathbb{R}^3)_{/Gl(3)}$ via the induced isomorphism*

$$\hat{\pi}_{\mathcal{K}} : \mathcal{I}(M;\mathbb{R}^3)_{/Gl(3)} \xrightarrow{\cong} \mathcal{K}, \quad [\gamma] \longmapsto \nabla[\gamma].$$

The projection $\pi_{\mathcal{K}} : \mathcal{I}(M; \mathbb{R}^3) \longrightarrow \mathcal{K}$ may be endowed with the structure of a trivial smooth Fréchet principal $Gl(3)$-bundle, cf. [18]. It follows from Theorem 7.1 that $\mathcal{K}$ is a smooth Fréchet manifold. Therefore, $\mathcal{K}$ is a configuration space in the sense of global analysis. Working with connections or, alternatively, with sections into the frame bundle is the more classical approach. However, from the point of view of global analysis, differential forms $\mathcal{I}(M; \mathbb{R}^3)$ are a much nicer space.

8. Dislocation densities as torsions

In classical terms, dislocation densities are described by torsions $T \in \Omega^2(M; TM)$ which stem from flat connections. This section characterises these *admissible* torsions by $O(3)$-valued functions, where $O(3)$ denotes the orthogonal group. A priori, the correspondence between torsions and connections is not one-to-one. The Ricci lemma tells us under which conditions this is the case, cf. [8].

Proposition 8.1 (Ricci lemma). *Let g be a metric on a Riemannian manifold M and $T \in \Omega^2(M; TM)$. Then there exists a unique connection ∇ which is metric with respect to g and has torsion T.*

In general, ∇ in Proposition 8.1 will have non-vanishing curvature. Thus, flat connections which are compatible with a given metric are characterised first.

Proposition 8.2. *Let $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$. Then set of all connection in $\mathcal{K}$ which are metric with respect to $m[\gamma]$ is given by*

$$\mathcal{K}_\gamma := \{\nabla[a\gamma] \mid a \in C^\infty(M; O(3))\}.$$

Proof. Let $\gamma, \beta \in \mathcal{I}(M; \mathbb{R}^3)$ be arbitrary. We have to show that $\nabla[\beta]$ is metric with respect to $m[\gamma]$ iff $\nabla[\beta] = \nabla[a\gamma]$, where $a \in C^\infty(M; O(3))$. Since $m[a\gamma] = m[\gamma]$ for all $a \in C^\infty(M; O(3))$, by Proposition 3.1, $\nabla[a\gamma]$ is compatible with the metric $m[\gamma]$.

For the converse observe that for any basis $w_1, w_2, w_3 \in \mathbb{R}^3$, a frame $Y_1, Y_2, Y_3 \in \Gamma(TM)$ is defined by setting $Y_k := \beta^{-1} w_k$, $k = 1, 2, 3$. In particular, we may choose the $w_k \in \mathbb{R}^3$ such that $m[\gamma(p_0)](Y_k(p_0), Y_l(p_0)) = \delta_{kl}$, $k, l = 1, 2, 3$, where $p_0 \in M$ is some fixed point. By Lemma 3.2, this frame is parallel with respect to $\nabla[\beta]$. From metricity $(\nabla[\beta] m[\gamma]) \equiv 0$ we obtain

$$\mathcal{L}_Z(m[\gamma](Y_k, Y_l)) = 0 \quad \forall Z \in \Gamma(TM), \quad k, l = 1, 2, 3,$$

i.e. $m[\gamma](Y_k, Y_l) \equiv \delta_{kl}$, $k, l = 1, 2, 3$ on M. This shows that $Y_1, Y_2, Y_3 \in \Gamma(TM)$ is $m[\gamma]$-orthonormal and parallel with respect to $\nabla[\beta]$. By Proposition 3.2, there exists $\bar{\gamma} \in \mathcal{I}(M; \mathbb{R}^3)$, such that Y_1, Y_2, Y_3 is $m[\bar{\gamma}]$-orthonormal and parallel with respect to $\nabla[\bar{\gamma}]$. The first property implies $m[\gamma] = m[\bar{\gamma}]$, yielding $\bar{\gamma} = a\gamma$ for some $a \in C^\infty(M; O(3))$. The second one then gives $\nabla[a\gamma] = \nabla[\beta]$, since flat connections are uniquely determined by orthonormal, parallel frames. □

