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Geometrical structure of two-dimensional crystals with non-constant dislocation density

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Geometrical structure of two-dimensional crystals with non-constant dislocation density

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Abstract We outline mathematical methods which seem to be necessary in order to discuss crystal structures with non-constant dislocation density tensor(ddt) in some generality. It is known that, if the ddt is constant (in space), then material points can be identified with elements of a certain Lie group, with group operation determined in terms of the ddt - the dimension of the Lie group equals that of the ambient space in which the body resides, in that case. When the ddt is non-constant, there is also a relevant Lie group (given technical assumptions), but the dimension of the group is strictly greater than that of the ambient space. The group acts on the set of material points, and there is a non-trivial isotropy group associated with the group action. We introduce and discuss the requisite mathematical apparatus in the context of Davini's model of defective crystals, and focus on a particular case where the ddt is such that a three dimensional Lie group acts on a two dimensional crystal state - this allows us to construct corresponding discrete structures too.

Keywords Crystals · Defects · Lie groups

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1 Introduction

In [1] Davini introduced a kinematical framework for defective solid crystals wherein three smooth linearly independent vector fields $\boldsymbol{l}_1(\cdot), \boldsymbol{l}_2(\cdot), \boldsymbol{l}_3(\cdot)$ are supposed to represent an averaged atomic structure, with these 'lattice vector fields' varying on a length scale coarser than interatomic distance. Let us write

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$$\Sigma = \{\{\boldsymbol{l}_a(\cdot)\}, \Omega; \quad a = 1, 2 \ldots n, \Omega \subseteq \mathbb{R}^n\} \tag{1}$$

to represent a so-called 'crystal state', where n smooth linearly independent lattice vector fields are defined on a region $\Omega \subseteq \mathbb{R}^n$. In this paper, n will be 2 or 3.

To set up continuum mechanics, in this context, it is natural to suppose that a continuum strain energy density function (per unit volume, say) depends on values of the lattice vector fields and their derivatives. In the simplest case, common in discussions of perfect crystals, one supposes that the energy density depends only on the values of the lattice vector fields (at a point) and that it has the symmetry of some underlying discrete structure — in linear elasticity theory, one might choose to assume that the energy density is such that the elastic moduli have cubic or tetragonal symmetry, say, and so *define* a continuum associated with a cubic or tetragonal perfect lattice.

The intention in this paper is to describe the mathematical apparatus that allows us to discuss an analogous set-up procedure systematically in the case where the material has defects, and to illustrate these generalities with a single, explicit, running example. We shall outline what is to be done in the case of defective crystals later in this introduction, but first it is worthwhile to consider the perfect crystal case in more depth, to understand the issues involved.

1.1 Perfect crystals, $n = 3$

Let $n = 3$ in (1) and introduce dual lattice vector fields $\boldsymbol{d}_1(\cdot), \boldsymbol{d}_2(\cdot), \boldsymbol{d}_3(\cdot)$ by

$$\boldsymbol{l}_a(x) \cdot \boldsymbol{d}_b(x) = \delta_{ab}, \boldsymbol{l}_a(\boldsymbol{x}) \otimes \boldsymbol{d}_a(\boldsymbol{x}) = \text{ identity}, \boldsymbol{x} \in \Omega, \tag{2}$$

where δ_{ab} is the Kronecker delta, summation convention operates on repeated indices, and $a, b = 1, 2, 3$. Denote the non-zero, assumed positive, determinant of those fields by

$$n(\boldsymbol{x}) = \boldsymbol{d}_1(\boldsymbol{x}) \cdot \boldsymbol{d}_2(\boldsymbol{x}) \wedge \boldsymbol{d}_3(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega. \tag{3}$$

Each of the quantities $\nabla \wedge \boldsymbol{d}_a(\cdot), a = 1, 2, 3$, will be referred to as a Burgers vector field.

Introduce a different crystal state

$$\Sigma^* = \left\{\{\boldsymbol{l}_a^*(\cdot)\}, \Omega^*; \quad a = 1, 2, 3, \quad \Omega^* \subseteq \mathbb{R}^3\right\}, \tag{4}$$

and say that states Σ, Σ^* are **elastically related** to one another if there exists a diffeomorphism $\boldsymbol{u} : \Omega \to \Omega^* = \boldsymbol{u}(\Omega)$ such that

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

Also, it is convenient to introduce the notion of *local* elastic relatedness: states Σ, Σ^* are **locally elastically related** to one another 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 $\boldsymbol{u}_{\boldsymbol{x}_0}(N_{\boldsymbol{x}_0}) \subseteq \Omega^*$ such that

$$\boldsymbol{l}_a^*(\boldsymbol{u}_{\boldsymbol{x}_0}(\boldsymbol{x})) = \nabla \boldsymbol{u}_{\boldsymbol{x}_0}(\boldsymbol{x}) \boldsymbol{l}_a(\boldsymbol{x}), \quad a = 1, 2, 3, \quad \boldsymbol{x} \in N_{\boldsymbol{x}_0}, \boldsymbol{x}_0 \in \Omega, \tag{6}$$

and vice versa.

Define the dislocation density tensor (ddt) $S(\cdot) \equiv (S_{ab}(\cdot))$, $a, b = 1, 2, 3$ by

$$S_{ab}(\boldsymbol{x}) = \frac{\nabla \wedge \boldsymbol{d}_a(\boldsymbol{x}) \cdot \boldsymbol{d}_b(\boldsymbol{x})}{n(\boldsymbol{x})}, \quad a, b, = 1, 2, 3, \boldsymbol{x} \in \Omega. \tag{7}$$

Let the ddt deriving from state Σ^* be denoted $S^*(\cdot)$. Then one calculates from (5) that if states Σ, Σ^* are elastically related to one another, then

$$S^*(\boldsymbol{u}(\boldsymbol{x})) = S(\boldsymbol{x}). \tag{8}$$

So each component of S is a *scalar elastic invariant*, being a function of the lattice vector fields and their first derivatives, unchanged in value by elastic deformation in the sense that (8) holds.

One accepts that in a *perfect crystal* each Burgers vector is identically zero, and so S is zero by (7). Let $\boldsymbol{x} = x_i \boldsymbol{e}_i \in \Omega$, where $\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3$ is an arbitrary basis of $\mathbb{R}^3$. Then there exists a vector potential $\boldsymbol{\tau} = \tau_i(\{x_j\})\, \boldsymbol{e}_i$, where $\{x_j\}$ denotes the set of three coordinates x_1, x_2, x_3, such that the components of $\boldsymbol{d}_a(\cdot)$ have the form $\partial \tau_a / \partial x_j$ (as $\nabla \wedge \boldsymbol{d}_a = \boldsymbol{0}$), and those of $\boldsymbol{l}_a(\cdot)$ have the form $\partial x_j / \partial \tau_a$. Now use (5) to calculate the fields $\boldsymbol{l}_a^*(\cdot)$ in a crystal state elastically related to Σ via the diffeomorphism defined by the potential $\boldsymbol{\tau}(\cdot)$ and find that

$$\boldsymbol{l}_a^*(\boldsymbol{\tau}(\boldsymbol{x})) = \boldsymbol{e}_a, \quad a = 1, 2, 3, \quad \boldsymbol{x} \in \Omega. \tag{9}$$

Thus when $S = 0$ one can assert that the crystal state consists of *constant* lattice vector fields modulo elastic deformation. We choose to recast this fact so as to allow generalization to defective crystals in due course. So introduce constant fields $\boldsymbol{e}_a(\cdot)$ by putting

$$\boldsymbol{e}_a(\boldsymbol{x}) = \boldsymbol{e}_a, \quad a = 1, 2, 3, \quad \boldsymbol{x} \in \Omega. \tag{10}$$

Let $\boldsymbol{u} : \mathbb{R}^3 \to \mathbb{R}^3$ be the *translation* ($\boldsymbol{y} \in \mathbb{R}^3$ is fixed and arbitrary, below)

$$\boldsymbol{u}(\boldsymbol{x}) \equiv \boldsymbol{x} + \boldsymbol{y}, \tag{11}$$

so $\nabla \boldsymbol{u}(\boldsymbol{x}) =$ identity, and rewrite (10) as

$$\boldsymbol{e}_a(\boldsymbol{u}(\boldsymbol{x})) = \nabla \boldsymbol{u}(\boldsymbol{x}) e_{\boldsymbol{a}}(\boldsymbol{x}), \quad a = 1, 2, 3, \quad \boldsymbol{x} \in \Omega. \tag{12}$$

