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The 'moving frame', and defects in crystals

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Abstract

I outline a special theory of defective crystals where the microstructure is represented by fields of lattice vectors and their spatial derivatives. Since these fields are assumed to be smooth, in the model, it is a central issue to be precise about the sense in which such fields can represent defects, and that is done by introducing elastic invariant integrals (of which the most elementary examples are the Bürger's integrals and the dislocation density).

It turns out that the notion of slip has a natural place in the analysis of these elastic invariant integrals, and moreover that the formulation invites one to draw results from Cartan's theory of 'equivalence' of vector fields, and also from the theory of Lie groups. Indeed, it is a remarkable fact that one can identify material points in a crystal that has constant dislocation density tensor with an appropriate Lie group, as a consequence of which one finds that such crystals have a self-similarity which generalises the classic idea of generating a perfect crystal (lattice) by translation of a particular unit cell. Generally, it seems that there is much to be done in adapting known mathematical results to this context.

Keywords: Crystal; Defect; Invariant integral; Lattice vector

1. Introduction

My intention, in this paper, is to describe aspects of a theory of defective crystals which have been developed in the past few years with Davini, Fonseca and Silhavy. In particular, I shall emphasise relevant mathematical notions which are not usually employed in a continuum mechanics context: Cartan's theory of equivalence, simple ideas involving Lie groups, Thurston's concept of groups with small generators. For the most part, I focus on kinematical aspects of the theory, and base the exposition on a simple model of defective crystals introduced by Davini (1986), wherein smoothly varying lattice vector fields are supposed to capture relevant averaged geometrical features of the distribution of atoms within a crystal.

The paper begins with a description of the model; three linearly independent vector fields are defined at each point of a region which represents the current position of material points which make up the body.

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The central notions of elastic deformation (or diffeomorphism) and elastic invariants are introduced. Some of the elastic invariants are widely known – in this category are the Bürgers integrals and the dislocation density tensor (which I shall refer to as the classic invariants, in the sequel) – but it is not generally appreciated that there is an infinite number of elastic invariants, with the same properties as the classic invariants. Here, one notes the first connection with a mathematical theory that is not usually referred to in this area – 'Cartan's theory of equivalence' relates to the classification of vector fields with respect to an equivalence, which places vector fields which are diffeomorphic to one another in the same class. The 'moving frame' of the title is just Cartan's name for the set of vector fields (more precisely, I suppose he called it the 'repere mobile'). The invariants that he used in his analysis are the generalisations of the classic invariants mentioned above, and it is an important result that there is a finite functional basis of such invariants. One notes that this basis of invariants contains elements other than the Bürgers integrals and dislocation density tensor. In fact, the specific nature and context of the model that we are interested in gives more invariants than Cartan derived, or employed, in his work, so that results of his need to be adapted a little for the specific applications here.

The following question is important: if all elastic invariants match in two crystal states, then how are the crystal states related? Plainly, the two states may be related elastically, but it turns out that such states may also be related by slip (where the term slip means a rearrangement of material points in sets where lattice vector fields are constant, just as one sees in phenomenological theories of plasticity). It seems to me that this result is a success of the theory; the slip mechanism has an abstract status, which emerges from ideas that do not anticipate the kinematics of particular types of defects in crystals, so the simple model and framework that we employ is sufficiently wide to encompass main features of inelastic behaviour.

Aspects of the theory of Lie groups also enter into the considerations, even though that is not generally realised. This can be seen most simply in the case where the dislocation density tensor is constant in a particular crystal state. It turns out that, in that case, the lattice vector fields vary in such a manner that there is an elastic deformation, which maps the vector fields in a neighbourhood of any given point to the vector fields in an appropriate neighbourhood of any other point in the same state. Thus, the state has a remarkable self-similarity corresponding to the set of such elastic deformations. (In the case of a perfect crystal, where the lattice vectors are constant, this particular set of elastic deformations consists of the translations which map lattice vectors unchanged from one point to another). It is a basic fact of the theory of Lie groups that one can (locally) reconstruct a Lie group from the corresponding Lie algebra, and that the Lie algebra is defined by the so-called 'structure constants'. In this context, the structure constants turn out to be the components of the dislocation density tensor; the elements of the Lie group are represented by the material points of the body and the composition function for the group (which effects multiplication of group elements) turns out to provide the set of elastic deformations, which gives the self-similarity of the crystal state.

Of course, one needs more than kinematics in a mechanical theory of defective crystals, and one has to accept that significant dissipation of energy occurs in inelastic deformation. So, the proper setting for an appropriate theory of inelastic behaviour is undoubtedly thermodynamical, even though a sufficiently general structure does not exist at the moment, so far as I know. This means that there is a place for simple treatments of the mechanics, and I illustrate such by outlining a variational problem which entirely ignores the dissipation of energy which is involved in slip. This problem deals with a perfect crystal which can deform elastically, and can also deform through slip; if one makes logical assumptions regarding the symmetry of the energy function, then one finds that the infimum of the energy functional is produced by the limit of piecewise differentiable functions (representing both elastic deformation and slip) with every increasing numbers of surfaces of discontinuity. The limit functions themselves are nowhere differentiable, in general, but significant volume averages are well defined. In particular, the average limiting Cauchy stress tensor is well defined, and one calculates that it is isotropic. If one accepts that, in a perfect crystal, shear stresses relax by developing sufficiently finely distributed properly oriented shear bands, then this rather

startling result might have some appeal. Realistically, though one needs to predict a small but finite shear strength, there is a need to refine the model, and various options are mentioned briefly in the text.

However, one chooses to proceed, to improve the mechanics; one has to concede that real crystals are never perfect, and so one has to reassess the symmetry assumptions that are used in a prototypical variational argument (say). To be specific, suppose that the dislocation density tensor is constant, once again, and ask if there is an analogue of the perfect lattice case where one envisages that atoms of a corresponding discrete model of the crystal are generated by translation using the constant lattice vectors. In the perfect lattice case, the symmetries of this discrete set of points (the Bravais lattice) are transferred to the energy function, so the passage from discrete to continuum models is the assumption that symmetries of relevant energy functions are transferred in an obvious way between the two levels of description.

There is indeed an analogue of the procedure outlined above, for some defective crystals. Thurston's treatment of groups with small generators appears to be relevant. I show, using his results, that for some choices of dislocation density tensor, an iterative procedure (akin to that which produces a perfect lattice from one atom by appropriate translations) gives discrete sets of points which have a non-zero minimum separation. If the lattice vectors are quantities of macroscopic order, then the discrete points so generated hardly represent the atoms of the crystal. Nevertheless, the discrete set of points obtained in this way encapsulates some aspect of a discrete structure which underlies the continuum model, and one may pass from the symmetries of this discrete structure to the symmetries of the continuum model as one traditionally does for a perfect crystal. This seems reasonable in the absence of any better ideas. Symmetry assumptions are quite critical, in this area (in the perfect crystal case, the lack of convexity of the variational problem derives from the symmetry assumptions, and that lack gives minimisers with infinitely fine oscillations). So, it seems that the study of the crystallography of defective crystals, by which I mean the classification of sets of points generated by iteration procedures like the one outlined above, must prefigure any analysis of corresponding variational problems, or any more realistic thermodynamical treatment of the continuum mechanics of such crystals.

2. Lattice vectors, elastic deformations

Let a region Ω be given and let $\boldsymbol{d}_a(\boldsymbol{x}),\ a=1,2,3$ denote three linearly independent vector fields defined at each point $\boldsymbol{x}\in\Omega$. Suppose that $1/n\equiv\det\{\boldsymbol{d}_a(\boldsymbol{x})\}>0$ for all $\boldsymbol{x}\in\Omega$. We call the set $\{\boldsymbol{d}_a(\boldsymbol{x})\}$, the lattice vector fields at a point $\boldsymbol{x}\in\Omega$, and call

$$\Sigma=\{\boldsymbol{d}_a(\cdot),\Omega\},\tag{1}$$

the state of the crystal. In any state Σ, the domain $\Omega\subset\boldsymbol{R}^3$ is to be a simply connected open set, and the lattice vector fields are to be smooth, $\boldsymbol{d}_a(\cdot)\in C^\infty(\Omega,\boldsymbol{R}^3)$.

Define

$$\boldsymbol{d}^a(\boldsymbol{x})=\tfrac{1}{2}n\varepsilon^{abc}\boldsymbol{d}_b(\boldsymbol{x})\wedge\boldsymbol{d}_c(\boldsymbol{x}),\tag{2}$$

so that

$$\boldsymbol{d}^a(\boldsymbol{x})\cdot\boldsymbol{d}_b(\boldsymbol{x})=\delta^a_b,\tag{3}$$

and call the set $\{\boldsymbol{d}^a(\boldsymbol{x})\}$, the dual lattice vector fields at the point $\boldsymbol{x}\in\Omega$. Thus, the state of the crystal is specified by three independent lattice vectors $\boldsymbol{d}_a$, assigned over that region of space Ω, occupied by the body. The lattice vectors are imagined to characterise the behaviour of the crystal on a macroscopic scale, and are envisaged as an average of vectors which represent interatomic positions. Accordingly, these vectors are assumed to vary smoothly on the macroscopic scale. Even if defects occur at the atomic scale, so that there is no recognisable lattice of atoms, it is assumed that these averages are observable at a coarser level. The

evolution of defects is then supposed to account for the discrepancy between the macroscopic deformation and the behaviour of the $\boldsymbol{d}_a$.

Definition 1. (i) A state $\Sigma = \{\boldsymbol{d}_a(\cdot), \Omega\}$ is *elastically related* to a state $\Sigma^* = \{\boldsymbol{d}_a^*(\cdot), \Omega^*\}$, if there exists a diffeomorphism $\boldsymbol{u} : \Omega \to \Omega^* = \boldsymbol{u}(\Omega)$ such that

$$\boldsymbol{d}_a^*(\boldsymbol{u}(\boldsymbol{x})) = \nabla\boldsymbol{u}(\boldsymbol{x})\boldsymbol{d}_a(\boldsymbol{x}), \quad a = 1,2,3, \ \ \boldsymbol{x} \in \Omega. \tag{4}$$

Then, write $\Sigma^* = \boldsymbol{u}\Sigma$, for brevity.

