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TORSION AND CURVATURE IN CONTINUOUSLY DEFECTIVE SOLID CRYSTALS

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ABSTRACT. I show how one can utilize the concept of a canonical connection on a homogeneous space to describe defectiveness of a continuous elastic crystal solid.

1. Introduction

The kinematic theory of continuously defective elastic crystals proposed by Davini (1986) has been developed over last 25 years by Davini and Parry, and their collaborators (see, for example, Parry and Šilhavý 1999; Parry and Sigrist 2012; Elżanowski and Parry 2020). The key assumption of this approach is that the state of a defective continuous crystal body is defined by three linearly independent smooth vector fields which are to represent an underlaying atomic structure. The defectiveness of such a state is described by the *dislocation density tensor* (see Eq. 13) measuring the first order interactions of the defining vector fields.

When the dislocation density tensor is position independent the underlying space can be identified with a Lie group acting on itself (Parry 2003). This allows one to use the techniques of the theory of Lie group to analyze in a systematic way the properties of the *uniformly defective crystal states*, in particular, its classification and symmetries. In contrast, when the defining vector fields are such that the corresponding dislocation density tensor is point dependent such an identification is no longer possible. Instead, one can show that the body manifold can be equipped with the properly defined homogeneous space structure (Elżanowski and Preston 2013; Elżanowski and Parry 2020). This in turn allows one to utilize, subject to some additional assumptions, the concept of a canonical connection on a homogeneous space (Wang 1958), the torsion and curvature of which can serve as additional characteristics of the defectiveness of a lattice.

In this paper I discuss the non-uniformly defective elastic crystal states. Continuing the work presented by Elżanowski and Parry (2019) (see also Elżanowski and Parry 2020) where we introduced the canonical connection as a tool in describing non-uniformly defective

Dedicated to the memory of my friend and colleague Serge Preston (1953-2020).

crystals, I show that for a certain subclass of states, called the *reductive states*, one can relate the torsion of a lattice canonical connection to the dislocation density tensor (and the Burgers vector: Parry 2003) while its curvature describes the second order interactions of the defining vector fields being possibly indicative of the existence of the disclinations (see, *e.g.*, Bowick and Giomi 2009; Yavari and Goriely 2013). I conclude the presentation by showing a couple of examples of different non-uniformly defective structures.

2. Continuous lattice and its Lie algebra

Following Davini's approach (Davini 1986), we assume that the kinematic state of a continuous crystal solid body is defined by a *continuous lattice* I, that is, three linearly independent smooth vector fields l_1, l_2, l_3 on the body manifold M of the same dimension. As our considerations are local, the reader may view the manifold M as an open neighborhood in \mathbb{R}^3 . We postulate that the vector fields l_i , i = 1, 2, 3, generate a finite dimensional complete¹ Lie subalgebra L of the algebra of all smooth vector fields on M. We call such an algebra L the *lattice algebra* of the continuous lattice l^2 .

Given the (Lie) algebra \mathbf{L} , there exists an abstract Lie group G, viewed as a subgroup of the group of all diffeomorphism of M, acting smoothly on the left on M, whose Lie algebra \mathfrak{g} is isomorphic to the algebra \mathbf{L} (Palais 1957; Kobayashi 1995). That is, there exists a smooth mapping

$$\Psi: G \times M \to M \tag{1}$$

such that for every $g, \overline{g} \in G$

$$\Psi_g = \Psi(g, \cdot) : M \to M \tag{2}$$

is a diffeomorphism and

$$\Psi(g\overline{g},p) = \Psi(g,\Psi(\overline{g},p)) \tag{3}$$

at any $p \in M$, where $g\overline{g}$ denote a group multiplication in *G*. We also postulate that the action Ψ is transitive on *M*. This implies that the (right) Lie algebra of the group *G* is isomorphic to the lattice algebra **L** via the tangent map

$$d\Psi_p: TG \to TM \tag{4}$$

where $\Psi_p : G \to M$ is the orbit map at $p \in M$ induced by the action Ψ .