Then the vector fields $\boldsymbol{e}_a(\cdot)$ are translation invariant in the sense that the elastic deformation $\boldsymbol{u}(\cdot)$ maps the vector fields to themselves, according to (12). Moreover this 'self-similarity' of the crystal state $\left\{\{\boldsymbol{e}_a(\cdot)\}, \mathbb{R}^2; a = 1, 2, 3\right\}$ can be associated, straightforwardly, with a discrete structure (i.e. a set of points with non-zero minimum separation of pairs of points) — simply choose three

linearly independent translations $\boldsymbol{y} = \boldsymbol{e}_a, a = 1, 2, 3$, and construct a non-trivial set of points T invariant under the three translations. Then if $\boldsymbol{x}_0 \in T$, it follows that $\boldsymbol{x}_0 + L \subseteq T$, where

$$L \equiv \{\boldsymbol{x} : \boldsymbol{x} = n_a \boldsymbol{e}_a, n_a \in \mathbb{Z}, a = 1, 2, 3\}. \tag{13}$$

L is the perfect crystal lattice with basis $\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3$, and this is the way that perfect crystal lattices are associated with continua that have zero ddt, $S = 0$. Also, as noted earlier, the symmetries of the perfect lattices are traditionally used as material symmetry groups for continuum strain energy densities (see e.g. Green and Adkins [2]) — elements of the corresponding point group can be represented as changes of basis of L. It is a fact that each such change of basis of L extends uniquely to a symmetry of the continuum crystal state, in the sense that each smooth bijection $\boldsymbol{\phi} : \mathbb{R}^3 \to \mathbb{R}^3$ that preserves addition (cf. (11)) determines and is determined by $\boldsymbol{\phi}(\boldsymbol{e}_a), a = 1, 2, 3$. This fact lies at the heart of the traditional procedure (of using symmetries of lattices as material symmetry groups for 'perfect crystal' continua) — it is a rather obvious fact in the case that $S = 0$, but the analogous result in the case of defective crystals (where $S \neq 0$) is not so obvious (see Parry and Sigrist [3], Nicks and Parry [4] for the case $S =$ constant, $S \neq 0$).

1.2 Defective crystals, $n = 3$

Now suppose that fields $\{\boldsymbol{l}_a(\cdot)\}$ are given, with $S \neq 0$, and consider the set of partial differential equations

$$\boldsymbol{l}_a(\boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{y})) = \nabla_1 \boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{y}) \boldsymbol{l}_a(\boldsymbol{x}), \quad a = 1, 2, 3, \boldsymbol{x}, \boldsymbol{y} \in \Omega, \tag{14}$$

for determination of the function $\boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{y})$. Note that (14) generalizes (12), recalling that $\boldsymbol{u}(\boldsymbol{x})$ depends on the parameter $\boldsymbol{y}$ in (11). In (14), $\nabla_1 \boldsymbol{\psi}(\cdot, \boldsymbol{y})$ denotes the gradient of $\boldsymbol{\psi} : \Omega \times \Omega \to \Omega$ with respect to its first argument.

It is one of the main result of Lie group theory that, if $S =$ constant, (14) has a solution for $\boldsymbol{\psi}$, and that $\boldsymbol{\psi}$ may be chosen to be invertible in both arguments with the additional properties:

$$\boldsymbol{\psi}(\boldsymbol{e}, \boldsymbol{x}) = \boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{e}) = \boldsymbol{x}, \boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{\psi}(\boldsymbol{y}, \boldsymbol{z})) = \boldsymbol{\psi}(\boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{y}), \boldsymbol{z}), \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z} \in \Omega, \tag{15}$$

where coordinates in Ω are chosen so that those of the point $\boldsymbol{e} \in \Omega$ are zero. So $\boldsymbol{\psi}$ can be viewed as a group composition function, with group identity element $\boldsymbol{e}$. (Note that properties (15) are evident in the case $S = 0, \boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{x} + \boldsymbol{y}$.)

So, *when the ddt is constant*, the continuum crystal state has the self-similarity (14). Note that this implies that Σ is locally elastically related to itself (put $\boldsymbol{u}_{\boldsymbol{x}_0} = \boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{x}_0), \boldsymbol{l}_a^*(\cdot) \equiv \boldsymbol{l}_a(\cdot), a = 1, 2, 3$ in (6)). We contend that this fact is useful when a continuum has strain energy density that includes a dependence on S:

$$w = \bar{w}(\{\boldsymbol{l}_a\}, S), \tag{16}$$

say, where $\boldsymbol{l}_a, S$ are interpreted as point values of fields $\boldsymbol{l}_a(\cdot), S(\cdot)$ calculated from a crystal state Σ - since only point values of $S(\cdot)$ are needed for the determination of the energy density, at that point, we can assume that the fields $\boldsymbol{l}_a(\cdot)$ are such that $S(\cdot)$ is constant. (We would not be able to make this assumption were the energy function in (16) to depend on derivatives of S). When (14) does hold, then, one can exploit the properties of the Lie group associated with the given ddt S to determine symmetries of corresponding discrete structures and examine whether or not these extend to symmetries of the continuum [3–5] .

We shall be concerned in this paper with a more general constitutive assumption than (16). To motivate the assumption made below, first allow that the energy depends on gradients of lattice vector fields up to some (arbitrary) finite order r (so it is a 'differential function' of order r, in the terminology of Olver [6]). Note that the components of $S(\cdot)$ are differential functions of order 1, and recall that they are scalar elastic invariants. In generalization of this note that

$$\boldsymbol{l}_a \cdot \nabla S, \boldsymbol{l}_b \cdot \nabla(\boldsymbol{l}_a \cdot \nabla S), \cdots, \quad a, b \cdots = 1, 2, 3 \tag{17}$$

are differential functions of order $2, 3, \cdots$, and that they are also scalar elastic invariants (see Davini and Parry [7]). In different terminology, they are **plastic strain variables**', unchanged by elastic deformation, and it is an old question in the theory of inelastic behaviour to determine a set of such kinematic variables which is sufficient to quantify inelastic behaviour, in some sense. In the context of this paper, this old question is answered below, see [8] for details.

Let $\mathfrak{F}$ be the (fields of) directional derivatives of S of order ≤ 3:

$$\mathfrak{F} = \{(S(\cdot), (\boldsymbol{l}_a \cdot \nabla S)(\cdot), (\boldsymbol{l}_b \cdot \nabla(\boldsymbol{l}_a \cdot \nabla S))(\cdot), (\boldsymbol{l}_c \cdot \nabla(\boldsymbol{l}_b \cdot \nabla(\boldsymbol{l}_a \cdot \nabla S)))(\cdot)) \, ; a, b, c = 1, 2, 3\} \, . \tag{18}$$

Then $\mathfrak{F}$ is a functional basis of all scalar elastic invariants deriving from the lattice vector fields in the sense that all scalar elastic invariants (of all orders) can be calculated if $\mathfrak{F}$ is known (let $\Delta^{(r)}$ consist of the fields of gradients of lattice vector fields $\boldsymbol{l}_a(\cdot)$ of order $\leq r$, and let $\Delta^{*(r)}$ derive, similarly, from lattice vector fields $\boldsymbol{l}^*_a(\cdot)$. Then $f : \Delta^{(r)} \to \mathbb{R}$ is a scalar elastic invariant if whenever (5) holds, $f(\Delta^{*(r)}(\boldsymbol{u}(\boldsymbol{x})) = f(\Delta^{(r)}(\boldsymbol{x})), \boldsymbol{x} \in \Omega$.)

Now let

$$\mathrm{CM}_\Sigma = \{\boldsymbol{g}(\boldsymbol{x}); \boldsymbol{x} \in \Omega, \boldsymbol{g} \in \mathfrak{F}\} \tag{19}$$

be the **classifying manifold** (of order 3) associated with Σ (cf. the remark following Theorem 8.19 in Olver [6]), and define CM_{Σ^*} via (4) similarly. Then the 'old question' is answered as follows: suppose that $\mathrm{CM}_\Sigma = \mathrm{CM}_{\Sigma^*}$ and that $\boldsymbol{g}(\boldsymbol{x}_0) = \boldsymbol{g}^*(\boldsymbol{x}^*_0)$ where $\boldsymbol{g}$ and $\boldsymbol{g}^*$ are corresponding elements of $\mathfrak{F}$ and $\mathfrak{F}^*$, for some $\boldsymbol{x}_0 \in \Omega, \boldsymbol{x}^*_0 \in \Omega^*$ in particular. Then Σ and Σ^* are locally elastically related to each other, and (6) holds with $u_{\boldsymbol{x}_0}(\boldsymbol{x}_0) = \boldsymbol{x}^*_0$.

That is, the plastic strain variables in $\mathfrak{F}$ are a 'complete' set of such variables, because if those variables match in two different states Σ, Σ^*, then the states are locally elastically related to one another. Loosely, the identity of the classifying manifolds is necessary and sufficient for local elastic relatedness.