(ii) A state $\Sigma = \{\boldsymbol{d}_a(\cdot), \Omega\}$ is *locally elastically related* to a state $\Sigma^* = \{\boldsymbol{d}_a^*(\cdot), \Omega^*\}$, if for each $\boldsymbol{x}_0 \in \Omega$ there exists a diffeomorphism $\boldsymbol{u}_{\boldsymbol{x}_0}$, defined on a neighbourhood $N_{\boldsymbol{x}_0}$ of $\boldsymbol{x}_0$ in Ω, with $\boldsymbol{u}_{\boldsymbol{x}_0}(N_{\boldsymbol{x}_0}) \subset \Omega^*$, such that

$$\boldsymbol{d}_a^*(\boldsymbol{u}_{\boldsymbol{x}_0}(\boldsymbol{x})) = \nabla\boldsymbol{u}_{\boldsymbol{x}_0}(\boldsymbol{x})\boldsymbol{d}_a(\boldsymbol{x}), \quad a = 1,2,3, \ \ \boldsymbol{x} \in N_{\boldsymbol{x}_0}, \ \ \boldsymbol{x}_0 \in \Omega. \tag{5}$$

3. Elastic invariants

The elastic deformations defined above occupy a pivotal position in the sequel; also, elastic invariant integrals which are unchanged by (any) elastic deformation will play an important role.

For any state Σ, and each $\boldsymbol{x} \in \Omega$, let

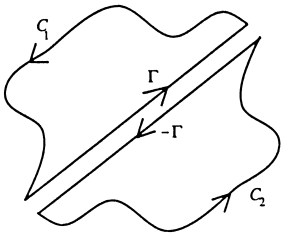
$$\Delta_\Sigma^{(r)}(\boldsymbol{x}) \equiv \left\{\boldsymbol{d}^a(\boldsymbol{x}), \ \nabla\boldsymbol{d}^a(\boldsymbol{x}), \ldots, \nabla^{(r)}\boldsymbol{d}^a(\boldsymbol{x}); \quad a = 1,2,3\right\}, \tag{6}$$

where $\nabla^{(r)}$ denotes the spatial gradient operator of order r. The elastic invariant integrals will be circuit, surface and volume integrals of the form

$$\oint_{\boldsymbol{C}} \boldsymbol{f} \cdot \mathrm{d}\boldsymbol{x}, \quad \int_{\boldsymbol{S}} \boldsymbol{g} \cdot \mathrm{d}\boldsymbol{S}, \quad \int_V h\,\mathrm{d}V, \tag{7}$$

where $\boldsymbol{C}$, $\boldsymbol{S}$, V are circuits, surfaces and subsets (with vol $(V) \neq 0$) of Ω, and each of $\boldsymbol{f}$, $\boldsymbol{g}$, h has argument $\Delta_\Sigma^r(\boldsymbol{x})$, for some integer r. The classic example of an elastic invariant integral is Bürger's integral $\oint_{\boldsymbol{C}} \boldsymbol{d}^a \cdot \mathrm{d}\boldsymbol{x}$ (Kondo, 1955; Bilby, 1960; Kröner, 1960, 1981). Although this integral appears centrally in the theory of continuous distributions of dislocations, its properties (which are the reasons I focus on it here) are not generally in evidence. Note that

(i)



Let $\boldsymbol{C} = \boldsymbol{C}_1 \cup \boldsymbol{C}_2$ and choose Γ, as shown, so that $\boldsymbol{C}_1 \cup \Gamma$, $\boldsymbol{C}_2 \cup (-\Gamma)$ are closed circuits. Then, it is clear that

$$\oint_{\boldsymbol{C}} \boldsymbol{d}^a \cdot \mathrm{d}\boldsymbol{x} = \int_{\boldsymbol{C}_1} \boldsymbol{d}^a \cdot \mathrm{d}\boldsymbol{x} + \int_{\boldsymbol{C}_2} \boldsymbol{d}^a \cdot \mathrm{d}\boldsymbol{x} = \oint_{\boldsymbol{C}_1 \cup \Gamma} \boldsymbol{d}^a \cdot \mathrm{d}\boldsymbol{x} + \oint_{\boldsymbol{C}_2 \cup (-\Gamma)} \boldsymbol{d}^a \cdot \mathrm{d}\boldsymbol{x}. \tag{8}$$

(ii) Write the transformation law (4) as

$$\boldsymbol{d}_a \to F\boldsymbol{d}_a = \boldsymbol{d}_a^*, \quad \text{where } F = \nabla\boldsymbol{u}, \tag{9}$$

and check that this implies

$$\boldsymbol{d}^a \to F^{-\mathrm{T}}\boldsymbol{d}^a = \boldsymbol{d}^{a*}, \tag{10}$$

where $F^{-\mathrm{T}}$ is the inverse transpose of F. Under elastic deformation $\boldsymbol{C} \to \boldsymbol{y}(\boldsymbol{C}) = \boldsymbol{C}^*$ and

$$\oint_{C^*} \boldsymbol{d}^{a*} \cdot \mathrm{d}\boldsymbol{y} = \oint_{C} F^{-\mathrm{T}}\boldsymbol{d}^a \cdot F\mathrm{d}\boldsymbol{x} = \oint_{C} \boldsymbol{d}^a \cdot \mathrm{d}\boldsymbol{x}. \tag{11}$$

Thus, Bürger's integral is additive over subregions of Ω (in the sense of (i)), and invariant under elastic deformations (this is (ii)). Now, notice that it is easy to construct an infinite number of elastic invariant integrals, satisfying analogues of properties (i) and (ii) above. To do this, let v be a real-valued *elastic scalar invariant of order r*, so that if Σ is elastically related to Σ^*, and

$$\Delta^{(r)}_{\Sigma^*}(\boldsymbol{x}^*) = \left\{\boldsymbol{d}^{a*}(\boldsymbol{x}^*), \nabla\boldsymbol{d}^{a*}(\boldsymbol{x}^*), \ldots, \nabla^{(r)}\boldsymbol{d}^{a*}(\boldsymbol{x}^*); \quad a = 1,2,3\right\}, \tag{12}$$

where $x^* = \boldsymbol{u}(\boldsymbol{x}) \in \Omega^*$, then

$$v\left(\Delta^{(r)}_{\Sigma^*}(\boldsymbol{x}^*)\right) = v\left(\Delta^{(r)}_{\Sigma}(\boldsymbol{x})\right). \tag{13}$$

Stated more simply, let v be a real-valued function of the (dual) lattice vectors and their derivatives (up to order r) which is unchanged in any elastic deformation. One calculates, by differentiation, that if v is such a scalar, then $\boldsymbol{d}_a \cdot \nabla v$ is a scalar of order $(r+1)$. So $\boldsymbol{d}_b \cdot \nabla(\boldsymbol{d}_a \cdot \nabla v)$ is a scalar of order $(r+2)$, and so on. If v is not constant, then at least one of $\boldsymbol{d}_a \cdot \nabla v$, $a = 1,2,3$, is non-zero, and so on. Generally, one non-constant scalar function will generate an infinite number of different scalars in this way. Moreover, given any particular scalar v, it is clear that $\oint_C v\boldsymbol{d}^a \cdot \mathrm{d}\boldsymbol{x}$ is an elastic invariant integral which satisfies analogues of (i) and (ii) above. Hence it is sufficient, for a proof of the result quoted, to construct just one scalar which is generally non-constant. Now, just note that $n \to (\det F)^{-1}n$, $\nabla \wedge \boldsymbol{d}^a \to (\det F)^{-1}F\nabla \wedge \boldsymbol{d}^a$, under elastic deformation, so

$$\frac{\boldsymbol{d}^b \cdot \nabla \wedge \boldsymbol{d}^a}{n} \quad \text{is a scalar.} \tag{14}$$

In fact, define

$$S^{ab} = \boldsymbol{d}^b \cdot \nabla \wedge \boldsymbol{d}^a \tag{15}$$

and refer to S^{ab}/n as the lattice components of the dislocation density tensor. Notice that

$$\oint_C \boldsymbol{d}^a \cdot \mathrm{d}x, \quad \int_V S^{ab}\,\mathrm{d}V, \quad \int_V n\,\mathrm{d}V \tag{16}$$

are elastic invariant integrals, and that the same is true of

$$\oint_C v\boldsymbol{d}^a \cdot \mathrm{d}x, \quad \int_V vS^{ab}\,\mathrm{d}V, \quad \int_V vn\,\mathrm{d}V \tag{17}$$

provided that v is any scalar. Thus, there is an 'overabundance' (cf. Olver, 1995) of elastic invariants, and it is natural to enquire if any specific invariant, or list of specific invariants, is sufficient to describe the 'defectiveness' of the crystal in some sense. This will be the thrust of Sections 4–6, culminating in a proof that there is a functional basis of invariants, which is sufficient for this purpose.