Proposition 8.2 motivates the following. If $T[\gamma]$ denotes the torsion of $\nabla[\gamma]$, then the set of all $m[\gamma]$-admissible torsions is defined by

$$\mathcal{T}_\gamma := \{T[a\gamma] \mid a \in C^\infty(M; O(3))\}, \quad \gamma \in \mathcal{I}(M; \mathbb{R}^3).$$

Clearly, $\mathcal{T}_\gamma \subset \Omega^2(M; TM)$ for all $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$. It is shown next that in the case where TM is trivialisable, $\mathcal{T}_\gamma$ may be identified with $C^\infty(M; O(3))$ up to $O(3)$-valued constant functions.

Proposition 8.3. *Let $\gamma, \beta \in \mathcal{I}(M; \mathbb{R}^3)$. Then*

$$m[\gamma] = m[\beta] \quad \textit{and} \quad T[\gamma] = T[\beta] \quad \Longleftrightarrow \quad \beta = a\gamma \quad \textit{with } a \in O(3).$$

Moreover, for each $T \in \mathcal{T}_\gamma$, $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$, the natural surjection

$$\pi_{\mathcal{T}_\gamma} : C^\infty(M; O(3)) \longrightarrow \mathcal{T}_\gamma, \quad a \longmapsto T[a\gamma],$$

satisfies $\pi_{\mathcal{T}_\gamma}^{-1}(T) \cong O(3)$.

Proof. Clearly,

$$m[\gamma] = m[\beta] \quad \Longleftrightarrow \quad \exists a \in C^\infty(M; O(3)) \ \text{ with } \beta = a\gamma. \tag{27}$$

From the equality of the torsions $T[\gamma] = T[\beta]$, the Ricci lemma implies $\nabla[\gamma] = \nabla[\beta]$. By Proposition 7.2 the latter is valid iff there exists $a \in Gl(3)$ such that $\beta = a\gamma$. By (27), $a \in O(3)$, yielding the first statement. The second statement then becomes obvious. □

Identifying constant $O(3)$-valued functions with $O(3)$, the quotient $C^\infty(M; O(3))_{/O(3)}$ is defined analogous to (26). This quotient is a Fréchet manifold, cf. [18]. Now, Proposition 8.3 yields the desired characterisation of dislocation densities.

Theorem 8.1. *Let $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$. Then the set of all $m[\gamma]$-admissible torsions $\mathcal{T}_\gamma$ is isomorphic with $C^\infty(M; O(3))_{/O(3)}$ via the induced isomorphism*

$$\hat{\pi}_{\mathcal{T}_\gamma} : C^\infty(M; O(3))_{/O(3)} \xrightarrow{\cong} \mathcal{T}_\gamma, \quad [a] \longmapsto T[a\gamma].$$

If $\gamma, \beta \in \mathcal{I}(M; \mathbb{R}^3)$ are closed forms $d\gamma = d\beta = 0$, then both connections $\nabla[\gamma]$ and $\nabla[\beta]$ have vanishing torsions $T[\gamma] = T[\beta] = 0$. As a consequence of Proposition 8.3, this yields the following.

Corollary 8.1. *If $\gamma, \beta \in \mathcal{I}(M; \mathbb{R}^3)$ are closed forms, then*

$$m[\gamma] = m[\beta] \quad \Longleftrightarrow \quad \beta = a\gamma \quad \textit{with } a \in O(3).$$

In particular, if $i, j \in E(M; \mathbb{R}^3)$, then

$$m[di] = m[dj] \quad \Longleftrightarrow \quad di = a\, dj \quad \textit{with } a \in O(3).$$

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Appendix A. The structure of $\mathcal{V}(M;\mathbb{R}^3)$