In the body of the paper we shall consider a strain energy density which is intermediate in generality between (16) and an energy which incorporates a dependence on all the invariants in $\mathfrak{F}$. One can motivate this assumption by restricting to crystal states that allow 'neutral deformation', in Davini and Parry's terminology [7], see also [8], however we do not go into this motivation here. So we suppose that

$$w = \bar{w}\left(\{\boldsymbol{l}_a\}, S, \{\boldsymbol{l}_a \cdot \nabla S\}\right), \tag{20}$$

because we intend to explore the mathematical landscape required in order to discuss crystal states where $S(\cdot)$ is not constant, and the particular group structure discussed above is not available. We shall investigate whether or not there is nevertheless some discrete structure corresponding to the constitutive fields listed in (20).

1.3 Reformulation of constitutive assumptions, $n = 3$

Recall, to begin with, that in the case $S(\cdot) =$ constant there is a group structure deriving from the existence of a solution $\boldsymbol{\psi} : \Omega \times \Omega \to \Omega$ of (14), and that the assumption $S(\cdot) =$ constant was motivated by the form (16) of the energy density. We choose to reexpress S using the Lie bracket of pairs of vector fields $\boldsymbol{v}(\cdot), \boldsymbol{w}(\cdot)$, thus

$$[\boldsymbol{v}, \boldsymbol{w}](\cdot) \equiv \{(\boldsymbol{w} \cdot \nabla)\boldsymbol{v} - (\boldsymbol{v} \cdot \nabla)\boldsymbol{w}\}(\cdot). \tag{21}$$

Note the sign convention in (21). Let

$$\boldsymbol{L}_3(\cdot) = [\boldsymbol{l}_1, \boldsymbol{l}_2](\cdot), \tag{22}$$

and likewise introduce $\boldsymbol{L}_1(\cdot), \boldsymbol{L}_2(\cdot)$, the Lie brackets of pairs of lattice vector fields. Then one may compute, as in [8], [9], that in general

$$\boldsymbol{L}_b = S_{ab}\boldsymbol{l}_a, [\boldsymbol{L}_b, \boldsymbol{l}_c] = S_{ac}[\boldsymbol{l}_a, \boldsymbol{l}_b] + (\boldsymbol{l}_b \cdot \nabla S_{ac})\boldsymbol{l}_a. \tag{23}$$

From (23) in the case $S(\cdot) =$ constant,

$$\boldsymbol{L}_b = S_{ab}\boldsymbol{l}_a, [\boldsymbol{L}_b, \boldsymbol{l}_c] = S_{ac}[\boldsymbol{l}_a, \boldsymbol{l}_b]. \tag{24}$$

We shall refer to terms such as $[\boldsymbol{l}_1, \boldsymbol{l}_2]$ as Lie brackets of second order, to terms such as $[\boldsymbol{L}_3, \boldsymbol{l}_c] = [[\boldsymbol{l}_1, \boldsymbol{l}_2], \boldsymbol{l}_c]$ as Lie brackets of third order, etc. (and to $\boldsymbol{l}_a$ as a Lie bracket of first order, for convenience). It is clear from (24) that, in the case $S(\cdot) =$ constant, Lie brackets of *all* orders may be expressed as (constant) linear combinations of the vector fields $\boldsymbol{l}_a(\cdot)$. So $\boldsymbol{l}_1(\cdot), \boldsymbol{l}_2(\cdot), \boldsymbol{l}_3(\cdot)$ provide a basis for the Lie algebra of vector fields formed by taking successive Lie brackets of the given fields. This gives the existence of a three dimensional Lie group with composition function $\boldsymbol{\psi}$ satisfying (14).

In fact, this perspective (in the last paragraph) gives a means to exploit the constitutive assumption (20). First when $S(\cdot) =$ constant, (24) gives $S_{ab} = \boldsymbol{L}_b \cdot \boldsymbol{d}_a$ so that (16) can be written in the form

$$w = w'\left(\{\boldsymbol{l}_a\}, \{\boldsymbol{L}_a\}\right) \tag{25}$$

and we have from the remarks above that $\{\boldsymbol{l}_a\}$ is a basis for the vector fields $\boldsymbol{L}_a(\cdot)$ and all higher order Lie brackets.

In the case that $S(\cdot)$ is not constant, note that from (23), S and $\boldsymbol{l}_b \cdot \nabla S_{ac}$ can be written in terms of $\{\boldsymbol{l}_a\}, \{\boldsymbol{L}_a\}$ and $\{[\boldsymbol{L}_a, \boldsymbol{l}_b]\}$. So (20) can be written as

$$w = w' \left(\{\boldsymbol{l}_a\}, \{\boldsymbol{L}_a\}, \{[\boldsymbol{L}_a, \boldsymbol{l}_b]\} \right). \tag{26}$$

By analogy with the reformulation of the assumption $S(\cdot) =$ constant, we **assume** that, corresponding to (26), the vector fields $\boldsymbol{l}_a(\cdot), \boldsymbol{L}_a(\cdot), a = 1, 2, 3$ provide (or rather, include) a basis for $\{[\boldsymbol{L}_a, \boldsymbol{l}_b]\}$ and all higher order brackets. So $\{\boldsymbol{l}_a(\cdot)\}, \{\boldsymbol{L}_a(\cdot)\}$ generate a Lie algebra of vector fields, called the 'lattice algebra' by Elżanowski and Preston [10]. Via a result of Palais [11], this gives a corresponding Lie group of dimension k, $3 < k \leq 6$, and this is the observation that we shall exploit in this paper. Note that, descriptively, the energy density (26) depends on the lattice vector fields, the Burgers vectors (which are determined by $\{\boldsymbol{l}_a\}, \{\boldsymbol{L}_a\}$) and on vectors $[\boldsymbol{L}_a, \boldsymbol{l}_b]$ determined by an *iteration* of the Burgers vector construction.

In the sequel we highlight, repeatedly, a particular class of two dimensional crystal states - states where $\boldsymbol{l}_1(\cdot)$, $\boldsymbol{l}_2(\cdot)$ and $[\boldsymbol{l}_1, \boldsymbol{l}_2](\cdot)$ generate a three dimensional lattice algebra, so that there exists a corresponding three dimensional Lie group, via Palais' result. This appears to be the simplest non-trivial case where the dimension of the Lie group associated with the lattice vector fields is greater than the number of lattice vector fields. This mathematical convenience allows us to focus on issues rather than detailed calculation, and to exploit familiar results, however we intend to catalogue and investigate more general low dimensional crystal states in future.

1.4 Two-dimensional crystal states

Let

$$\Sigma = \left\{ \boldsymbol{l}_1(\cdot), \boldsymbol{l}_2(\cdot), \Omega; \Omega \subseteq \mathbb{R}^2 \right\}, \tag{27}$$

and in a **new notation** define the Lie bracket $\boldsymbol{l}_3(\cdot)$ of $\boldsymbol{l}_1(\cdot)$ and $\boldsymbol{l}_2(\cdot)$ by

$$\boldsymbol{l}_3(\cdot) \equiv [\boldsymbol{l}_1, \boldsymbol{l}_2](\cdot) \equiv \{(\boldsymbol{l}_2 \cdot \nabla)\boldsymbol{l}_1 - (\boldsymbol{l}_1 \cdot \nabla)\boldsymbol{l}_2\}(\cdot). \tag{28}$$

We shall consider the case where $\boldsymbol{l}_1(\cdot), \boldsymbol{l}_2(\cdot)$ and $\boldsymbol{l}_3(\cdot)$ provide a basis for all vector fields generated by taking successive Lie brackets of $\boldsymbol{l}_1(\cdot), \boldsymbol{l}_2(\cdot)$. To simplify even more we shall assume that all Lie brackets of order ≥ 3 are zero. The corresponding Lie algebra has dimension 3, in this case, as does the associated Lie group. Thus

$$[\boldsymbol{l}_1, \boldsymbol{l}_2] \equiv \boldsymbol{l}_3, [\boldsymbol{l}_2, \boldsymbol{l}_3] = \boldsymbol{0}, [\boldsymbol{l}_3, \boldsymbol{l}_1] = \boldsymbol{0}. \tag{29}$$

Note that

$$\boldsymbol{l}_3(\boldsymbol{x}) = \alpha(\boldsymbol{x})\boldsymbol{l}_1(\boldsymbol{x}) + \beta(\boldsymbol{x})\boldsymbol{l}_2(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega, \tag{30}$$

for some functions $\alpha, \beta : \Omega \to \mathbb{R}$ which are the analogues of the ddt in this case (recall (23)), and recall that we are interested in the case where at least

one of the functions $\alpha(\cdot), \beta(\cdot)$ is not constant. The Lie group corresponding to (29) is called the Heisenberg group — it is well known, and many useful result are available. These results will allow us to determine a discrete structure (of points in Ω) associated with Σ, in generalization of the way that a perfect lattice is associated with the case $S = 0$ (for $n = 3$).