Some of the integral invariants in Eq. (17) have a topological interpretation, which is not immediately apparent. I follow Arnol'd (1986) and consider the invariant $\int_V S^{ab}\,\mathrm{d}V$. For simplicity choose $a = b = 1$, put $\boldsymbol{d}^1 \equiv \boldsymbol{d}$ and suppose that $\nabla \wedge \boldsymbol{d}$ is tangential to the boundary of V. (So the analysis applies, for example, if $\nabla \wedge \boldsymbol{d}$ vanishes outside some subset of V of Ω.) Let

$$S(\boldsymbol{d}(\cdot)) = \int_V \boldsymbol{d}\cdot\boldsymbol{\nabla}\wedge\boldsymbol{d}\,\mathrm{d}V. \tag{18}$$

Then,

$$S(\boldsymbol{d}(\cdot)) = S(\{\boldsymbol{d}+\boldsymbol{\nabla}\phi\}(\cdot)), \tag{19}$$

where $\phi(\boldsymbol{x})$ is an arbitrary function for

$$\int_V (\boldsymbol{d}+\boldsymbol{\nabla}\phi)\cdot\boldsymbol{\nabla}\wedge[\boldsymbol{d}+\boldsymbol{\nabla}\phi]\,\mathrm{d}V = \int_V (\boldsymbol{d}+\boldsymbol{\nabla}\phi)\cdot\boldsymbol{\nabla}\wedge\boldsymbol{d}\,\mathrm{d}V = S(\boldsymbol{d}(\cdot)) + \int_V \boldsymbol{\nabla}\phi\cdot\boldsymbol{\nabla}\wedge\boldsymbol{d}\,\mathrm{d}V,$$

and,

$$\int_V \boldsymbol{\nabla}\phi\cdot\boldsymbol{\nabla}\wedge\boldsymbol{d}\,\mathrm{d}V = \int_V \boldsymbol{\nabla}\cdot\{\phi\boldsymbol{\nabla}\wedge\boldsymbol{d}\}\,\mathrm{d}V = \int_{\partial V}\phi\boldsymbol{\nabla}\wedge\boldsymbol{d}\cdot\mathrm{d}\boldsymbol{S} = 0,$$

where ∂V is the boundary of V, since $\boldsymbol{\nabla}\wedge\boldsymbol{d}$ is tangential to ∂V. Now, define

$$\boldsymbol{\eta}(\boldsymbol{x}_1) = -\frac{1}{4\pi}\int_V \{\boldsymbol{\nabla}\wedge\boldsymbol{d}\}(\boldsymbol{x}_2)\wedge\frac{(\boldsymbol{x}_1-\boldsymbol{x}_2)}{|\,\boldsymbol{x}_1-\boldsymbol{x}_2\,|}\,\mathrm{d}V(\boldsymbol{x}_2) \tag{20}$$

and check that

$$\boldsymbol{\nabla}\wedge\boldsymbol{\eta} = \boldsymbol{\nabla}\wedge\boldsymbol{d}. \tag{21}$$

It follows that $\boldsymbol{\eta} = \boldsymbol{d}+\boldsymbol{\nabla}\phi$, for some ϕ, and so $S(\boldsymbol{d}(\cdot)) = S(\boldsymbol{\eta}(\cdot))$. Hence,

$$S(\boldsymbol{d}(\cdot)) = -\frac{1}{4\pi}\int_V\int_V (\boldsymbol{\nabla}\wedge\boldsymbol{d})(\boldsymbol{x}_1)\cdot(\boldsymbol{\nabla}\wedge\boldsymbol{d})(\boldsymbol{x}_2)\wedge\frac{(\boldsymbol{x}_1-\boldsymbol{x}_2)}{|\,\boldsymbol{x}_1-\boldsymbol{x}_2\,|^3}\,\mathrm{d}V(\boldsymbol{x}_1)\,\mathrm{d}V(\boldsymbol{x}_2). \tag{22}$$

Now Gauss' integral formula for the linking number $N(\boldsymbol{C}_1,\boldsymbol{C}_2)$ of two closed curves

$$\boldsymbol{C}_i = \{x_i(t_i); t_i\in[0,T_i],\ x_i(0) = x_0(T_i)\}, \tag{23}$$

where $i = 1,2$ is

$$N(\boldsymbol{C}_1,\boldsymbol{C}_2) = \frac{1}{4\pi}\int_0^{T_1}\int_0^{T_2}\dot{\boldsymbol{x}}_1(t_1)\cdot\dot{\boldsymbol{x}}_2(t_2)\wedge\frac{(\boldsymbol{x}_1(t_1)-\boldsymbol{x}_2(t_2))}{|\,\boldsymbol{x}_1(t_1)-\boldsymbol{x}_2(t_2)\,|^3}\,\mathrm{d}t_1\,\mathrm{d}t_2. \tag{24}$$

This (integer) linking number is the algebraic number of times that one curve passes through a surface which has the other curve as boundary.

Define *dislocation lines* C_1, C_2 emanating from given points $\boldsymbol{x},\boldsymbol{y}$ as

$$\begin{aligned} C_1 &= \{\boldsymbol{x}_1(t_1); \dot{\boldsymbol{x}}_1 = \{\boldsymbol{\nabla}\wedge\boldsymbol{d}\}(\boldsymbol{x}_1),\ \boldsymbol{x}_1(0) = \boldsymbol{x},\ t_1\in[0,T_1]\},\\ C_2 &= \{\boldsymbol{x}_2(t_2); \dot{\boldsymbol{x}}_2 = \{\boldsymbol{\nabla}\wedge\boldsymbol{d}\}(\boldsymbol{x}_2),\ \boldsymbol{x}_2(0) = \boldsymbol{y},\ t_2\in[0,T_2]\}. \end{aligned} \tag{25}$$

Then,

$$\lim_{T_1,T_2\to\infty}\frac{1}{T_1T_2}N(C_1,C_2) \tag{26}$$

gives the asymptotic linking number of these two curves (which are not closed in general). Moreover, the integrand in the two expressions (22) and (26) is the same; the right hand side of Eq. (22) is proportional to the *space average* of that integrand and the right hand side of Eq. (26) is its *time average*. It is (Birkhoff's) theorem of ergodic theory that the space average of the time average equals the space average, and it follows that

$S(\boldsymbol{d}(\cdot))$ is the space integral of the (asymptotic) linking numbers of the dislocation lines. (27)

So, the invariant integral $\int_V \boldsymbol{d}\cdot\nabla\wedge\boldsymbol{d}\,\mathrm{d}V$ measures the degree of entanglement of the dislocation lines, or dislocation loops, in precise fashion.

It is appropriate, here, to give a representation theorem for elastic scalar invariants of order r; see Parry and Silhavy (1999) for a proof. The result emphasises the importance of the dislocation density tensor.

Theorem 1. *v is an elastic scalar invariant of order r if and only if it can be represented in the form*

$$v = v\big(E^{(r)}\big), \tag{28}$$

where $E^{(r)} = \big(W^{(1)}, W^{(2)}\ldots W^{(r)}\big)$ and $W^{(k)}, \quad k = 1,2,\ldots,r$ is defined below.

For $r = 1$, $Z^{(1)}$ is a collection

$$Z^{(1)} = \{Z^{(1)ab},\ a,b = 1,2,3\},$$

and $Y^{(1)}, W^{(1)}$ are similarly defined collections of $Y^{(1)ab}, W^{(1)ab}$, respectively, where

$$Z^{(1)ab} := Y^{(1)ab} := W^{(1)ab} := S^{ab}/n.$$

For each $r > 1$, let further $Z^{(r)}$ be the collection

$$Z^{(r)} = \{Z^{(r)ab}_{c_1\ldots c_{r-1}},\ a,b,c_1,\ldots,c_{r-1} = 1,2,3\},$$

and $Y^{(r)}, W^{(r)}$ similarly defined collections of $Y^{(r)ab}_{c_1\ldots c_{r-1}}$, $W^{(r)ab}_{c_1\ldots c_{r-1}}$, respectively, where

$$Z^{(r)ab}_{c_1\ldots c_{r-1}} := \boldsymbol{d}_{c_{r-1}}\cdot\nabla Z^{(r-1)ab}_{c_1\ldots c_{r-2}},$$

$$Y^{(r)ab}_{c_1\ldots c_{r-1}} := \textit{the symmetrization with respect to } c_1,\ldots,c_{r-1} \textit{ of } Z^{(r)ab}_{c_1\ldots c_{r-1}},$$

and

$$W^{(r)ab}_{c_1\ldots c_{r-1}} = Y^{(r)ab}_{c_1\ldots c_{r-1}} - \frac{1}{(r+1)}\big(\delta^b_{c_1}Y^{(r)am}_{mc_2\cdots c_{r-1}} + \cdots + \delta^b_{c_{r-1}}Y^{(r)am}_{mc_1\ldots c_{r-2}}\big).$$

The last is the traceless part of $Y^{(r)ab}_{c_1\ldots c_{r-1}}$ in the sense

$$W^{(r)am}_{mc_2\ldots c_{r-1}} = \ldots = W^{(r)am}_{c_1\ldots c_{r-2}m} = 0.$$

That is to say, every scalar can be represented as a function of appropriately symmetrized combinations of (directional) derivatives of the dislocation density tensor. This result should be useful from the point of view of constitutive theory, in due course.

Finally, note the following definition:

Definition 2. Let $\Sigma = \{(\cdot), \Omega\}$ be given, and let the fields $S^{ab}(\cdot)$, $n(\cdot)$ be calculated as above. The fundamental set $\mathscr{F}$ of scalar invariants consists of the fields

$$\left\{1, \frac{S^{ab}}{n}(\cdot),\ (\boldsymbol{d}_c\cdot\nabla)\frac{S^{ab}}{n}(\cdot);\ a,b,c = 1,2,3\right\}. \tag{29}$$

This particular set of scalars will be useful when it comes to classifying vector fields which are equivalent with respect to diffeomorphism.

4. Neutrally related states

If two crystal states are elastically related, then (by definition) the elastic invariant integrals correspond in the two states (cf. property (ii) of Bürger's integral). It turns out to be productive to answer the converse question: if all elastic invariant integrals correspond in two different states, then how are those states related?