Selecting a point, say, $p_0 \in M$, the *isotropy group* G_{p_0} of the action Ψ at p_0

$$G_{p_0} = \{g \in G : \Psi(g, p_0) = p_0\}$$
(5)

is a closed subgroup of the group G. Although, in general, the isotropy group is point p_0 dependent, the isotropy groups at different points are conjugate due to the transitivity of the action Ψ .

Selecting specific isotropy group G_{p_0} , one can show that the body manifold M becomes a *homogeneous space* as it can be identified diffeomorphically with the left quotient $G \setminus G_{p_0}$. The identification is provided by the map $\psi : G \setminus G_{p_0} \to M$ such that

$$\Psi(gG_{p_0}) = \Psi_{p_0}(g) = \Psi(g, p_0) \tag{6}$$

¹These are purely technical assumptions which, as far as I know, have no physical significance.

²The presentation is mathematically correct in any finite dimension. However, for physical reasons we assume that body manifold M is either of dimension three or two.

where gG_{p_0} denotes a coset of the isotropy group G_{p_0} generated by an element $g \in G$. Moreover, the group G acts on the quotient $G \setminus G_{p_0}$ on the left mimicking the corresponding left action of Ψ on M. That is,

$$\psi(h(gG_{p_0})) = \Psi_{p_0}(hg) = \Psi(h(\Psi(g, p_0)) = \Psi(h, \psi(gG_{p_0})).$$
(7)

This, together with the fact that the isotropy group acts freely of *G* on the right preserving individual fiber, implies that one may view the group *G* as a total space of a principal fiber bundle $\pi : G \to M$ with the structure group G_{p_0} where $\pi = \Psi_{p_0}$. In turn, the bundle $\pi : G \to M$ induces on L(M), the bundle of linear frames on *M*, an isomorphic structure by representing the isotropy group as a subgroup of the general linear group $GL(3,\mathbb{R})$. Indeed, given $h \in G_{p_0}$, the tangent mapping $d_{p_0}\Psi_h$ is an automorphism of the tangent space $T_{p_0}M$. Selecting a frame in $T_{p_0}M$, that is a linear isomorphism $u_0 : \mathbb{R}^3 \to T_{p_0}M$ assigning coordinates to a vector, one obtains a representation of the isotropy group G_{p_0} in the general linear group. It is a straightforward exercise to show that the mapping $\lambda : G_{p_0} \to GL(3,\mathbb{R})$.

$$\lambda(h) = u_0^{-1} \circ d_{p_0} \Psi_h \circ u_0, \tag{8}$$

called as a *linear isotropy representation* of G_{p_0} , is a group homomorphism (see, *e.g.*, Kobayashi and Nomizu 1996). Consequently, the collection of mappings

$$L(M,G_0) = \{ d_{p_0} \Psi_g \circ u_0 : \mathbb{R}^3 \to M : g \in G \}$$

$$\tag{9}$$

is a reduction of the bundle of linear frames of *M* to the *linear isotropy group* $G_0 = \lambda(G_{p_0})$. It is easy to show that the principle bundles $\pi : G \to M$ and $L(M, G_0)$ are isomorphic.

3. Lattice connection

A continuous lattice $l = \{l_1, l_2, l_3\}$, defining a state of a crystal body *M*, not only induces a homogeneous space structure on *M* but it also introduces a long-distance parallelism on the body manifold *M*. Such a parallelizm implies the existence of a linear connection characterized by a vanishing curvature. We shall call this connection a *lattice connection*. Its Christoffel's coefficients Γ_{ik}^i , i, j, k = 1, 2, 3, take the form (see, *e.g.*, Epstein 2010)

$$\Gamma^{i}_{jk} = -(l^{a}_{j})^{-1} \frac{\partial l^{i}_{a}}{\partial x_{k}}$$
(10)

where the matrix l_a^i (viewed as mappings from \mathbb{R}^3 to \mathbb{R}^3) represents the vector fields l_a , a = 1, 2, 3 in the natural basis of the coordinate system x_1, x_2, x_3 and where the summation convention over the repeated indices is enforced. Its torsion tensor

$$T = T^i_{jk} l_i \otimes \eta^j \wedge \eta^k, \tag{11}$$

where $T_{jk}^i = \Gamma_{[jk]}^i$ and where η^l , l = 1, 2, 3 denote the co-frame dual to the frame I. In terms of the Lie brackets of the lattice algebra **L** the components of the torsion tensor *T* are given by

$$[l_j, l_k] = T^i_{ik} l_i, \quad i, j, k = 1, 2, 3.$$
(12)