Note that one associates a three dimensional Lie group with lattice vector fields $\boldsymbol{l}_1(\cdot), \boldsymbol{l}_2(\cdot), \boldsymbol{l}_3(\cdot) \equiv [\boldsymbol{l}_1, \boldsymbol{l}_2](\cdot)$ defined on $\Omega \subseteq \mathbb{R}^2$ by means of the following result (a particular case of Theorem 1.57 Olver [12]).

Theorem 1 *Suppose that lattice vector fields $\boldsymbol{l}_1(\cdot), \boldsymbol{l}_2(\cdot), \boldsymbol{l}_3(\cdot)$ defined on $\Omega \subset \mathbb{R}^2$ are given, such that (cf.* (29))

$$[\boldsymbol{l}_i, \boldsymbol{l}_j] = C_{kij}\boldsymbol{l}_k, \quad i, j, k = 1, 2, 3, \tag{31}$$

where the structure constants C_{ijk} *are zero except that $C_{312} = -C_{321} = 1$. Then there exists a Lie group G, a corresponding Lie algebra $\mathfrak{g}$ with the* same structure constants *relative to some basis $\boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3$ of $\mathfrak{g}$, and a local group action $\boldsymbol{\lambda} : G \times \Omega \to \Omega$ such that*

$$\nabla_1 \boldsymbol{\lambda}(\boldsymbol{e}, \boldsymbol{x})\boldsymbol{v}_i = \boldsymbol{l}_i(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega, \tag{32}$$

where $\boldsymbol{e}$ is the identity element of G, $\nabla_1 \boldsymbol{\lambda}(\cdot, \boldsymbol{x})$ is the gradient of λ with respect to its first argument, and

$$\boldsymbol{\lambda}(\boldsymbol{e}, \boldsymbol{x}) = \boldsymbol{x}, \boldsymbol{\lambda}(\boldsymbol{g}_1, \boldsymbol{\lambda}(\boldsymbol{g}_2, \boldsymbol{x})) = \boldsymbol{\lambda}(\boldsymbol{\psi}(\boldsymbol{g}_1, \boldsymbol{g}_2), \boldsymbol{x}), \boldsymbol{g}_1, \boldsymbol{g}_2 \in G, \boldsymbol{x} \in \Omega, \tag{33}$$

where $\boldsymbol{\psi} : G \times G \to G$ is the composition function in G.

It is the group action $\boldsymbol{\lambda}$ that links the higher dimensional group structure to the flow defined by the lattice vector fields, and it will turn out that iteration of the corresponding discrete flows gives a discrete set of points in $\Omega \subseteq \mathbb{R}^2$, in some cases.

One important further point is that, since $\boldsymbol{\lambda}(\cdot, \boldsymbol{x})$ maps a three dimensional group to $\mathbb{R}^2$, for each $\boldsymbol{x} \in \Omega$, the *isotropy group* of $\boldsymbol{x} \in \Omega$, defined by

$$I_{\boldsymbol{x}} \equiv \{\boldsymbol{g} \in G : \lambda(\boldsymbol{g}, \boldsymbol{x}) = \boldsymbol{x}\}. \tag{34}$$

is non-trivial. Clearly $I_{\boldsymbol{x}}$ is determined by the group action $\boldsymbol{\lambda}$, but it is also true that $\boldsymbol{\lambda}$ is determined by $I_{\boldsymbol{x}}$, see section 2.4 below. This observation will be useful when it comes to classifying 'canonical' forms of the vector fields $\boldsymbol{l}_1(\cdot), \boldsymbol{l}_2(\cdot)$ with the properties mentioned.

1.5 Outline of content

We start by briefly recalling salient facts from the theory of Lie groups and algebras, highlighting the three dimensional case (bearing section 1.4 in mind) and we recall the notions of homomorphic and isomorphic groups and algebras. The groups and algebras of interest in this paper (i.e. those such that (29) holds) are **nilpotent**, and this term is defined.

Next we list some useful facts regarding nilpotent groups — foremost amongst these facts are the following: one may choose coordinates so that the elements of the group and the elements of the corresponding algebra can be identified, and in those coordinates, the automorphisms of the group are represented as linear transformations (they can be thought of as 'homogeneous deformations', in continuum mechanical terms).

We have indicated in section 1.4 that in the case of a three dimensional nilpotent Lie group G acting on a region $\Omega \subseteq \mathbb{R}^2$, the corresponding isotropy groups (34) are non-trivial. For transitive group actions this leads to the theory of homogeneous spaces, and we recall some general results, in particular the construction of the group action from the isotropy group. This allows us to construct 'inequivalent' group actions, for a given G — it is a straightforward calculation once the automorphisms of G are known.

With these general results at hand, we next calculate canonical forms of the lattice vector fields satisfying (29), modulo elastic deformation and change of basis. These lattice vector fields may be obtained from a particular three dimensional nilpotent Lie group via relations of the form (32) — they are the *infinitesimal generators* of the group action, in different jargon. We investigate what choices of group, algebra, Lie algebra basis and group action produce the given lattice vector fields — since the lattice vector fields are the 'primary' kinematical variables, we may and do choose coordinates in the group in canonical fashion (i.e. the different choices of coordinates in the group have no effect on the lattice vector fields, so we make a particular, convenient, choice of coordinates).

At this stage we have enough information/apparatus to calculate the set of points obtained by iterating the flow along the lattice vector fields, and so obtain the analogues of the perfect lattices of traditional crystallography, in this case where the crystals are defective. Theorem 2 connects group multiplication in G to flow along $\boldsymbol{l}_1(\cdot), \boldsymbol{l}_2(\cdot), \boldsymbol{l}_3(\cdot)$, and this allows us to use results obtained by Cermelli and Parry [13]. The final result is simple, but the main point of the paper is to lay out methods which we hope will allow generalization to a wider class of defective crystals, with non-constant $S(\cdot)$, than the particular one considered here.

2 Lie groups and algebras

2.1 Generalities

A Lie group G is a group with the structure of a manifold, such that the group multiplication and inverse maps are smooth. In this paper we consider groups G such that an element $\boldsymbol{x} \in G$ is uniquely specified by three real numbers x_1, x_2, x_3 (called the coordinates of $\boldsymbol{x}$), and write $\boldsymbol{x} = x_i \boldsymbol{e}_i$, where $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3\}$ is a basis of $\mathbb{R}^3$ in recognition of this fact. The group multiplication function $\boldsymbol{\psi}$ satisfies relations (15) above, and the coordinates are chosen so that the group identity element has each coordinate zero.

As an alternative notation for the product of group elements $\boldsymbol{x}, \boldsymbol{y}$, which is $\boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{y})$, we shall often write

$$\boldsymbol{x}\boldsymbol{y} \equiv \boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{y}). \tag{35}$$

Let $(\boldsymbol{x}, \boldsymbol{y})$ denote the commutator of two group elements:

$$(\boldsymbol{x}, \boldsymbol{y}) \equiv \boldsymbol{x}^{-1}\boldsymbol{y}^{-1}\boldsymbol{x}\boldsymbol{y}. \tag{36}$$

Then the quadratic term in the Taylor expansion of $(\boldsymbol{x}, \boldsymbol{y})$ is $\boldsymbol{\gamma}(\boldsymbol{x}, \boldsymbol{y})$ (cf. Gorbatsevich, Onishchik, Vinberg [14]), where

$$\boldsymbol{\gamma}(\boldsymbol{x}, \boldsymbol{y}) \equiv C_{ijk} x_j y_k \boldsymbol{e}_i, \tag{37}$$

(with $\boldsymbol{y} = y_i \boldsymbol{e}_i$), and

$$C_{ijk} \equiv \left(\frac{\partial^2 \psi_i}{\partial x_j \partial y_k}(\boldsymbol{x}, \boldsymbol{y})\bigg|_{\boldsymbol{x}=\boldsymbol{y}=\boldsymbol{e}} - \frac{\partial^2 \psi_i}{\partial x_k \partial y_j}(\boldsymbol{x}, \boldsymbol{y})\bigg|_{\boldsymbol{x}=\boldsymbol{y}=\boldsymbol{e}} \right). \tag{38}$$

For our purposes, the vector space $\mathbb{R}^3$, with the operation $[\cdot, \cdot] : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^3$ defined by

$$[\boldsymbol{x}, \boldsymbol{y}] = \boldsymbol{\gamma}(\boldsymbol{x}, \boldsymbol{y}) \tag{39}$$

is the Lie algebra of the group G, and $[\cdot, \cdot]$ is called the Lie bracket. The Lie bracket satisfies

$$[\boldsymbol{x}, [\boldsymbol{y}, \boldsymbol{z}]] + [\boldsymbol{y}, [\boldsymbol{z}, \boldsymbol{x}]] + [\boldsymbol{z}, [\boldsymbol{x}, \boldsymbol{y}]] = \boldsymbol{0}.$$

The constants C_{ijk} which define the form $\boldsymbol{\gamma}$ are called the structure constants of the Lie algebra.