Precisely, if states $\Sigma = \{\boldsymbol{d}_a(\cdot), \Omega\}$, $\Sigma^* = \{\boldsymbol{d}^*_a(\cdot), \Omega^*\}$ are given, if there exists a C^∞ diffeomorphism $\boldsymbol{u} : \Omega \to \Omega^* = \boldsymbol{u}(\Omega)$ such that

$$\oint_{\boldsymbol{C}} \boldsymbol{f}\left(\Delta^{(r)}_{\Sigma}(\boldsymbol{x})\right) \cdot \mathrm{d}\boldsymbol{x} = \oint_{\boldsymbol{u}(\boldsymbol{C})} \boldsymbol{f}\left(\Delta^{(r)}_{\Sigma^*}(\boldsymbol{x}^*)\right) \cdot \mathrm{d}\boldsymbol{x}^* \tag{30}$$

for all elastic invariant line integrals, and with similar requirements for all the invariant surface and volume integrals, then how are Σ and Σ^* related to each other? The question can be put in a slightly different form, to simplify later considerations, by applying the elastic deformation $\boldsymbol{u}^{-1} : \Omega^* \to \Omega$ to the state Σ^*, leaving the elastic invariant integrals unchanged, mapping circuits $\boldsymbol{u}(\boldsymbol{C})$ to $\boldsymbol{C}$, etc., producing a new state $\Sigma' = \boldsymbol{u}^{-1}\Sigma^* = \{\boldsymbol{d}'_a(\cdot), \Omega\}$. Then requirement (30) becomes

$$\oint_{\boldsymbol{C}} \boldsymbol{f}\left(\Delta^{(r)}_{\Sigma}(\boldsymbol{x})\right) \cdot \mathrm{d}\boldsymbol{x} = \oint_{\boldsymbol{C}} \boldsymbol{f}\left(\Delta^{(r)}_{\Sigma'}(\boldsymbol{x})\right) \cdot \mathrm{d}\boldsymbol{x} \tag{31}$$

and it is necessary and sufficient for Eq. (31) to hold that

$$\boldsymbol{\nabla} \wedge \left\{\boldsymbol{f}\left(\Delta^{(r)}_{\Sigma}(\boldsymbol{x})\right)\right\} = \boldsymbol{\nabla} \wedge \left\{\boldsymbol{f}\left(\Delta^{r}_{\Sigma'}(\boldsymbol{x})\right)\right\}, \quad \boldsymbol{x} \in \Omega, \tag{32}$$

as the circuit $\boldsymbol{C} \subset \Omega$ is arbitrary. Eq. (32) and its analogues are to be solved, given Σ, given the function f and its analogues, to find the state Σ'.

Note that if $\Sigma^* = \boldsymbol{u}\Sigma$, then $\Sigma' = \boldsymbol{u}^{-1}\Sigma^* = \Sigma$, so that solving Eq. (32) and its analogues for states $\Sigma' \neq \Sigma$ amounts to finding the inelastic deformations which preserve the elastic invariant integrals.

However, it is a fact that if a certain finite number of the (infinite number of) equations analogous to Eq. (32) is satisfied, then all (the infinite number of) such equations are satisfied. The proof of this fact is outlined later. The following definition selects a finite number of conditions analogous to Eq. (32) and is motivated by this last result.

Definition 3. States Σ, Σ' are neutrally related to one another if $\boldsymbol{\nabla} \wedge (\boldsymbol{d}^a - \boldsymbol{d}^{a\prime}) = 0, \quad \nu n = \nu' n'$, $\boldsymbol{\nabla}\nu \wedge (\boldsymbol{d}^a - \boldsymbol{d}^{a\prime}) = 0, \quad \nu \in \mathscr{F}$, where $\nu'(x) := \nu\left(\Delta^{(r)}_{\Sigma'}(\boldsymbol{x})\right)$.

One should note that some of the invariants used for Definition 3 explicitly involve gradients of the dislocation density tensor, e.g. $\oint_{\boldsymbol{C}} \{(\boldsymbol{d}_a \cdot \boldsymbol{\nabla})(S^{bc}/n)\} d^e \cdot \mathrm{d}\boldsymbol{x}$ is an elastic invariant with density listed in Eq. (29). The list that is given is almost certainly not optimal (in that shorter lists may be sufficient for later results), but it is known that invariants other than the classic invariants must be involved (Section 6).

5. Canonical states

There are geometrical compatibility conditions on states Σ such that there exists $\Sigma' \neq \Sigma$ neutrally related to Σ. Such states may be put in canonical form by using appropriate elastic deformations. To get the flavour of this, consider the simple example where $\boldsymbol{\nabla} \wedge \boldsymbol{d}^a = 0$ for each a. Then, there exist potentials τ^a such that $\boldsymbol{d}^a = \boldsymbol{\nabla}\tau^a$, and if one puts $\boldsymbol{\tau} \equiv (\tau^1, \tau^2, \tau^3)$ then $\det(\boldsymbol{\nabla}\boldsymbol{\tau}) \neq 0$ by the linear independence of the lattice vectors. So $\boldsymbol{\tau}\Sigma = \{\boldsymbol{e}_a, \boldsymbol{\tau}(\Omega)\}$, where $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3\}$ is the canonical Cartesian basis of $\mathbb{R}^3$. That is, the lattice vector fields

are 'straightened out' using the potentials $\{\tau^1, \tau^2, \tau^3\}$, and one recovers the continuum analogue of the perfect crystal lattice, in this case. States neutrally related to $\boldsymbol{\tau}\Sigma$ are then easily obtained from $\boldsymbol{\nabla} \wedge \boldsymbol{d}^{a\prime} = \boldsymbol{0}$, $\det(\boldsymbol{d}^{a\prime}) = 1$: this implies that $\boldsymbol{d}^{a\prime} = \boldsymbol{\nabla} v^a$ for some potentials v^a, and if $\boldsymbol{v} \equiv (v^1, v^2, v^3)$, then $\det(\boldsymbol{\nabla v}) = 1$. If one superimposes an elastic deformation $\boldsymbol{u} : \boldsymbol{\tau}(\Omega) \to \boldsymbol{u} \cdot \boldsymbol{\tau}(\Omega)$, the dual lattice vector becomes $(\boldsymbol{\nabla u})^{-\mathrm{T}} \boldsymbol{\nabla} v^a$, the corresponding state becomes $(\boldsymbol{u} \cdot \boldsymbol{\tau})\Sigma = \left\{\boldsymbol{d}_a^+(\cdot),\ \boldsymbol{u} \cdot \boldsymbol{\tau}(\Omega)\right\}$ with

$$\boldsymbol{d}_a^+(\boldsymbol{u}(\boldsymbol{y})) = \boldsymbol{\nabla u}(\boldsymbol{y})[\boldsymbol{\nabla v}(\boldsymbol{y})]^{-1} \boldsymbol{e}_a, \quad \text{where } \det(\boldsymbol{\nabla v}) = 1,\ \ \boldsymbol{y} \in \boldsymbol{\tau}(\Omega). \tag{33}$$

This is a representation of lattice vectors in states elastically related to states neutrally related to $\boldsymbol{\tau}\Sigma$. One can interpret this representation in a different way: suppose that material points in $\boldsymbol{\tau}\Sigma$ are *rearranged* in the sense that lattice vectors are transported unchanged, as points $\boldsymbol{x} \in \boldsymbol{\tau}(\Omega)$ are moved to $\boldsymbol{v}(\boldsymbol{x}) \in \boldsymbol{v}(\boldsymbol{\tau}(\Omega))$. Thus, a state $\hat{\Sigma} = \left\{\hat{\boldsymbol{d}}_a(\cdot),\ \boldsymbol{v}(\boldsymbol{\tau}(\Omega))\right\}$ is produced by rearrangement of $\boldsymbol{\tau}\Sigma$, where

$$\hat{\boldsymbol{d}}_a(\boldsymbol{v}(\boldsymbol{y})) = \boldsymbol{d}_a(\boldsymbol{y}) = \boldsymbol{e}_a, \quad \det(\boldsymbol{\nabla v}) = 1, \quad \boldsymbol{y} \in \boldsymbol{\tau}(\Omega). \tag{34}$$

A further elastic deformation of $\hat{\Sigma}$, through the diffeomorphism $\boldsymbol{u} \cdot \boldsymbol{v}^{-1}$, gives lattice vectors $\boldsymbol{\ell}_a(\boldsymbol{u} \cdot \boldsymbol{v}^{-1}(\boldsymbol{v}(\boldsymbol{y})))$, defined by

$$\boldsymbol{\ell}_a(\boldsymbol{u}(\boldsymbol{y})) = \left[\boldsymbol{\nabla}(\boldsymbol{u} \cdot \boldsymbol{v}^{-1})\right](\boldsymbol{v}(\boldsymbol{y}))\, \hat{\boldsymbol{d}}_a(\boldsymbol{v}(\boldsymbol{y})) = \boldsymbol{\nabla u}(\boldsymbol{y})\left(\boldsymbol{\nabla} \boldsymbol{v}^{-1}\right)(\boldsymbol{v}(\boldsymbol{y}))\boldsymbol{e}_a. \tag{35}$$

Since $(\boldsymbol{\nabla} \boldsymbol{v}^{-1})(\boldsymbol{v}(\boldsymbol{y})) = (\boldsymbol{\nabla v})^{-1}(\boldsymbol{y})$, one sees that

$$\boldsymbol{\ell}_a(\boldsymbol{u}(\boldsymbol{y})) \equiv \boldsymbol{d}_a^+(\boldsymbol{u}(\boldsymbol{y})), \quad \boldsymbol{y} \in \boldsymbol{\tau}(\Omega). \tag{36}$$

The state $(\boldsymbol{u} \cdot \boldsymbol{\tau})\Sigma$ is obtained, then, by a rearrangement $\boldsymbol{v}$, followed by an elastic deformation $\boldsymbol{u} \cdot \boldsymbol{v}^{-1}$. In the rearrangement, lattice vectors are transported unchanged, with the material points, whereas in the elastic deformation, lattice vectors behave as do material line elements. In a suggestive notation, let F_{e}^1 denote the elastic deformation, $\boldsymbol{\tau}$, F_{p} denote the rearrangement $\boldsymbol{v}$, F_{e}^2 denote the elastic deformation $\boldsymbol{u} \cdot \boldsymbol{v}^{-1}$. Then lattice vectors $\boldsymbol{d}_a^+(\cdot)$ in state $(\boldsymbol{u} \cdot \boldsymbol{\tau})\Sigma$ are realised by the sequence of operations

$$F_{\mathrm{e}}^2 \cdot F_{\mathrm{p}} \cdot F_{\mathrm{e}}^1 \tag{37}$$

and in this rigorous decomposition F_{e}^1 and F_{e}^2 are truly elastic deformations, F_{p} "simply introduces a change of shape". The quote is from Lee (1969), Lee and Liu (1967) (out of context) where the famous "elastic–plastic" decomposition

$$F = F_{\mathrm{e}} F_{\mathrm{p}} \tag{38}$$

is introduced, based on a thought experiment, which envisages that the body is "cut up into small elements, and with the removal of the load on the elements, the unstressed state is approached as the element size approaches zero".