As it was mentioned in the introduction, we postulate that the *defectiveness* of a continuous lattice I is characterized by the *dislocation density tensor* (ddt) S^{ij} (Davini 1986; Parry 2003)

defined by the equations

$$n(p)S^{ij}(p) = \nabla \wedge \eta^i(p) \cdot \eta^j(p), \quad i, j = 1, 2, 3, \ p \in M,$$
(13)

where n(p) is the lattice volume element. It can be shown (Elżanowski and Parry 2004) that the dislocation density tensor and the torsion *T* are related by

$$T^i_{jk} = \varepsilon_{rjk} S^{ir} \tag{14}$$

where ε_{rjk} is the alternating tensor.

The following three cases are particularly relevant both mathematically and physically. First, if the torsion of the lattice connection Γ_{jk}^i vanishes the connection is trivial and the lattice vector fields defining the corresponding parallelism commute. The lattice **l** is holonomic and the lattice Lie algebra **L** is abelian. Physically, the kinematic state the lattice **l** represents is *homogenoeus*, that is, no defects are present and the dislocation density tensor S^{ij} vanishes identically. The group G the algebra **L** induces can be viewed, without the loss of generality, as a group of linear translations on \mathbb{R}^3 . In fact, G can be identify with \mathbb{R}^3 acting on itself by translations. In other words, the kinematic state the lattice **l** defines is invariant under translations.

Next, assume that the torsion of the lattice connection does not vanish but its value is base point independent. This implies that the components of the torsion tensor T_{jk}^i are identical to the Lie algebra constants of the lattice algebra **L**, *i.e.*, the dislocation density tensor is constant. We say that such a kinematic state is *uniformly defective*. As before, the Lie group *G* is diffeomorphic to \mathbb{R}^3 but its action is non-trivial.

Finally, if the torsion of the lattice connection is a non-trivial function of position, the lattice algebra **L** is of a finite dimension $m > \dim M$, and the kinematic state \mathfrak{l} is said to be *non-uniformly defective*. The lattice algebra **L** induces an m-parameter connected Lie group G acting on M in such a way that the isotropy group G_{p_0} is non-trivial and of dimension $m - \dim M$. As the isotropy group is a Lie subgroup of the Lie group G its (left) Lie algebra \mathfrak{g}_0 is a Lie subalgebra of the (left) Lie algebra \mathfrak{g} . Viewing \mathfrak{g} as the algebra of all left-invariant vector fields on G, it can always be presented as a simple sum of the isotropy algebra \mathfrak{g}_0 and a vector space complement $\mathbf{V} \subsetneq \mathfrak{g}$, that is,

$$\mathfrak{g} = \mathfrak{g}_0 \oplus \mathbf{V},\tag{15}$$

where the vector space \mathbf{V} is not uniquely defined. Note that, in general, \mathbf{V} is not a subalgebra of \mathfrak{g} . In what follows we shall consider non-uniformly defective kinematic states.

4. Lattice canonical connection

Consider a lattice $l = \{l_1, l_2, l_3\}$ representing a non-uniformly defective kinematic state of the solid M. In other words, the frame l_i , i = 1, 2, 3, is non-holonomic and the corresponding lattice algebra \mathbf{L} is of dimension bigger than the dimension of M. This implies that the isotropy group G_{p_0} of the action of the Lie group G on M is non-trivial and its algebra \mathfrak{g} can be represented as $\mathfrak{g} = \mathfrak{g}_0 \oplus \mathbf{V}$ for some 3-dimensional vector space $\mathbf{V} \subset \mathfrak{g}$ of left-invariant vector fields on G. As the choice of the subspace \mathbf{V} is not unique, we shall assume that \mathfrak{g} admits a *reductive decomposition*(Kobayashi and Nomizu 1996), that is, a decomposition $\mathfrak{g}_0 \oplus \mathbf{V}$ in which the vector complement \mathbf{V} is such that

$$[\mathfrak{g}_0,\mathbf{V}]\subseteq\mathbf{V}.\tag{16}$$

We should point out here that although given a subalgebra $\mathfrak{g}_0 \subsetneq \mathfrak{g}$ there is always a vector space $\mathbf{V} \subseteq \mathfrak{g}$ such that $\mathfrak{g} = \mathfrak{g}_0 \oplus \mathbf{V}$, not every such decomposition is reductive. In fact, given \mathfrak{g} there may not exists a complement \mathbf{V} making the decomposition $\mathfrak{g} = \mathfrak{g}_0 \oplus \mathbf{V}$ reductive (Poor 1981).