Vector fields $\boldsymbol{\nu}(\cdot)$ defined on G which satisfy

$$\boldsymbol{\nu}\left(\boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{y})\right) = \nabla_1 \boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{y}) \boldsymbol{\nu}(\boldsymbol{x}), \tag{40}$$

are said to be right invariant on G, so the lattice vector fields which satisfy (14) are right invariant. Let $\boldsymbol{\nu}(\cdot)$ be right invariant on G and consider the integral curve of $\boldsymbol{\nu}(\cdot)$ through the point $\boldsymbol{x}_0$: this is the set $\{\boldsymbol{x}(t) : \ t \in \mathbb{R}\}$ which represents the solution of

$$\frac{d\boldsymbol{x}}{dt}(t) = \boldsymbol{\nu}\left(\boldsymbol{x}\left(t\right)\right), \ \boldsymbol{x}(0) = \boldsymbol{x}_0, \quad t \in \mathbb{R}. \tag{41}$$

It is a standard result that, if $\boldsymbol{x}_0 = \boldsymbol{e}$, the corresponding integral curve is a one parameter subgroup of G, and that conversely, any one parameter subgroup of G represents the integral curve of a right invariant field on G, through $\boldsymbol{e}$.

Define

$$\boldsymbol{\ell}_a(\boldsymbol{x}) = \nabla_1 \boldsymbol{\psi}(\boldsymbol{e}, \boldsymbol{x}) \boldsymbol{e}_a, \quad a = 1, 2, 3. \tag{42}$$

Then one can show that these fields are right invariant, and that the fields $\boldsymbol{\ell}_1(\cdot), \boldsymbol{\ell}_2(\cdot), \boldsymbol{\ell}_3(\cdot)$ defined by (42) provide a basis for the vector space of all right invariant fields on G. Also the vector field $\boldsymbol{\nu}(\cdot)$ on G is specified once

$\boldsymbol{\nu}(\boldsymbol{e})$ is prescribed. By virtue of this remark one can think of the Lie algebra of G either as the vector space $\mathbb{R}^3$, with Lie bracket (39), or as the vector space of right invariant vector fields on G, with the Lie bracket of vector fields defined by (21). (Note that the Lie bracket of right invariant fields is right invariant.)

Now (41) has a solution defined for all $t \in \mathbb{R}$, and thereby one defines a mapping $\exp(t\boldsymbol{\nu}) : G \to G$ given by

$$\exp(t\boldsymbol{\nu})(\boldsymbol{x}_0) = \boldsymbol{x}(t), \tag{43}$$

and a group element $e^{(t\boldsymbol{\nu})} \in G$ (as opposed to the *mapping* $\exp(t\boldsymbol{\nu})$) by

$$e^{(t\boldsymbol{\nu})} = \exp(t\boldsymbol{\nu})(\boldsymbol{e}). \tag{44}$$

Note that $e^{(\,)} : \mathbb{R}^3 \to G$. $e^{(\,)}$ is called the *exponential* mapping of the Lie algebra (here $\mathbb{R}^3$) to the Lie group. It is a standard result that

$$\exp(t\boldsymbol{\nu})(\boldsymbol{x}) = \boldsymbol{\psi}\left(e^{(t\boldsymbol{\nu})}, \boldsymbol{x}\right) \equiv e^{(t\boldsymbol{\nu})}\boldsymbol{x}, \quad t\boldsymbol{\nu} \in \mathbb{R}^3,\ \boldsymbol{x} \in G. \tag{45}$$

2.2 Group and algebra homomorphisms

Let $\mathfrak{g}$ and $\mathfrak{h}$ be Lie algebras with Lie brackets $[\cdot,\cdot]_{\mathfrak{g}}$, $[\cdot,\cdot]_{\mathfrak{h}}$ respectively. (In the context of this paper, both brackets $[\cdot,\cdot]_{\mathfrak{g}}, [\cdot,\cdot]_{\mathfrak{h}}$ map $\mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^3$). A Lie algebra homomorphism is a linear transformation $L : \mathfrak{g} \to \mathfrak{h}$ which satisfies

$$[L\boldsymbol{x}, L\boldsymbol{y}]_{\mathfrak{h}} = L\,[\boldsymbol{x}, \boldsymbol{y}]_{\mathfrak{g}}\,, \quad \boldsymbol{x}, \boldsymbol{y} \in \mathfrak{g}. \tag{46}$$

If $C^{\mathfrak{g}}_{ijk}, C^{\mathfrak{h}}_{ijk}$ are the structure constants for $\mathfrak{g}, \mathfrak{h}$ respectively, then (13),(16),(24) imply

$$C^{\mathfrak{h}}_{ijk} L_{jp} L_{kq} = L_{ir} C^{\mathfrak{g}}_{rpq}, \tag{47}$$

where $L\boldsymbol{e}_i = L_{ji}\boldsymbol{e}_j,\ i, j = 1, 2, 3.$

Let G and H be Lie groups with group multiplication functions $\boldsymbol{\psi}_G, \boldsymbol{\psi}_H$ respectively. A smooth mapping $\boldsymbol{\phi} : G \to H$ is a Lie group homomorphism if

$$\boldsymbol{\psi}_H\left(\boldsymbol{\phi}(\boldsymbol{x}), \boldsymbol{\phi}(\boldsymbol{y})\right) = \boldsymbol{\phi}\left(\boldsymbol{\psi}_G(\boldsymbol{x}, \boldsymbol{y})\right), \quad \boldsymbol{x}, \boldsymbol{y} \in G. \tag{48}$$

If $\mathfrak{g}$ is the Lie algebra of G, and $\mathfrak{h}$ is the Lie algebra of H, and $\boldsymbol{\phi} : G \to H$ is a Lie group homomorphism, then $\nabla\boldsymbol{\phi}(\mathbf{0}) \equiv L$ is a Lie algebra homomorphism. Conversely if L satisfies (46), then there exists a Lie group homomorphism $\boldsymbol{\phi}$ such that $\nabla\boldsymbol{\phi}(\mathbf{0}) = L$. Also,

$$\boldsymbol{\phi}\left(e^{\boldsymbol{\nu}}\right) = e^{(\nabla\boldsymbol{\phi}(\mathbf{0})\boldsymbol{\nu})}, \quad \boldsymbol{\nu} \in \mathfrak{g} \equiv \mathbb{R}^3, \tag{49}$$

where $\boldsymbol{\phi}$ satisfies (48), where the exponential on the left hand side of (49) is the exponential which maps $\mathfrak{g}$ to G, and that on the right hand side maps $\mathfrak{h}$ to H. Relation (49) allows one to calculate the Lie group homomorphisms explicitly if the Lie algebra homomorphisms are found by solving (47). $\phi(\cdot)$ (resp. L) is called a Lie group (resp. algebra) isomorphism if it (resp. L) is invertible. An isomorphism $\boldsymbol{\phi} : G \to G$ (resp. $L : \mathfrak{g} \to \mathfrak{g}$) is called an automorphism. ($\phi(\cdot)$ and $\phi^{-1}(\cdot)$ have to be smooth).

2.3 Nilpotent groups and algebras, Canonical Group J

Let G be a three dimensional Lie group, with commutator $(\boldsymbol{x},\boldsymbol{y}) \equiv \boldsymbol{x}^{-1}\boldsymbol{y}^{-1}\boldsymbol{x}\boldsymbol{y}$. Let $G \equiv G_0$ and define $G_1 \equiv (G, G_0)$, the group generated by elements of the form $(\boldsymbol{x},\boldsymbol{y}), \boldsymbol{x} \in G, \boldsymbol{y} \in G_0$. Define $G_k \equiv (G, G_{k-1})$ inductively, $k \geq 1$. G is called nilpotent if and only if G_k is the trivial group $\{\boldsymbol{e}\}$ for sufficiently large k. For three dimensional nilpotent groups, $G \equiv G_0 \supseteq G_1 \supseteq G_2 = \{\boldsymbol{e}\}$.