It is worth emphasising, and reiterating, that Eq. (37) is a rigorous result for this continuum model of a crystal, obtained for a particular class of inelastic changes of state without recourse to any notion of stress.

Features of this simple example turn out to hold generally: there is a canonical state, which is rearranged and elastically deformed to produce states elastically related to the neutrally related states, and the rearrangement transports material points through sets where the lattice vector fields are constant.

Theorem 2. *Suppose that Σ' is neutrally related to Σ, and that $\Sigma' \neq \Sigma$. Then either (a) there exists an elastic deformation with gradient F such that $\{F^{-\mathrm{T}} \boldsymbol{d}^a\}$ depends just on a single Cartesian coordinate, x^3 say; or (b) the fields $\{S^{ab}/n(\cdot)\}$ are constant and rank $\{\boldsymbol{\nabla} \wedge \boldsymbol{d}^a\} = 1$, in which case $(S^{ab}/n) = \boldsymbol{b} \otimes \boldsymbol{a}$ for some vectors $\boldsymbol{a}, \boldsymbol{b}$ and an elastic deformation gives dual lattice vectors of the form*

$$\boldsymbol{d}^a = \boldsymbol{e}^a + \boldsymbol{b}^a \boldsymbol{a} \wedge \boldsymbol{x} \phi(t), \tag{39}$$

where $t = \boldsymbol{a} \wedge \boldsymbol{x} \cdot \boldsymbol{b}$ and $\phi(t) = \frac{1}{2!} + \frac{t}{3!} + \frac{t^2}{4!} + \cdots = (e^t - 1 - t)/t^2$.

With the canonical states explicitly given by this last theorem, one can prove (Parry, 1992) that neutrally related states can be reconstructed, one from the other, by a sequence of unions, divisions, elastic deformations and rearrangements. The essential ingredient of the proof is the observation that, as lattice vectors may be assumed constant in planes $x^3 =$ constant, for example, finite slices of crystal (sliced by planes $x^3 =$ constant) are elastically related to one another. After subdivision and elastic deformation, then, Σ and Σ' can be reduced to (the same number of) copies of one "small element" of a specific slice. Finally, the rearrangement, elastic deformation and union of these small elements reconstructs Σ' from Σ. Again, this is a rigorous result where the suggestive ideas of Lee and Liu (1967) are prominent (though the result is obtained without any notion of stress).

6. Neutrally related states are locally elastically related

Given $\Sigma = \{\boldsymbol{d}_a(\cdot), \Omega\}$, define the *classifying manifold* T as

$$T = \{(v(\boldsymbol{x}), (\boldsymbol{d}_a \cdot \nabla)v(x),\ (\boldsymbol{d}_b \cdot \nabla)\ (\boldsymbol{d}_a \cdot \nabla)v(\boldsymbol{x}));\quad a, b = 1, 2, 3,\quad v \in \mathscr{F},\quad \boldsymbol{x} \in \Omega\}. \tag{40}$$

Then, one of the main results of Cartan's theory of equivalence, somewhat adapted to this context, is the following theorem.

Theorem 3. *Let $\Sigma = \{\boldsymbol{d}_a(\cdot), \Omega\}$ $\Sigma^* = \{\boldsymbol{d}^*_a(\cdot), \Omega^*\}$ have classifying manifolds T, T^*, respectively. Suppose that T and T^* overlap, in the sense that*

$$\mu_\Sigma(\boldsymbol{y}_0) = \mu_{\Sigma^*}(\boldsymbol{y}^*_0) \quad \text{for all } \mu_\Sigma \in \{v(\cdot),\ (\boldsymbol{d}_a \cdot \nabla)v(\cdot),\ (\boldsymbol{d}_b \cdot \nabla)\ (\boldsymbol{d}_a \cdot \nabla)v(\cdot);\quad a, b = 1, 2, 3,\quad v \in \mathscr{F}\} \tag{41}$$

for all $(\boldsymbol{y}_0, \boldsymbol{y}^*_0)$ in some neighbourhood of a point $(\boldsymbol{x}_0, \boldsymbol{x}^*_0) \in \Omega \times \Omega^*$. Then for any such $(\boldsymbol{x}_0, \boldsymbol{x}^*_0)$, there exists a diffeomorphism $\boldsymbol{u}_{\boldsymbol{x}_0}$ defined on a neighbourhood $N_{\boldsymbol{x}_0}$ of $\boldsymbol{x}_0$ in Ω such that $\boldsymbol{u}_{\boldsymbol{x}_0}(\boldsymbol{x}_0) = \boldsymbol{x}^*_0$ and

$$\boldsymbol{d}^*_a(\boldsymbol{u}_{\boldsymbol{x}_0}(\boldsymbol{x})) = \nabla \boldsymbol{u}_{\boldsymbol{x}_0}(\boldsymbol{x}) \boldsymbol{d}_a(\boldsymbol{x}), \quad \boldsymbol{x} \in N_{\boldsymbol{x}_0}. \tag{42}$$

That is, if the classifying manifolds overlap, the corresponding states are locally elastically related.

The result was proved, in effect, by brute force consideration of an exhaustive list of special cases in Davini and Parry (1989, 1991). Olver (1995) gives a proof via a dual version of Frobenius' theorem, stated in terms of differential forms.

Theorem 4. *Suppose that Σ and Σ' are neutrally related. Then Σ and Σ' are locally elastically related.*

Proof. If $\theta \in \mathscr{F},\ \theta(\boldsymbol{x}) = \theta'(\boldsymbol{x}),\ \ x \in \Omega$ (from Definition 3). Hence, the classifying manifolds T, T' are identical to each other in this case, and the result follows by the previous theorem (with $(\boldsymbol{x}_0, \boldsymbol{x}^*_0) = (\boldsymbol{x}_0, \boldsymbol{x}_0)$).

This result allows us to prove that a certain finite list of integrals is a *basis* for the elastic invariant integrals. □

Theorem 5. *Suppose that Σ and Σ' are neutrally related, then all elastic invariant integrals of the form $\oint_C \mu(\boldsymbol{x}) \boldsymbol{d}^a(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x},\ \int_V \mu(\boldsymbol{x}) n(\boldsymbol{x})\, \mathrm{d}V_x$, where μ is a scalar, match in Σ and Σ'.*

Proof. (a) If Σ and Σ' are neutrally related, then by Theorem 4, given $\boldsymbol{x}_0 \in \Omega$, there exists $\boldsymbol{u}_{\boldsymbol{x}_0} : N_{\boldsymbol{x}_0} \to \Omega$ such that $\boldsymbol{u}_{\boldsymbol{x}_0}(\boldsymbol{x}_0) = \boldsymbol{x}_0$ and $\boldsymbol{d}'_a(\boldsymbol{u}_{\boldsymbol{x}_0}(\boldsymbol{x})) = \nabla \boldsymbol{u}_{\boldsymbol{x}_0}(\boldsymbol{x}) \boldsymbol{d}_a(\boldsymbol{x}),\ \ \boldsymbol{x} \in N_{\boldsymbol{x}_0}$. Suppose μ is a scalar, in that Eq. (13) holds, then putting $\boldsymbol{x} = \boldsymbol{x}_0,\ \boldsymbol{u} = \boldsymbol{u}_{\boldsymbol{x}_0}$ in Eq. (13), one obtains

$$\mu(\boldsymbol{x}_0, \boldsymbol{d}_a(\boldsymbol{x}_0),\ \nabla\boldsymbol{d}_a(\boldsymbol{x}_0), \dots) = \mu(\boldsymbol{x}_0, \boldsymbol{d}'_a(\boldsymbol{x}_0),\ \nabla\boldsymbol{d}'_a(\boldsymbol{x}_0), \dots), \quad \boldsymbol{x}_0 \in \Omega. \tag{43}$$

(b) Suppose each S^{ab}/n is constant. Then the classifying manifold of $\Sigma = \{\boldsymbol{d}_a(\cdot), \Omega\}$ is a point, and choosing $\Sigma^* = \Sigma$ in Theorem 3 one deduces that if $\boldsymbol{x}_0,\ \boldsymbol{y} \in \Omega$, there exists a diffeomorphism $\boldsymbol{u}_{\boldsymbol{x}_0} : N_{\boldsymbol{x}_0} \to \Omega$ such that $\boldsymbol{u}_{\boldsymbol{x}_0}(\boldsymbol{x}_0) = \boldsymbol{y}$ and

$$\boldsymbol{d}_a(\boldsymbol{u}_{\boldsymbol{x}_0}(\boldsymbol{x})) = \nabla\boldsymbol{u}_{\boldsymbol{x}_0}(\boldsymbol{x})\boldsymbol{d}_a(\boldsymbol{x}). \tag{44}$$

Then, putting $\boldsymbol{x} = \boldsymbol{x}_0,\ \boldsymbol{u} = \boldsymbol{u}_{\boldsymbol{x}_0}$ in Eq. (13), one obtains

$$\mu(\boldsymbol{x}_0, \boldsymbol{d}_a(\boldsymbol{x}_0),\ \nabla\boldsymbol{d}_a(\boldsymbol{x}_0), \dots) = \mu(\boldsymbol{y}, \boldsymbol{d}_a(\boldsymbol{y}),\ \nabla\boldsymbol{d}_a(\boldsymbol{y}), \dots), \quad \boldsymbol{x}_0,\ \boldsymbol{y} \in \Omega. \tag{45}$$

That is to say, $\mu(\cdot)$ is constant in this case.