The vector space **V** forms a horizontal distribution on the principle bundle $\pi : G \to M$ in the sense that it depends smoothly on *G* and the projection $d\pi : TG \to TM$ is surjective with the subalgebra \mathfrak{g}_0 as its kernel. Moreover, **V** defines a horizontal distribution of a left invariant principle bundle connection on $\pi : G \to M$. Indeed, the fact that the decomposition $\mathfrak{g} = \mathfrak{g}_0 \oplus \mathbf{V}$ is reductive implies that **V** is also invariant under the right action of the isotropy group (Wang 1958; Elżanowski and Parry 2020). Such a principle bundle connection is called a *canonical connection* of the homogeneous space $M \cong G \setminus G_{p_0}$.

As the bundles $\pi: G \to M$ and $L(M, G_0) \subset L(M)$ are isomorphic, the principal connection associated with the distribution V induces a linear connection on *M* (Wang 1958; Kobayashi and Nomizu 1996). To this end, let Π be an equivariant linear mapping from the Lie algebra g to the Lie algebra $gl(3,\mathbb{R})$ of the general linear group $GL(3,\mathbb{R})$ such that

$$\Pi(X) = \begin{cases} d\lambda(X), & X \in \mathfrak{g}_0, \\ 0, & X \in \mathbf{V}, \end{cases}$$
(17)

where $d\lambda$ denotes the tangent map of the linear isotropy representation λ . The corresponding *linear canonical connection* on the reduced frame bundle $L(M, G_0)$ is given by a $gl_0(3, \mathbb{R})$ -valued one-form ω (a connection form) such that

$$\omega(\tilde{X}) = \Pi(X), \quad X \in \mathfrak{g}, \tag{18}$$

where \widetilde{X} is the *natural lift*³ of a vector field X to the bundle $L(M, G_0)$ and $gl_0(n, \mathbb{R})$ denotes the Lie algebra of the linear isotropy group $G_0 \subseteq Gl(n, \mathbb{R})$ (Kobayashi and Nomizu 1996). Note that thus defined linear canonical connection ω is left-invariant under the induced action of G on $L(M, G_0)$ and that its horizontal distribution is simply the image of the vector space V under the said principle bundle isomorphism⁴. Consequently, identifying V with \mathbb{R}^3 via the projection π and the frame u_0 , one is able to obtain its torsion and curvature (Kobayashi and Nomizu 1996).

Theorem 1. Let \mathbf{l} be continuous lattice defined on a body manifold M. Select a base point $p_0 \in M$ and a frame $u_0 : \mathbb{R}^3 \to T_{x_0}M$. Assume also that the homogenous space $G \setminus G_{p_0}$ associated with the lattice \mathbf{l} is reductive, that is, that the Lie algebra $\mathfrak{g} = \mathfrak{g}_0 \oplus \mathbf{V}$ for some vector complement \mathbf{V} such that $[\mathfrak{g}_0, \mathbf{V}] \subseteq \mathbf{V}$. Then, relative to the choice of the frame u_0 , the torsion and curvature of the corresponding linear canonical connection are given at p_0 by

- (a) $T(X,Y) = -[X,Y]_{\mathbf{V}}$,
- (b) $R(X,Y)Z = -[[X,Y]_{g_0},Z]$

for any $X, Y, Z \in \mathbf{V}$ where $[\cdot, \cdot]_{\mathbf{V}}$ and $[\cdot, \cdot]_{\mathfrak{g}_0}$ denote respectively the \mathbf{V} and \mathfrak{g}_0 components of the Lie algebra bracket in \mathfrak{g} . In addition, both tensors are covariantly constant.