Let $\mathfrak{g}$ be the Lie algebra corresponding to a Lie group G, with Lie bracket $[\boldsymbol{x},\boldsymbol{y}], \boldsymbol{x},\boldsymbol{y} \in \mathfrak{g}$. Let $\mathfrak{g} \equiv \mathfrak{g}_0$ and define $\mathfrak{g}_1 \equiv [\mathfrak{g}, \mathfrak{g}_0]$, the subspace generated by elements of the form $[\boldsymbol{x},\boldsymbol{y}],\ \boldsymbol{x} \in \mathfrak{g}, \boldsymbol{y} \in \mathfrak{g}_0$. Define $\mathfrak{g}_k \equiv \left[\mathfrak{g}, \mathfrak{g}_{k-1}\right]$ inductively, $k \geq 1$. $\mathfrak{g}$ is called nilpotent if and only if $\mathfrak{g}_k$ is the trivial subspace $\{\boldsymbol{0}\}$ for sufficiently large k. For three dimensional nilpotent algebras, $\mathfrak{g} \equiv \mathfrak{g}_0 \supseteq \mathfrak{g}_1 \supseteq \mathfrak{g}_2 = \{\boldsymbol{0}\}$.

A Lie group is nilpotent if and only if the corresponding Lie algebra is nilpotent (Gorbatsevich, Onishchik, Vinberg [14]).There is a one–to–one correspondence between isomorphism classes of Lie algebras and isomorphism classes of (connected and simply connected) Lie groups (c.f.Varadarajan [15] Theorem 2.8.2).

By the remarks in the introduction (Theorem 1) we are concerned with a three dimensional Lie group G, with Lie algebra $\mathfrak{g}$, that has nonzero structure constants $C_{312} = -C_{321} = 1$ with respect to a particular choice of basis, $\boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3$ of $\mathfrak{g}$. Thus

$$[\boldsymbol{v}_1, \boldsymbol{v}_2] = \boldsymbol{v}_3, [\boldsymbol{v}_2, \boldsymbol{v}_3] = \boldsymbol{0}, [\boldsymbol{v}_3, \boldsymbol{v}_1] = \boldsymbol{0}. \tag{50}$$

Define $\boldsymbol{\psi} : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^3$

$$\boldsymbol{\psi}(\boldsymbol{r},\boldsymbol{s}) \equiv \boldsymbol{r} + \boldsymbol{s} + \frac{1}{2}[\boldsymbol{r},\boldsymbol{s}] \tag{51}$$

so that if $\boldsymbol{\psi} = \psi_i \boldsymbol{v}_i, \boldsymbol{r} = r_i \boldsymbol{v}_i, s = s_i \boldsymbol{v}_i$, then

$$(\psi_i) = \left(r_1 + s_1, r_2 + s_2, r_3 + s_3 + \frac{1}{2}(r_1 s_2 - r_2 s_1)\right). \tag{52}$$

One can check that $\boldsymbol{\psi}$ has the properties required to be a Lie group composition function on $\mathbb{R}^3 \times \mathbb{R}^3$, and that the corresponding nonzero structure constants are $C_{312} = -C_{321} = 1$, with respect to $\boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3$. We shall denote the Lie group defined on $\mathbb{R}^3$, with $\boldsymbol{\psi}$ given by (51), or (52), by J — it is the three dimensional Heisenberg group (see [16]). J is a particular Lie group in the isomorphism class of Lie groups that have Lie algebra isomorphic to that defined by (50). We shall call J the *canonical group* with Lie algebra (50).

We shall show below that it does not matter what particular choice of group is made when it comes to exploiting group properties in order to describe discrete structures associated with the lattice vector fields. The above choice seems to be the simplest, for we have the following results, particular to J (see Parry [17]:

(i)
$$e^{(\boldsymbol{x})} = \exp(\boldsymbol{x})(\boldsymbol{e}) = \boldsymbol{x}, \quad \boldsymbol{x} \in \mathbb{R}^3, \tag{53}$$
this implies that Lie group elements in J may be identified with corresponding Lie algebra elements;

(ii)
$$(\boldsymbol{x}, \boldsymbol{y}) = [\boldsymbol{x}, \boldsymbol{y}], \quad \boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^3, \tag{54}$$
this implies that the group commutator (which represents the 'finite' Burgers vector obtained by successive flow along the right invariant fields defined by $\boldsymbol{y}, \boldsymbol{x}, \boldsymbol{y}^{-1}, \boldsymbol{x}^{-1}$) may be identified with the corresponding Lie bracket of algebra elements;

(iii) Given a (uniform) discrete subgroup D of J, there exist group elements $\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2, \boldsymbol{\alpha}_3$ such that
$$D = \{\boldsymbol{\alpha}_1^{n_1} \boldsymbol{\alpha}_2^{n_2} \boldsymbol{\alpha}_3^{n_3}; n_1, n_2, n_3 \in \mathbb{Z}\}, \tag{55}$$
in simple generalization of the definition of a perfect lattice, (13). Note that $\boldsymbol{\alpha}_3$ must be a generating element of $D \cap (J, J)$.

(iv) If $L : \boldsymbol{j} \to \boldsymbol{j}$ ($\boldsymbol{j}$ the Lie algebra of J) is a Lie algebra automorphism, then there exists a Lie group automorphism $\boldsymbol{\phi} : J \to J$ such that
$$\boldsymbol{\phi}(\boldsymbol{x}) = L\boldsymbol{x}, \quad \boldsymbol{x} \in \boldsymbol{j} \equiv J, \tag{56}$$
so
$$L = \nabla\boldsymbol{\phi}(\boldsymbol{0}). \tag{57}$$
It is straightforward to calculate the Lie algebra automorphisms of $\boldsymbol{j}$ — this is done in [17] and one finds that
$$L_{13} = L_{23} = 0, L_{33} = L_{11}L_{22} - L_{12}L_{21} \neq 0, \tag{58}$$
where $L\boldsymbol{x} = L(x_i\boldsymbol{v}_i) = x_i(L\boldsymbol{v}_i) \equiv x_i(L_{ji}\boldsymbol{v}_j) = (L_{ji}x_i)\boldsymbol{v}_j$.

(v) There are precisely two inequivalent one dimensional subgroups of J, modulo automorphisms of J.

Proof (of (v))The one dimensional subgroups of J have the form
$$H_{\boldsymbol{v}} = \{t\boldsymbol{v}; \boldsymbol{v} \in \boldsymbol{j}, t \in \mathbb{R}\}, \tag{59}$$
by (i) above. Let $\boldsymbol{\phi} : J \to J$ be an automorphism of J, with $L \equiv \nabla\boldsymbol{\phi}(0)$. Then
$$\boldsymbol{\phi}(H_{\boldsymbol{v}}) = H_{L\boldsymbol{v}}. \tag{60}$$
Recall that $\boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3$ is a basis of J. We have that:

1. $H_{\boldsymbol{h}}$ is equivalent to $H_{\boldsymbol{v}_3}$ modulo automorphism provided that $L\boldsymbol{v}_3 = \boldsymbol{h}$ for some L satisfying (58). So $\boldsymbol{h} = L_{33}\boldsymbol{v}_3$ and $\boldsymbol{h}$ must be parallel to $\boldsymbol{v}_3$.
2. $H_{\boldsymbol{h}}$ is equivalent to $H_{\boldsymbol{v}_1}$ provided $L\boldsymbol{v}_1 = \boldsymbol{h}$. This requires that, and is satisfied if, $\boldsymbol{h}$ is any vector not parallel to $\boldsymbol{v}_3$.

2.4 Homogeneous spaces

Let $\boldsymbol{\lambda} : G \times \Omega \to \Omega$ be a group action, satisfying (33). Suppose that the action is transitive, so that $\lambda(G, \boldsymbol{x}) = \Omega$, for all $\boldsymbol{x} \in \Omega$. Then (G, Ω) is called a *homogeneous space*. Let $I_{\boldsymbol{x}}$ be the isotropy group of $\boldsymbol{x}$, cf. (34).

Let H be a subgroup of G and introduce the left coset space G/H by

$$G/H = \{kH; k \in G\}. \tag{61}$$

Note that $k_1 H = k_2 H$ if and only if $k_1 = k_2 h$ for some $h \in H$. Then G/H is a homogeneous space with respect to the group action $\boldsymbol{\lambda} = G \times G/H \to G/H$ defined by

$$\boldsymbol{\lambda}(\boldsymbol{g}, \boldsymbol{k}H) = (\boldsymbol{g}\boldsymbol{k})H, \tag{62}$$

for if $\boldsymbol{k}H$ is given and $\boldsymbol{l}H \in G/H$ is chosen arbitrarily, then $\boldsymbol{\lambda}(\boldsymbol{l}\boldsymbol{k}^{-1}, \boldsymbol{k}H) = \boldsymbol{l}H$, so the action is transitive.