(c) Suppose that (at least) one of S^{ab}/n is non-constant, call it θ. Choose points $\boldsymbol{x}_0,\ \boldsymbol{x}_0^*$ such that $\theta(\boldsymbol{x}_0) = \theta(\boldsymbol{x}_0^*)$, and choose $\Sigma^* = \Sigma$ in Theorem 3. It follows that $\mu_\Sigma(\boldsymbol{x}_0) = \mu_\Sigma(\boldsymbol{x}_0^*)$ and hence that $\mu_\Sigma(\cdot) = \mu(\theta(\cdot))$.

(d) Finally, since $\mu_\Sigma(\cdot) = \mu_{\Sigma'}(\cdot)$ from Eq. (43), and $n(\cdot) = n'(\cdot)$ from Definition 3,

$$\mu_\Sigma n = \mu_{\Sigma'} n' \quad \text{and so} \quad \int_V \mu_\Sigma(\boldsymbol{x}) n(\boldsymbol{x})\,\mathrm{d}V_x = \int_V \mu_{\Sigma'}(\boldsymbol{x}) n'(\boldsymbol{x})\,\mathrm{d}V_x. \tag{46}$$

Also, if μ_Σ is a constant, then $\mu_{\Sigma'}$ is the same constant, by Eq. (43), and so

$$\nabla \wedge \mu_\Sigma(\boldsymbol{x})\boldsymbol{d}^a(\boldsymbol{x}) = \nabla \wedge \mu_{\Sigma'}(\boldsymbol{x})\boldsymbol{d}^{a'}(\boldsymbol{x}),$$

since $\nabla \wedge (\boldsymbol{d}^a - \boldsymbol{d}^{a'}) = \boldsymbol{0}$ by Definition 3. If μ_Σ is not a constant, then $\mu = \mu(\tau^a)$ since $\mu = \mu(\theta(\cdot))$ by (c) and $\theta = \theta(\tau^a)$, see below. Recall that $\boldsymbol{d}^a - \boldsymbol{d}^{a'} = \nabla\tau^a$. Hence,

$$\nabla \wedge (\mu_\Sigma(\boldsymbol{x})\boldsymbol{d}^a(\boldsymbol{x})) - \nabla \wedge (\mu_{\Sigma'}(\boldsymbol{x})\boldsymbol{d}^{a'}(\boldsymbol{x})) = \mu_\Sigma(\boldsymbol{x})\nabla \wedge (\boldsymbol{d}^a - \boldsymbol{d}^{a'}) + \nabla\mu \wedge (\boldsymbol{d}^a - \boldsymbol{d}^{a'}) = 0,$$

since $\mu_\Sigma(\cdot) = \mu_{\Sigma'}(\cdot)$ by Eq. (43). Quite generally then, $\oint_C \mu_\Sigma \boldsymbol{d}^a\,\mathrm{d}\boldsymbol{x} = \oint_C \mu_{\Sigma'}\boldsymbol{d}^{a'} \cdot \mathrm{d}\boldsymbol{x}$, and this concludes the proof. □

Notice some straightforward implications of Definition 3. First, $\boldsymbol{d}^a - \boldsymbol{d}^{a'} = \nabla\tau^a$ for some potentials $\tau^a(\boldsymbol{x})$, not all of them constant. Then, $\nabla v \wedge \nabla\tau^a = 0$, so $v = v(\tau^a)$ for any index a, where $\nabla\tau^a \neq 0$. Let $v_1, v_2 \in \mathscr{F}$. Suppose that v_1 is non-constant, then $\nabla v_1 = \lambda\nabla\tau^a,\ \lambda \neq 0$, so since $\nabla v_2 \wedge \nabla\tau^a = 0,\ \nabla v_2 \wedge \nabla v_1 = 0$ and $v_2 = v_2(v_1)$. Clearly $v_2 = v_2(v_1)$, if $v_2(\cdot)$ is constant. Therefore, either all the elements of $\mathscr{F}$ are constant, or each element of $\mathscr{F}$ is a function of some non-constant element θ, say (and clearly $\theta(\cdot) = S^{ab}/n(\cdot)$ for some choice of a, b). In any case, then $v = v(\theta), v \in \mathscr{F}$. In particular, $\bar{v} := (\boldsymbol{d}_c \cdot \nabla)S^{ab}/n$ is a function of θ, and it follows that

$$(\boldsymbol{d}_d \cdot \nabla)(\boldsymbol{d}_c \cdot \nabla)\frac{S^{ab}}{n} = (\boldsymbol{d}_d \cdot \nabla)\{\bar{v}(\theta)\} = \bar{v}'(\theta)(\boldsymbol{d}_d \cdot \nabla)\theta \tag{47}$$

is a function of θ, since $(\boldsymbol{d}_a \cdot \nabla)\theta \in \mathscr{F}$. In the same way, it follows that $(\boldsymbol{d}_e \cdot \nabla)(\boldsymbol{d}_d \cdot \nabla)(\boldsymbol{d}_c \cdot \nabla)S^{ab}/n$ is a function of θ, and so on.

Now, one can show that the fundamental set $\mathscr{F}$ of scalar invariants must include more than just the classic invariants, i.e. it is not enough just to require that

$$\nabla \wedge \boldsymbol{d}^a = \nabla \wedge \boldsymbol{d}^{a'}, \qquad S^{ab} = S^{ab'}, \qquad n = n', \tag{48}$$

if one is to deduce that all invariants match in neutrally related states. To see this, let $\Sigma = \{\boldsymbol{d}_a(\cdot), \Omega\}$ correspond to

$$\boldsymbol{d}^{\alpha} = \boldsymbol{e}^{\alpha} + x^{\alpha}\boldsymbol{e}^{3}, \quad \boldsymbol{d}^{3} = \boldsymbol{\nabla}\xi + x^{1}x^{2}\boldsymbol{e}^{3}, \quad \xi = x^{2}x^{3}, \quad \alpha = 1,2, \tag{49}$$

and suppose that $\oint_{\boldsymbol{C}} \boldsymbol{d}^{a} \cdot \mathrm{d}\boldsymbol{x}$, $\int_{V} S^{ab}\,\mathrm{d}V$, $\int_{V} n\,\mathrm{d}V$ match in states $\Sigma, \Sigma' = \{\boldsymbol{d}'_{a}(\cdot), \Omega\}$. Then from Definition 3, one finds that

$$\boldsymbol{d}^{a\prime} = \boldsymbol{d}^{a} + f^{a}(x^{3})\boldsymbol{e}^{3}, \quad \text{where } f^{\alpha} = f^{\alpha}(x^{3}), \quad \alpha = 1,2 \quad \text{and} \quad f^{3} = x^{3}f^{2}(x^{3}). \tag{50}$$

Also,

$$S^{21} = 1, \quad S^{31} = x^{1}, \quad S^{32} = -x^{2}, \quad S^{13} = -x^{3}. \tag{51}$$

Suppose, for the sake of contradiction, that Σ, Σ', are locally elastically related. Then there exists an invertible $\boldsymbol{y}(\boldsymbol{x})$ such that (locally)

$$\boldsymbol{d}'_{a}(\boldsymbol{y}(\boldsymbol{x})) = (\boldsymbol{\nabla}\boldsymbol{y})(\boldsymbol{x})\boldsymbol{d}_{a}(\boldsymbol{x}), \tag{52}$$

$$(S^{ab\prime}/n')(\boldsymbol{y}) = (S^{ab}/n)(\boldsymbol{x}), \tag{53}$$

since S^{ab}/n is a scalar. Since the S^{ab}, n match in Σ and Σ', and in particular $S^{21\prime} = S^{21} = 1$, it follows that $n'(\boldsymbol{x}) = n(\boldsymbol{x})$ and hence

$$S^{ab}(\boldsymbol{y}) = S^{ab}(\boldsymbol{x}). \tag{54}$$

Thus, taking those S^{ab} that appear in Eq. (51), we deduce that

$$\boldsymbol{y}(\boldsymbol{x}) = \boldsymbol{x} \tag{55}$$

for all $\boldsymbol{x} \in \Omega$. But then, Eq. (52) implies that $\boldsymbol{d}_{a}(\cdot) = \boldsymbol{d}'_{a}(\cdot)$ and this contradicts the fact that $\Sigma \neq \Sigma'$.

Remark: It is vitally important to realise that generally, there is no elastic deformation mapping Ω to itself, which takes Σ to Σ'. To see this, consider neutrally related states, with $\Sigma = \{\boldsymbol{e}^{a}, \Omega\}, \Sigma' = \{\boldsymbol{\nabla}\theta^{a}(\cdot), \Omega\}$, where $\{\boldsymbol{e}^{a}\}$ is an orthonormal basis, the functions θ^{a} are independent and $\det(\boldsymbol{\nabla}\theta^{a}) = 1$ but otherwise they are arbitrary, and Ω is the unit cube. Also, suppose that there is an elastic deformation $\boldsymbol{y}$, which takes Σ' to Σ, for contradiction. Then, since $\boldsymbol{d}^{a}(\boldsymbol{y}(\boldsymbol{x})) = F^{-\mathrm{T}}(\boldsymbol{x})\boldsymbol{d}^{a'}(\boldsymbol{x})$,

$$\boldsymbol{e}^{a} = (\boldsymbol{\nabla}\boldsymbol{y})^{-\mathrm{T}}\boldsymbol{d}^{a'}(\boldsymbol{x}), \quad \text{so} \quad (\boldsymbol{\nabla}\boldsymbol{y})^{\mathrm{T}}\boldsymbol{e}^{a} = (\boldsymbol{\nabla}\theta^{a}) \quad \text{in } \Sigma. \tag{56}$$

It follows that $y^{a} = \theta^{a} +$ constant, for each a, which implies that $\theta(\Omega)$ is a translation of Ω (since $\boldsymbol{y}(\Omega) = \Omega$). But this is false, in general, since $\theta = (\theta^{a})$ is arbitrary, except that $\det(\boldsymbol{\nabla}\theta^{a}) = 1$.