We turn to the question when $\mathrm{d}j+\beta \in \mathcal{I}(M;\mathbb{R}^3)$ where $j \in E(M;\mathbb{R}^3)$, $\beta \in \mathcal{D}(M;\mathbb{R}^3)$. We need an appropriate criterion for β being relatively 'small' as compared to $\mathrm{d}j$. Each metric $g \in \mathcal{M}(M)$ defines a (fibre-) norm on TM given by

$$|v_p|_g := \sqrt{g(p)(v_p, v_p)}, \quad v_p \in T_pM,\ p \in M.$$

On the vector bundle of all strong bundle endomorphisms $\mathrm{End}(TM)$ this norm induces the fibre norm

$$|A_p|_g := \sup_{|v_p|_g=1} |A_p v_p|_g, \quad A \in \mathrm{End}(TM),\ v_p \in T_pM,\ p \in M, \tag{A.1}$$

which in turn on the module of sections $\Gamma(\mathrm{End}(TM))$ induces the maximum norm

$$\|\cdot\|_{g,\infty} := \max_{p\in M} |\cdot|_g. \tag{A.2}$$

The latter is well defined since M is compact. The norm (A.1) is fibrewise an operator norm on $\mathrm{End}(TM)$, i.e. in particular

$$\|A\circ B\|_{g,\infty} \le \|A\|_{g,\infty}\|B\|_{g,\infty} \qquad \forall A, B \in \Gamma(\mathrm{End}(TM)).$$

Let $\eta_g \in \mathcal{I}(M;\mathbb{R}^3)$ be a one-form with $g = m[\eta_g]$ given by Lemma 3.1. Since η_g is injective for each $\alpha \in \Omega^1(M;\mathbb{R}^3)$, there exists a unique $A[\eta_g] \in \Gamma(\mathrm{End}(TM))$ with $\alpha = \eta_g\circ A[\eta_g]$. Thus the norm (A.1) induces a fibre norm on $\Lambda^1(M;\mathbb{R}^3)$, again denoted by $|\cdot|_g$, given by

$$|\alpha_p|_g := |A[\eta_g]_p|_g \qquad \forall \alpha \in \Lambda^1(M;\mathbb{R}^3),\ p \in M. \tag{A.3}$$

This norm is well defined, since for each one-form $\hat{\eta}_g \in \mathcal{I}(M;\mathbb{R}^3)$ with $m[\hat{\eta}_g] = m[\eta_g] = g$ the bundle isomorphism $O \in \mathrm{Aut}(TM)$ given by $\hat{\eta}_g = \eta_g\circ O$ is fibrewise isometric with respect to g. Then $O\circ A[\hat{\eta}_g] = A[\eta_g]$ and we have

$$|A[\hat{\eta}_g]_p|_g = |O_p\circ A[\hat{\eta}_g]_p|_g = |A[\eta_g]_p|_g \quad \forall \alpha \in \Lambda^1(M;\mathbb{R}^3),\ p \in M.$$

On $\Omega^1(M;\mathbb{R}^3)$ the analogue of (A.2) is given by the maximum norm

$$\|\alpha\|_{g,\infty} := \max_{p\in M} |\alpha_p|_g \qquad \forall \alpha \in \Omega^1(M;\mathbb{R}^3). \tag{A.4}$$

It is shown in [18] that the norm (A.3) is equivalent to the norm induced by the fibre metric $\mathcal{G}$. Also, for any two Riemannian metrics $g, \bar{g} \in \mathcal{M}(M)$, the induced norms (A.4) are equivalent. A criterion for the injectivity of one-forms of type $\mathrm{d}j + \beta$ may now be stated in slightly more general form.

Proposition A.1. *Let $g = m[\eta_g] \in \mathcal{M}(M)$ be a fixed Riemannian metric and $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$ be arbitrary. Then there exists a positive constant $c > 0$ such that $\gamma + \beta \in \mathcal{I}(M; \mathbb{R}^3)$ for all $\beta \in \Omega^1(M; \mathbb{R}^3)$ with $\|\beta\|_{g,\infty} < c$.*

Proof. For arbitrary $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$ and each $\beta \in \Omega^1(M; \mathbb{R}^3)$ there are a unique $C[\eta_g] \in \Gamma(\mathrm{Aut}(TM))$ and $B[\eta_g] \in \Gamma(\mathrm{End}(TM))$ such that $\gamma = \eta_g\, C[\eta_g]$ and $\beta = \eta_g\, B[\eta_g]$, respectively. We write

$$\gamma + \beta = \eta_g(id_{TM} + B[\eta_g] \circ C[\eta_g]^{-1}) \circ C[\eta_g],$$

which implies

$$\gamma + \beta \in \mathcal{I}(M; \mathbb{R}^3) \quad \Longleftrightarrow \quad (id_{TM} + B[\eta_g] \circ C[\eta_g]^{-1}) \in \Gamma(\mathrm{Aut}(TM)).$$