Define the *projection* mapping $\boldsymbol{\pi} : G \to G/H$ by

$$\boldsymbol{\pi}(\boldsymbol{g}) = \boldsymbol{g}H, \tag{63}$$

and choose a *section* $\boldsymbol{\sigma} : G/H \to G$ such that $\boldsymbol{\sigma}$ is a smooth right inverse to $\boldsymbol{\pi}$:

$$\boldsymbol{\pi}(\boldsymbol{\sigma}(\boldsymbol{g}H)) = \boldsymbol{g}H. \tag{64}$$

(The considerations in this paper are local - we do not discuss the existence of global smooth sections). Note that for the particular crystal state introduced in section 1.4, G is a three dimensional Lie group, $H \subset G$ will be a one dimensional subgroup, G/H will be parameterized by two real variables and identified with $\Omega \subseteq \mathbb{R}^2$.

Also note that one may define $\boldsymbol{\lambda} : G \times G/H \to G/H$ by

$$\boldsymbol{\lambda}(\boldsymbol{g}, \boldsymbol{k}H) = \boldsymbol{\pi}(\boldsymbol{g}\boldsymbol{\sigma}(\boldsymbol{k}H)), \tag{65}$$

and check two things: (i) $\boldsymbol{\lambda}$ satisfies (33), (ii) $\boldsymbol{\lambda}$ is independent of the choice of section, $\boldsymbol{\sigma}$. We also have (Komrakov et al [18]):

Proposition 1 *1. Let (G, Ω) be a homogeneous space and let $I_{\boldsymbol{x}}$ be the isotropy group of $\boldsymbol{x} \in \Omega$. Then $I_{\boldsymbol{x}}$ is a closed subgroup of G.*
2. Let H be a closed subgroup of a Lie group G, then G/H has the structure of a manifold, with $\boldsymbol{\lambda} : G \times G/H \to G/H$ (defined by (65)) smooth.

That is, given a group action $\boldsymbol{\lambda}$, any isotropy group $I_{\boldsymbol{x}}$ is a closed subgroup of G, and given any closed subgroup of G one can construct a corresponding group action. In fact, given a closed subgroup $H \subset G$ and the group action defined by (65), we have that

$$H = I_{\boldsymbol{\pi}(\boldsymbol{e})}, \tag{66}$$

for $\boldsymbol{\lambda}(\boldsymbol{g}, \boldsymbol{\pi}(\boldsymbol{e})) = \boldsymbol{\pi}(\boldsymbol{g}\boldsymbol{\sigma}(\boldsymbol{\pi}(\boldsymbol{e}))) = \boldsymbol{\pi}(\boldsymbol{g}\boldsymbol{h}) = \boldsymbol{g}H (\boldsymbol{h} \in H)$, so that $\boldsymbol{\lambda}(\boldsymbol{g}, \boldsymbol{\pi}(\boldsymbol{e})) = \boldsymbol{\pi}(\boldsymbol{e}) = H$ if and only if $\boldsymbol{g} \in H$, as stated.

Recall that, given a lattice algebra of vector fields, from Theorem 1 there exists a Lie group G and corresponding group action $\boldsymbol{\lambda}$ from which may recover the given vector fields via (32). According to the above proposition, one can now catalogue all group actions by listing the closed subgroups of G.

The following result connects flow along right invariant fields in G with flow along the lattice vector fields in Ω, when (G, Ω) is a homogeneous space. It shows that 'iteration commutes with projection', and is surely well-known. Recall that from (32)

$$\nabla_1 \boldsymbol{\lambda}(\boldsymbol{e}, \boldsymbol{x})\boldsymbol{v} \equiv \boldsymbol{l}_{\boldsymbol{v}}(\boldsymbol{x}), \quad x \in \Omega, \boldsymbol{v} \in \boldsymbol{g} \tag{67}$$

is the vector field corresponding to the Lie alebra element $\boldsymbol{v}$ (if we set $\boldsymbol{l}_i(\cdot) \equiv \boldsymbol{l}_{\boldsymbol{v}_i}(\cdot)$).

Theorem 2 *Let $\boldsymbol{x}(\varepsilon), \varepsilon \in \mathbb{R}, \boldsymbol{x}(\varepsilon) \in \Omega$ be defined by*

$$\boldsymbol{x}(\varepsilon) = \boldsymbol{\lambda}(e^{\varepsilon \boldsymbol{v}}\boldsymbol{g}, \boldsymbol{x}). \tag{68}$$

Then $\boldsymbol{x}(\varepsilon)$ solves

$$\begin{cases} \frac{d}{d\varepsilon}\boldsymbol{x}(\varepsilon) &= \boldsymbol{l}_{\boldsymbol{v}}(\boldsymbol{x}(\varepsilon)), \quad \varepsilon \in \mathbb{R}, \\ \boldsymbol{x}(0) &= \boldsymbol{\lambda}(\boldsymbol{g}, \boldsymbol{x}). \end{cases} \tag{69}$$

Proof Let $\boldsymbol{v}(\boldsymbol{g})$ be the right invariant field on G with $\boldsymbol{v}(\boldsymbol{e}) = \boldsymbol{v} \in \boldsymbol{g}$, i.e.

$$\boldsymbol{v}(\boldsymbol{\psi}(\boldsymbol{h}, \boldsymbol{g})) = \nabla_1 \boldsymbol{\psi}(\boldsymbol{h}, \boldsymbol{g})\boldsymbol{v}(\boldsymbol{h}), \boldsymbol{v}(\boldsymbol{g}) = \nabla_1 \boldsymbol{\psi}(\boldsymbol{e}, \boldsymbol{g})\boldsymbol{v}, \quad \boldsymbol{h}, \boldsymbol{g} \in G. \tag{70}$$

Note also that by differentiating $(33)_2$ with respect to $\boldsymbol{g}$, setting $\boldsymbol{g} = \boldsymbol{e}$ and replacing $\boldsymbol{h}$ by $\boldsymbol{g}$, one obtains

$$\nabla_1 \boldsymbol{\lambda}(\boldsymbol{g}, \boldsymbol{x})\boldsymbol{v}(\boldsymbol{g}) = \boldsymbol{l}_{\boldsymbol{v}}(\boldsymbol{\lambda}(\boldsymbol{g}, \boldsymbol{x})). \tag{71}$$

Clearly if $\boldsymbol{x}(\varepsilon)$ is defined by (68), then $(69)_2$ holds. Then as

$$\frac{d}{d\varepsilon}(e^{\varepsilon \boldsymbol{v}}\boldsymbol{g}) = \frac{d}{d\varepsilon}(\boldsymbol{\psi}(e^{\varepsilon \boldsymbol{v}}, \boldsymbol{g})) = \nabla_1 \boldsymbol{\psi}(e^{\varepsilon \boldsymbol{v}}, \boldsymbol{g})\boldsymbol{v}(e^{\varepsilon \boldsymbol{v}}) = \boldsymbol{v}(e^{\varepsilon \boldsymbol{v}}\boldsymbol{g}), \tag{72}$$

by $(70)_1$, we find

$$\frac{d}{d\varepsilon}\boldsymbol{\lambda}(e^{\varepsilon \boldsymbol{v}}\boldsymbol{g}, \boldsymbol{x})) = \nabla_1 \boldsymbol{\lambda}(e^{\varepsilon \boldsymbol{v}}\boldsymbol{g}, \boldsymbol{x})\boldsymbol{v}(e^{\varepsilon \boldsymbol{v}}\boldsymbol{g}) = \boldsymbol{l}_{\boldsymbol{v}}(\boldsymbol{\lambda}(e^{\varepsilon v}\boldsymbol{g}, \boldsymbol{x})), \tag{73}$$

by (72), (71). The result follows by uniqueness of solution of this last differential equation, with initial condition $\boldsymbol{\lambda}(\boldsymbol{g}, \boldsymbol{x}) \equiv \boldsymbol{x}(0)$.