7. Lie group structure of crystal states

For illustrative purposes, I work with crystal states where each S^{ab}/n is constant. Then, the classifying manifold of Σ consists of a single point, and so given $\boldsymbol{x}_{0}, \boldsymbol{x}_{0}^{*} \in \Omega$, there exists a diffeomorphism $\boldsymbol{u}_{\boldsymbol{x}_{0}}$ defined on a neighbourhood $N_{\boldsymbol{x}_{0}}$ of $\boldsymbol{x}_{0}$ in Ω such that

$$\boldsymbol{d}_{a}(\boldsymbol{u}_{\boldsymbol{x}_{0}}(\boldsymbol{x})) = \boldsymbol{\nabla}\boldsymbol{u}_{\boldsymbol{x}_{0}}(\boldsymbol{x})\boldsymbol{d}_{a}(\boldsymbol{x}), \quad \boldsymbol{u}_{\boldsymbol{x}_{0}}(\boldsymbol{x}_{0}) = \boldsymbol{x}_{0}^{*}, \quad \boldsymbol{x} \in N_{\boldsymbol{x}_{0}}. \tag{57}$$

Thus, the lattice vector fields in the neighbourhoods of any two distinct points in Ω may be obtained, one from the other, by elastic deformation (a result incidental to the proof of the last theorem). Note that

$$\boldsymbol{\nabla} \wedge \boldsymbol{d}^{a} = (\boldsymbol{d}^{b} \cdot \boldsymbol{\nabla} \wedge \boldsymbol{d}^{a})\boldsymbol{d}_{b} = \left(S^{ab}/n\right)\frac{1}{2}\,\varepsilon_{brs}\boldsymbol{d}^{r} \wedge \boldsymbol{d}^{s}, \tag{58}$$

and taking the divergence

$$\left(S^{ab}/n\right)\varepsilon_{brs}S^{rs} = 0. \tag{59}$$

Eq. (59) is the analogue of the Jacobi identity for the structure constants $C_{ij}^k = -C_{ji}^k$ of a three-dimensional Lie algebra, which is

$$C_{ij}^m C_{mk}^r + C_{jk}^m C_{mi}^r + C_{ki}^m C_{mj}^r = 0. \tag{60}$$

To see this, put $C_{ij}^k = \varepsilon_{ijp} S^{kp}/n$ and check that Eq. (60) reduces to Eq. (59). Now, one can recover a (local) Lie group from its Lie algebra, and so it is natural to wonder if there is any connection between the lattice vector fields $\{\boldsymbol{d}_a(\cdot)\}$ and the local Lie group corresponding to the structure constants $\varepsilon_{ijp} S^{kp}/n$. There is indeed a connection, and it is made explicit by the construction of Maurer–Cartan forms on the group. Denote the three group parameters by $(X_1, X_2, X_3) = \boldsymbol{X}$ and solve the following initial value problem for the variables $D_j^a(t, \boldsymbol{X}),\ t \in \mathbb{R}$

$$\dot{D}_j^a = \delta_j^a + \varepsilon_{k\ell t}(S^{ta}/n) X^k D_j^\ell, \qquad D_j^a(0, \boldsymbol{X}) = 0. \tag{61}$$

Here, the dot signifies a partial derivative with respect to the first argument, t, and I took the general ruse from Sattinger and Weaver (1986). Now put

$$\theta_r^a = \varepsilon_{rpq} D_{q,p}^a - \frac{1}{2}\left(S^{ab}/n\right) \varepsilon_{bcd} \varepsilon_{rjk} D_j^c D_k^d,$$

and calculate from Eq. (61) that

$$\dot{\theta}_r^m = \varepsilon_{k\ell i} X^k (S^{im}/n)\, \theta_r^\ell, \qquad \theta_r^i(0, \boldsymbol{X}) = 0. \tag{62}$$

It follows that θ_r^i is identically zero. Let $\boldsymbol{D}^i$ be the vector with components $D_j^i(1, \boldsymbol{X})$, then

$$\boldsymbol{\nabla} \wedge \boldsymbol{D}^a = \left(S^{ab}/n\right) \frac{1}{2} \varepsilon_{brs} \boldsymbol{D}^r \wedge \boldsymbol{D}^s. \tag{63}$$

Moreover, $D_j^a(t, \boldsymbol{0}) = \delta_j^a t,\ D_j^a(1, \boldsymbol{0}) = \delta_j^a$; it follows that $\det\{\boldsymbol{D}^a\}$ is positive in a neighbourhood of $\boldsymbol{X} = 0$ and that one can regard the fields as lattice vector fields. So, define a state

$$\Sigma^{mc} = \{\boldsymbol{D}_a(\cdot), \Omega^{mc}\}, \tag{64}$$

where $\boldsymbol{D}_a(\boldsymbol{X}) \cdot \boldsymbol{D}^b(\boldsymbol{X}) = \delta_a^b,\ \boldsymbol{X} \in \Omega^{mc} \subset \Omega$. (One can always arrange that Ω contains the point $\boldsymbol{X} = \boldsymbol{0}$.) Thus,

$$\frac{\boldsymbol{D}^b \cdot \boldsymbol{\nabla} \wedge \boldsymbol{D}^a}{\det\{\boldsymbol{D}^a\}} = S^{ab}/n = \text{ constant}. \tag{65}$$

So from Theorem 3, there is a local diffeomorphism between Σ and Σ^{mc}. Also, if Σ is neutrally related to Σ', there is a local diffeomorphism between Σ' and Σ^{mc}.

It is the vectors $\boldsymbol{D}^a(\cdot)$ that reflect the group structure. Let the relevant Lie group be denoted $\mathscr{G}$, so that group elements g are parametrised by the points $\boldsymbol{X} \in \Omega^{mc}$ and there is a mapping $\Psi(\boldsymbol{X}, \boldsymbol{Y})$ which corresponds to the composition of group elements, $g(\boldsymbol{X})g(\boldsymbol{Y}) = g(\Psi(\boldsymbol{X}, \boldsymbol{Y}))$. The mapping $\Psi : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^3$ reflects the associativity of the group operation and is such that the Lie algebra (in $\mathbb{R}^3$) deriving from the Lie product $g(\boldsymbol{X})g(\boldsymbol{Y})g^{-1}(\boldsymbol{X})g^{-1}(\boldsymbol{Y})$ is that corresponding to the structure constants $\varepsilon_{ijp} S^{kp}/n$. The vectors $\boldsymbol{D}^a$ are determined by the mapping Ψ, and they satisfy

$$D_k^a(\Psi(\boldsymbol{Y}, \boldsymbol{X})) \frac{\partial \Psi^k}{\partial X^\ell}(\boldsymbol{Y}, \boldsymbol{X}) = D_\ell^a(\boldsymbol{X}), \tag{66}$$

identically in $\boldsymbol{Y}$. Note that, once the structure constants are given, the construction which starts at Eq. (61) provides fields $\{\boldsymbol{D}_a(\cdot)\}$; then solving Eq. (66) for $\Psi(\boldsymbol{Y}, \boldsymbol{X})$ tells us the (composition function for the) group operation in $\mathscr{G}$. Moreover, fixing $\boldsymbol{Y} = \boldsymbol{Y}_0$ in Eq. (59) gives

$$\boldsymbol{D}^a(\boldsymbol{u}(\boldsymbol{X})) = (\boldsymbol{\nabla u})^{-\mathrm{T}}(\boldsymbol{X}) \boldsymbol{D}^a(\boldsymbol{X}), \tag{67}$$

if one puts

$$\boldsymbol{u}(\boldsymbol{X}) = \Psi(\boldsymbol{Y}_0, \boldsymbol{X}), \tag{68}$$

and writes $-\mathrm{T}$ for the inverse transpose of a matrix. Eq. (67) states that the fields $\boldsymbol{D}^a(\cdot)$ transform as dual lattice vector fields in the *elastic* deformation $\boldsymbol{X} \to \Psi(\boldsymbol{Y}_0, \boldsymbol{X}) \equiv \boldsymbol{u}(\boldsymbol{X})$, defined by the group composition function. In the Lie group literature, such fields (forms) are called left-invariant. Knowing $\boldsymbol{D}^a(0) = \boldsymbol{e}^a$, the canonical basis in $\mathbb{R}^3$, and knowing the group composition function Ψ (deriving from the structure constants), the lattice vector fields in Σ^{mc} are fixed by the transformation rule (67). Thus, Σ^{mc} provides a canonical form of states which allow neutral deformation; the lattice vector fields are Maurer–Cartan fields on the group corresponding to (S^{ab}/n), the corresponding coordinates are canonical of the first kind in the terminology of Pontryagin (1955).

Theorem 6. *Suppose that Σ and Σ' are neutrally related and that each (S^{ab}/n) is constant. Then, Σ is locally elastically related to a state Σ^{mc}, where the dual lattice vectors are left invariant under the local Lie group $\mathscr{G}$ defined above.*

Thus, the study of neutral deformations in states, where the lattice components of dislocation density are constant amounts to a study of mappings between different subsets of the Lie group $\mathscr{G}$.