By the theorem on *Neumann* series (cf. [1]), the latter holds true for

$$\|B[\eta_g] \circ C[\eta_g]^{-1}\|_{g,\infty} = \|\beta \circ C[\eta_g]^{-1}\|_{g,\infty} < 1.$$

In particular, we have $\gamma + \beta \in \mathcal{I}(M; \mathbb{R}^3)$ for all β such that

$$\|\beta\|_{g,\infty} < \frac{1}{\|C[\eta_g]^{-1}\|_{g,\infty}} =: c\,.$$

This completes the proof. □

Note that the constant c appearing in Proposition A.1 depends on the chosen metric g only. In particular, for $j \in E(M; \mathbb{R}^3)$ we have $\|\mathrm{d}j\|_{m[\mathrm{d}j],\infty} = \|id_{TM}\|_{m[\mathrm{d}j],\infty} = 1$ by definition.

Corollary A.1. *Let $\beta \in \Omega^1(M; \mathbb{R}^3)$. Then $\mathrm{d}j + \beta \in \mathcal{I}(M; \mathbb{R}^3)$ for all $j \in E(M; \mathbb{R}^3)$ such that $\|\beta\|_{m[\mathrm{d}j],\infty} < 1$.*

Corollary A.1 implies that an embedding $j \in E(M; \mathbb{R}^3)$ can bear a given dislocation density $\mathrm{d}\beta$ as long as $\beta \in \mathcal{D}(M; \mathbb{R}^3)$ is small enough such that $\mathrm{d}j + \beta \in \mathcal{I}(M; \mathbb{R}^3)$. The converse is also true:

Theorem A.1. *Let $\mathrm{d}\xi \in \Omega^2(M; \mathbb{R}^3)$ be an arbitrary exact two-form. Then there exists $\gamma \in \mathcal{I}(M; \mathbb{R}^3)$ such that $\mathrm{d}\gamma = \mathrm{d}\xi$. In particular, $\gamma = \mathrm{d}j + \beta \in \mathcal{V}(M; \mathbb{R}^3)$, where β is the divergence-free part of ξ.*

Proof. The Helmholtz decomposition of ξ yields $\xi = \mathrm{d}h + \beta$ with $k \in C^\infty(M; \mathbb{R}^3)$, $\beta \in \mathcal{D}(M; \mathbb{R}^3)$. For any embedding j' and any sufficiently large positive number λ,

$$\|\beta\|_{m[\lambda\,\mathrm{d}j'],\infty} = \tfrac{1}{|\lambda|}\|\beta\|_{m[\mathrm{d}j'],\infty} < 1.$$

By Corollary A.1, setting $j = \lambda \cdot j'$, yields $\gamma := \mathrm{d}j + \beta \in \mathcal{V}(M; \mathbb{R}^3)$. □

Proposition A.1 implies that $\mathcal{V}(M; \mathbb{R}^3) \subset \mathcal{I}(M; \mathbb{R}^3)$ is an open subset of $\mathcal{I}(M; \mathbb{R}^3)$ endowed with the Fréchet topology. Due to the norm equivalence mentioned above, this topology is independent of the metric g on M. Furthermore, one can show that $\mathrm{d}E(M; \mathbb{R}^3) \subset \mathcal{V}(M; \mathbb{R}^3)$ is a Fréchet submanifold of $\mathcal{I}(M; \mathbb{R}^3)$. Thus, $\mathrm{d}E(M; \mathbb{R}^3)$ becomes a submanifold of $\mathcal{V}(M; \mathbb{R}^3)$, see [18] for details.

Proposition A.2. *The configuration space $\mathcal{V}(M; \mathbb{R}^3)$ is an open Fréchet submanifold of $\mathcal{I}(M; \mathbb{R}^3)$ which contains $\mathrm{d}E(M; \mathbb{R}^3)$ as a Fréchet submanifold.*

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