³A vector field X on the group G generates a one-parameter group of left translations which in turn induces a one-parameter group of transformation of $L(M, G_0)$ the tangent vector of which is defined as a natural lift of X (Kobayashi and Nomizu 1996).

⁴For a more detailed derivation (see, for example, Kobayashi and Nomizu 1996; Elżanowski and Parry 2020).

Given a continuous lattice l, let w_1, w_2, w_3 denote right-invariant vector fields on G such that

$$d_g \Lambda_{x_0}(w_i) = l_i, \quad i = 1, 2, 3.$$
⁽¹⁹⁾

As the mapping $d_g \Lambda_{p_0}$ is of rank 3 and as the vector fields l_1, l_2, l_3 are linearly independent, the right-invariant vector fields w_1, w_2, w_3 are also linearly independent. Let v_1, v_2, v_3 be the *equivalent set* of left-invariant vector fields on G, that is, the set of elements of the algebra g such that

$$v_i = di(w_i), \quad i = 1, 2, 3,$$
 (20)

where i is the inverse map on the group G, *i.e.*, $i(g) = g^{-1}$, $g \in G$. It can be shown (Olver 1995) that

$$[v_i, v_j] = -[w_i, w_j], \quad [v_i, w_j] = 0, \quad i, j = 1, 2, 3.$$
(21)

Let a vector space $\mathbf{V}_l = \operatorname{span}\{v_1, v_2, v_3\}$. Clearly, \mathbf{V}_l is a vector subspace of the Lie algebra \mathfrak{g} and $\mathfrak{g} = \mathfrak{g}_0 \oplus \mathbf{V}_l$ as the isotropy subalgebra \mathfrak{g}_0 is the kernel of the projection $d\pi : TG \to TM$. Assume that the lattice \mathfrak{l} is such that the decomposition $\mathfrak{g} = \mathfrak{g}_0 \oplus \mathbf{V}_l$ is reductive, a property which cannot be guaranteed in general (see the lattice (30)). We call the corresponding linear canonical connection ω_l the *lattice canonical connection* of a *continuous reductive lattice* \mathfrak{l} .

As shown by Wang (1958) (see also Kobayashi and Nomizu 1996), the coefficients of the torsion tensor of the lattice canonical connection ω_l (in the frame v_1, v_2, v_3) are the smooth functions $\widehat{T}_{ik}^i: M \to \mathbb{R}, i, j, k = 1, 2, 3$, such that

$$\widehat{T}_{jk}^{i} v_{i} = [v_{j}, v_{k}]_{\mathbf{V}_{l}},\tag{22}$$

where $[\cdot, \cdot]_{\mathbf{V}_l}$ denotes the \mathbf{V}_l -component of the Lie bracket of the algebra \mathfrak{g} . Respectively, the coefficients of the curvature tensor of the connection ω_l are the smooth functions $\widehat{R}^i_{ikl}: M \to \mathbb{R}$ defined by

$$\widehat{R}^i_{jkl}v_i = [[v_j, v_k]_{\mathfrak{g}_0}, v_l]$$
(23)

where $[\cdot, \cdot]_{\mathfrak{g}_0}$ is the \mathfrak{g}_0 component of the Lie bracket in \mathfrak{g}^5 .

The following corollary is the immediate consequence of Theorem 1 and the definition and the properties of the equivalent set of left-invariant vector fields (19), (20), (21).

Corollary 1. If a continuous lattice l defined by the vector fields l_i , i = 1, 2, 3, admits a reductive decomposition $\mathfrak{g}_0 \oplus \mathbf{V}_l$, then the torsion of the lattice canonical connection ω_l is minus the torsion of the lattice connection Γ^i_{ik} .

In conclusion, the defectiveness of a kinematic state defined by a continuous reductive lattice is described not only by the dislocation density tensor

$$S^{ir} = \frac{1}{2} \varepsilon^{rkl} T^i_{kl} = -\frac{1}{2} \varepsilon^{rkl} \widehat{T}^i_{kl}$$
(24)

but also by the curvature \hat{R}^i_{jkl} of the corresponding lattice canonical connection ω_l measuring the second order interactions of the defining vector fields.