8. Equilibrium of a perfect crystal which can deform elastically and through slip

I consider a variational problem where lattice vector fields are represented in the form (33), appropriate to states where the elastic invariant integrals match those in a perfect crystal and recall that the diffeomorphism $\boldsymbol{u}$ represents the elastic part of the change of state, and that $\boldsymbol{v}$ represents the slip, or rearrangement. So (letting $\boldsymbol{\tau}(\Omega) \to \Omega$),

$$\text{find} \quad \inf \mathscr{P}, \quad \text{where } \mathscr{P} = \int_\Omega W\Big((\nabla \boldsymbol{u})(\nabla \boldsymbol{v})^{-1}\Big)\,\mathrm{d}V, \tag{69}$$

when W is a non-negative energy density function with $w(\mathbf{1}) = 0$, with symmetry properties appropriate to a perfect crystal (Chipot and Kinderlehrer, 1988; Fonseca, 1987; Fonseca and Parry, 1992), assuming displacement boundary conditions $\boldsymbol{y} = A\boldsymbol{x}$ on the boundary of Ω (A is a constant matrix). One tries to minimise $\mathscr{P}$ by choice of the two functions $\boldsymbol{u}, \boldsymbol{v}$ with $\det(\nabla \boldsymbol{v}) = 1$.

It follows from these assumptions that W is not quasi-convex, so the corresponding function is not lower semicontinuous, and the minimising sequences may develop oscillations. Information on the minimising state is stored in the corresponding Young measure (Young, 1942; Tartar, 1979) – this is a field of probability measures which holds enough information that the limit of continuous functions (of sequences that oscillate) may be calculated. In the present context, it is the lattice vectors given by Eq. (33) that may oscillate; the set of lattice vectors takes values in the space of 3×3 matrices with positive determinant, $M^{3\times 3}_+$, so the relevant Young measure is a field of probability measures $\mu_{\boldsymbol{x}}(M)$, $M \in M^{3\times 3}_+$, $\boldsymbol{x} \in \Omega$. The limiting value of the continuous function representing the Cauchy stress, defined by

$$\sigma(M) = \frac{1}{\det M}\left(\frac{\partial W}{\partial M}(M)\right)M^{\mathrm{T}} \tag{70}$$

is then given by

$$\bar{\sigma}(\boldsymbol{x}) = \int_{M^{3\times 3}_+} \sigma(M)\,\mathrm{d}\mu_{\boldsymbol{x}}(M), \tag{71}$$

and a calculation given in Fonseca and Parry (1992) shows that

$$\bar{\sigma}(\boldsymbol{x}) \text{ is isotropic} \quad \text{for almost all } \boldsymbol{x} \in \Omega. \tag{72}$$

Thus, $\bar{\sigma}(\boldsymbol{x}) = \lambda \mathbb{I}$, where $\mathbb{I}$ is the identity matrix, and the function λ turns out to be the convex minorant of the 'subenergy' function $\inf\{W(M); \det M = t\}$, introduced by Ericksen and Flory.

It is worth noting that the structure of the neutrally related states (not just the particular case considered above) is 'stable' in the sense that the (L^∞ weak *) limit of a sequence of states neutrally related to some Σ, is also neutrally related to Σ. This 'weak closure' of the neutrally related states is derived from Murat and Tartar's div–curl lemma (Fonseca and Parry, 1992).

9. Defective crystallography

I shall show how to construct a discrete set of points which seems to be naturally associated with the continuum model of interest, in the case where the dislocation density tensor is constant throughout Ω and equals either (i) zero or (ii) $\lambda \boldsymbol{v} \otimes \boldsymbol{v}$ for some number λ, vector $\boldsymbol{v}$. In fact, since case (i) just represents the case of perfect crystal (as far as constructing a related lattice is concerned), I focus just on case (ii). As mentioned earlier, this construction is to motivate the choice of symmetry group for the continuum model.

The simplest mechanical problem for a defective crystal (with some $S^{ab}/n \neq 0$) would be a variational problem with energy density having the symmetry group deriving from the appropriate discrete set of points, with lattice vectors having elastic invariants consistent with constant (S^{ab}/n) equal to $\lambda \boldsymbol{v} \otimes \boldsymbol{v}$. Here, I indicate how ideas of Thurston (1997) are instrumental in constructing the relevant discrete set of points, but leave the associated variational problem aside (one would guess that non-zero S^{ab}/n would lead to non-trivial shear strength, since by Arnol'd's work, $\int_V S^{ab}\,\mathrm{d}V \neq 0$ implies that dislocation lines are knotted around one another, this knottedness is preserved in neutrally related states, and so the material cannot rearrange in arbitrary directions, thereby relaxing the shear stresses).

First of all, a set of points is generated from an arbitrary initial point $\boldsymbol{x}_0$ in the following way. Define the (exponential) mapping $\boldsymbol{x} \to \exp_a(\boldsymbol{x})$ by

$$\exp_a(\boldsymbol{x}) = \boldsymbol{x}(1), \tag{73}$$

where $\boldsymbol{x}(t)$ satisfies

$$\dot{\boldsymbol{x}}(t) = \boldsymbol{d}_a(\boldsymbol{x}(t)), \quad \boldsymbol{x}(0) = \boldsymbol{x}_0. \tag{74}$$

Thus, $\boldsymbol{x}_0$ generates three points $\boldsymbol{x}_1^a \equiv \exp_a(\boldsymbol{x}_0)$, the three points $\boldsymbol{x}_1^a$ generate nine points $\boldsymbol{x}_2^{ab} \equiv \exp_b(\boldsymbol{x}_1^a)$, and so on. So the iterations correspond to flow (through time 1) along the integral lines of the three lattice vectors. Note that the iteration is an "elastic invariant procedure"; it is an easy calculation to show that if the analogous iteration is carried out for lattice vector fields elastically related to $\boldsymbol{d}_a(x)$, then there is the obvious correspondence of the relevant iterates.

Moreover, when $(S^{ab}/n) = \lambda \boldsymbol{v} \otimes \boldsymbol{v}$, one deduces from Eq. (39) that

$$\boldsymbol{d}^a = \boldsymbol{e}^a + \frac{1}{2}\lambda \boldsymbol{v}^a (\boldsymbol{v} \wedge \boldsymbol{x}), \tag{75}$$

and calculates that

$$\boldsymbol{d}_a = \boldsymbol{e}_a - \frac{1}{2}\lambda (\boldsymbol{v} \wedge \boldsymbol{x} \cdot \boldsymbol{e}_a)\boldsymbol{v}. \tag{76}$$

Solving Eq. (66) for the composition function, it turns out that

$$\Psi(\boldsymbol{x},\boldsymbol{y}) = \boldsymbol{x} + \boldsymbol{y} + \frac{1}{2}\lambda \boldsymbol{v}(\boldsymbol{v}\cdot\boldsymbol{x}\wedge\boldsymbol{y}), \tag{77}$$

so that

$$\Psi(\boldsymbol{e}_a,\boldsymbol{y}) = \boldsymbol{e}_a + \boldsymbol{y} + \frac{1}{2}\lambda \boldsymbol{v}(\boldsymbol{e}_a\cdot\boldsymbol{x}\wedge\boldsymbol{y}). \tag{78}$$

The exponential mapping, in this case, derives from

$$\dot{\boldsymbol{x}}(t) = \boldsymbol{e}_a - \frac{1}{2}\lambda(\boldsymbol{v}\wedge\boldsymbol{x}\cdot\boldsymbol{e}_a)\boldsymbol{v} \tag{79}$$

and if $\boldsymbol{x}(0) = \boldsymbol{y}$, one deduces that

$$\exp_a(\boldsymbol{y}) = \Psi(\boldsymbol{e}_a,\boldsymbol{y}). \tag{80}$$

So the iteration procedure, which is exponentiation, translates to group multiplication by an element which corresponds to a (canonical) basis vector.

Let $S(\Sigma)$ be the set of points obtained by forward and backward iteration of $\boldsymbol{x}_0 = \boldsymbol{0}$. It follows, from Eq. (80), that $S(\Sigma)$ is a subgroup of the relevant Lie group, $\mathscr{G}$ say; it is the subgroup generated by the three elements corresponding to $\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3$. One expects that $S(\Sigma)$ is an infinite group, and it is natural to ask if there is a minimum separation between its elements (in traditional crystallography, the minimum separation property of a regular array of atoms is what gives the so-called 'crystallographic restriction' that only certain rotational symmetries are possible).

In the general case (with no restriction on the constants (S^{ab}/n)), one might as a first step try to characterise the particular (S^{ab}/n) which produce subgroups Γ of $\mathscr{G}$ with the minimum separation property (which I refer to as discrete subgroups, henceforward). Further, one might try to characterise such discrete subgroups, and ask if there is a relation between the geometrical symmetry of the corresponding set of points and the subgroup itself. These are the kinds of questions that Thurston (1997) addresses and answers conditional on one extra assumption:

Assumption. The subgroup Γ is generated by elements which are close to the identity.

In physical terms, this is an assumption that 'atoms' of the structure which are close to the atom at the origin generate all other atoms, by the relevant analogue of translation in a crystal lattice (which is the iteration procedure described above).

Thurston shows that the group $\mathscr{G}$ must be nilpotent, in this case, and this gives a restriction on the values of the dislocation density tensor. This restriction (in the three-dimensional case that is of concern) is precisely that (S^{ab}/n) is either (i) zero or (ii) $\lambda\boldsymbol{v}\otimes\boldsymbol{v}$, for some number λ, vector $\boldsymbol{v}$ and that is what motivated the consideration of case (ii), above.

After Thurston, it seems that a classification of discrete structures associated with continuum models of defective crystals is possible, and my opinion is that this study must precede any serious attempt to analyse variational problems or thermodynamical issues in this context.

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