⁵Note that the curvature \hat{R}^i_{ikl} is not defined for a non-reductive decomposition of a lattice.

5. Examples

In this last section I briefly discuss two different lattice structures. Namely, I show that the first lattice is reductive, thus allowing for the existence of the lattice canonical connection ω_l , while the second lattice is not reductive and the only characteristic of its defectiveness is provided by the torsion of its lattice connection Γ_{ik}^i .

(A) Consider a continuous lattice l in \mathbb{R}^3 defined (in the standard coordinate system) by the vector fields

$$l_1 = (1,0,0), \ l_2 = (-y,1,0), \ l_3 = (x,y,1).$$
 (25)

Straightforward calculations show, that it generates a four dimensional lattice algebra L such that

$$T_{13}^1 = T_{23}^2 = 1, \ T_{23}^1 = y \tag{26}$$

while all other Lie algebra constants vanish. It induces on \mathbb{R}^3 a left action Λ of a four parameter group $G = \{(a, b, c, d) : a, b, c, d \in \mathbb{R}\}$ such that

$$g\overline{g} = \left(\overline{a} + ae^{-\overline{d}} - b(\overline{b} + \overline{c}), b + \overline{b}, (b + c)e^{-\overline{d}} + \overline{c} - b, d + \overline{d}\right)$$
(27)

and

$$\Lambda((a,b,c,d),(x,y,z) = \left((x+a-yb)e^d,(y+b+c)e^d,z+d\right)$$
(28)

for any $x, y, z) \in \mathbb{R}^3$. The isotropy group of the action Λ at $p_0 = (x_0, y_0, z_0)$ is

$$G_0 = \{ (y_0 b, b, -b, 0) : b \in \mathbb{R} \}.$$
(29)

As the algebra g of all left-invariant vector fields on *G* is spanned by $v_1 = (1,0,0,0)$, $v_2 = (-b,1,0,0)$, $v_3 = (-b,0,1,0)$ and $v_4 = (-a,0,-b-c,1)$ and as the Lie algebra of the isotropy group g_0 is generated by $(y_0,1,-1,0)$, the decomposition $g = g_0 \oplus V_l$, where $V_l = \text{span}\{v_1, v_2, v_4\}$ is reductive and V_l is consistent, (20), with the lattice frame $I = \{l_1, l_2, l_3\}$. The torsion of the corresponding lattice canonical connection is such that $\hat{T}_{13}^1 = \hat{T}_{23}^2 = -1$, $\hat{T}_{23}^1 = -y$ and has only two non-zero curvature coefficients $\hat{R}_{232}^1 = -\hat{R}_{233}^1 = 1$.

(B) Let the lattice l in \mathbb{R}^2 be defined by the vector fields

$$l_1 = (x, 0), l_2 = (1, 1).$$
 (30)

It generates an action of a three parameter group G given by the function Λ : $G \times \mathbb{R}^2 \to \mathbb{R}^2$ such that

$$\Lambda(g,(x,y)) = (xe^a + b + c, y + c) \tag{31}$$

where $g = (a, b, c) \in G$ and where the group multiplication is given by

$$g\overline{g} = (a + \overline{a}, (b + \overline{c})e^a + b - \overline{c}, c + \overline{c}).$$
(32)

The isotropy group of the action Λ at a point $p_0 = (x_0, y_0)$ is $G_{p_0} = \{(a, -x_0e^a, 0) : a \in \mathbb{R}\}$ and its Lie algebra \mathfrak{g}_0 is defined by the left invariant vector field $(1, -x_0e^a, 0)$. It is easy to show that its \mathbf{V}_l complement to the Lie algebra \mathfrak{g} is spanned by the left invariant vector fields (1, 0, 0) and $(0, e^a - 1, 1)$. However, it is also easy to

show that the decomposition $\mathfrak{g} = \mathfrak{g}_0 \oplus \mathbf{V}_l$ is not reductive. Thus, a lattice canonical connection ω_l is not available. The only measure of defectiveness available for this lattice is the torsion of the lattice connection

$$T_{12}^1 = \frac{1}{x}, \ T_{12}^2 = 0.$$
 (33)

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