Remark 1 Regarding (67), it can be shown that $\nabla_1 \boldsymbol{\lambda}(\boldsymbol{e}, \boldsymbol{x})$ is a Lie algebra homomorphism from $\boldsymbol{g}$ to the lattice algebra, ie.

$$\nabla_1 \boldsymbol{\lambda}(\boldsymbol{e}, \boldsymbol{x})[\boldsymbol{v}, \boldsymbol{w}] = [\nabla_1 \boldsymbol{\lambda}(\boldsymbol{e}_1 \boldsymbol{x})\boldsymbol{v}, \nabla_1 \boldsymbol{\lambda}(\boldsymbol{e}, \boldsymbol{x})\boldsymbol{w}], \boldsymbol{v}, \boldsymbol{w} \in \boldsymbol{g}. \tag{74}$$

3 Three dimensional nilpotent lattice algebras of vector fields in $\mathbb{R}^2$

First we show that Lie brackets of order ≥ 3, in such lattice algebras, are zero. We are given that the algebra has dimension 3, so $[\boldsymbol{l}_1, \boldsymbol{l}_2](\cdot) \neq \mathbf{0}$ and

$$\alpha[\boldsymbol{l}_1, \boldsymbol{l}_2](\cdot) \ + \beta \boldsymbol{l}_1(\cdot) + \gamma \boldsymbol{l}_2(\cdot) = \mathbf{0}, \alpha, \beta, \gamma, \in \mathbb{R}, \text{ implies } \alpha = \beta = \gamma = 0. \quad (75)$$

Let N_p be the set of Lie brackets of order $p \in \mathbb{N}$. Since the algebra is nilpotent, there exists a least integer k such that $N_k \neq \phi, N_{k+1} = \phi$. We show that $k = 2$. Set

$$\big[[\boldsymbol{l}_1, \boldsymbol{l}_2], \boldsymbol{l}_i\big](\cdot) = a_i \boldsymbol{l}_1(\cdot) + b_i \boldsymbol{l}_2(\cdot) + c_i [\boldsymbol{l}_1, \boldsymbol{l}_2](\cdot), i = 1, 2, \quad (76)$$

where $a_i, b_i, c_i \in \mathbb{R}, i = 1, 2$. Also, for $\boldsymbol{N} \in N_k$ set

$$\boldsymbol{N} = r\boldsymbol{l}_1(\cdot) + s\boldsymbol{l}_2(\cdot) + t[\boldsymbol{l}_1, \boldsymbol{l}_2](\cdot), r, s, t \in \mathbb{R}. \quad (77)$$

Hence

$$\begin{aligned} [\boldsymbol{N}, \boldsymbol{l}_1](\cdot) &= s[\boldsymbol{l}_2, \boldsymbol{l}_1] + t\{a_1 \boldsymbol{l}_1(\cdot) + b_1 \boldsymbol{l}_2(\cdot) + c_1 [\boldsymbol{l}_1, \boldsymbol{l}_2](\cdot)\} = \mathbf{0} \in N_{k+1}, \\ [\boldsymbol{N}, \boldsymbol{l}_2](\cdot) &= r[\boldsymbol{l}_1, \boldsymbol{l}_2] + t\{a_2 \boldsymbol{l}_1(\cdot) + b_2 \boldsymbol{l}_2(\cdot) + c_2 [\boldsymbol{l}_1, \boldsymbol{l}_2](\cdot)\} = \mathbf{0} \in N_{k+1}. \end{aligned} \quad (78)$$

Hence by (75)

$$ta_1 = tb_1 = tc_1 - s = 0 \text{ and } ta_2 = tb_2 = tc_2 + r = 0. \quad (79)$$

Now $t \neq 0$, for if $t = 0$ then $r = s = 0$ contradicting $N_k \neq \phi$. Then given $t \neq 0$ we have from (79) that $a_1 = b_1 = a_2 = b_2 = 0$ so from (76)

$$\big[[\boldsymbol{l}_1, \boldsymbol{l}_2], \boldsymbol{l}_i\big](\cdot) = c_i [\boldsymbol{l}_1, \boldsymbol{l}_2](\cdot), \quad i = 1, 2. \quad (80)$$

Forming brackets of order (k+1), (80) implies in particular

$$c_i^{k-1} [\boldsymbol{l}_1, \boldsymbol{l}_2](\cdot) = \mathbf{0}, \quad (81)$$

and this gives the result (as $k \geq 2$, and $N_3 = \phi$ by (81)).

3.1 Canonical form of vector fields in $\mathbb{R}^2$ with three dimensional nilpotent lattice algebra

We shall construct all vector fields, $\boldsymbol{l}_1(\cdot), \boldsymbol{l}_2(\cdot)$, whose components are real analytic in Ω, which solve (cf. (29))

$$[\boldsymbol{l}_1, \boldsymbol{l}_2](\cdot) \ = \boldsymbol{l}_3(\cdot), [\boldsymbol{l}_2, \boldsymbol{l}_3](\cdot) = \mathbf{0}, [\boldsymbol{l}_3, \boldsymbol{l}_1](\cdot) = \mathbf{0}, \quad (82)$$

and continue to write (cf. (30))

$$\boldsymbol{l}_3(\boldsymbol{x}) = \alpha(\boldsymbol{x}) \boldsymbol{l}_1(\boldsymbol{x}) + \beta(\boldsymbol{x}) \boldsymbol{l}_2(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega. \quad (83)$$

Note that since $\boldsymbol{l}_1(\cdot)$ and $\boldsymbol{l}_2(\cdot)$ are linearly independent at each $\boldsymbol{x} \in \Omega$, the components of the dual lattice vector fields are analytic, and therefore so are the functions $\alpha(\cdot), \beta(\cdot)$. From (82) and (83),

$$[\alpha\boldsymbol{l}_1 + \beta\boldsymbol{l}_2, \boldsymbol{l}_1] = \boldsymbol{l}_1(\boldsymbol{l}_1 \cdot \nabla\alpha) + \boldsymbol{l}_2(\boldsymbol{l}_1 \cdot \nabla\beta) - \beta(\alpha\boldsymbol{l}_1 + \beta\boldsymbol{l}_2) = \boldsymbol{0},$$
$$[\alpha\boldsymbol{l}_1 + \beta\boldsymbol{l}_2, \boldsymbol{l}_2] = \boldsymbol{l}_1(\boldsymbol{l}_2 \cdot \nabla\alpha) + \boldsymbol{l}_2(\boldsymbol{l}_2 \cdot \nabla\beta) + \alpha(\alpha\boldsymbol{l}_1 + \beta\boldsymbol{l}_2) = \boldsymbol{0},$$

so

$$\boldsymbol{l}_1 \cdot \nabla\alpha = \alpha\beta,\ \boldsymbol{l}_2 \cdot \nabla\alpha = -\alpha^2,\ \boldsymbol{l}_1 \cdot \nabla\beta = \beta^2,\ \boldsymbol{l}_2 \cdot \nabla\beta = -\alpha\beta. \tag{84}$$

These relations, (84), imply that

$$\beta\nabla\alpha - \alpha\nabla\beta = 0, \tag{85}$$

as $\boldsymbol{l}_1(\cdot)$ and $\boldsymbol{l}_2(\cdot)$ are linearly independent. We are assuming that not both of $\alpha(\cdot)$ and $\beta(\cdot)$ are identically zero in Ω — suppose initially that $\alpha(\cdot)$ is not identically zero. Let $\boldsymbol{x}_0 \in \Omega$ be such that $\alpha(\boldsymbol{x}_0) = 0$. Then $(84)_{1,2}$ give that $\nabla\alpha(\boldsymbol{x}_0) = \boldsymbol{0}$, and by successive directional differentiation of $(84)_{1,2}$ we find all derivatives of α (of all orders) are zero. Since α is analytic this leads to a contradiction. Hence α has one sign in Ω, suppose $\alpha > 0$. Then from (85)

$$\beta = \lambda\alpha, \quad \lambda \in \mathbb{R}, \tag{86}$$

and (84) gives

$$\boldsymbol{l}_1 \cdot \nabla\alpha = \lambda\alpha^2, \boldsymbol{l}_2 \cdot \nabla\alpha = -\alpha^2. \tag{87}$$

Introduce $\bar{l}_1 = \boldsymbol{l}_1 + \lambda\boldsymbol{l}_2$, $\bar{l}_2 = l_2$, so that from (87), (83)

$$\bar{\boldsymbol{l}}_1 \cdot \nabla\lambda = 0, \bar{\boldsymbol{l}}_2 \cdot \nabla\alpha = -\alpha^2, [\bar{\boldsymbol{l}}_1, \bar{\boldsymbol{l}}_2] = \alpha\bar{\boldsymbol{l}}_1. \tag{88}$$

Now, as $\alpha > 0$, we may change coordinates in Ω by defining $\boldsymbol{u} : \mathbb{R}^2 \to \mathbb{R}^2$ as follows:

$$\boldsymbol{u}(x, y) = (t(x, y), y), \quad t(x, y) \equiv -\ln\alpha(x, y), \quad (x, y) \in \mathbb{R}^2. \tag{89}$$

Let

$$\boldsymbol{l}_i'(\boldsymbol{u}(x, y)) \equiv \nabla\boldsymbol{u}(x, y)\bar{\boldsymbol{l}}_i(x, y), \quad i = 1, 2$$

and calculate that

$$\boldsymbol{l}_1'(t, y) = (0, \tau(t, y)),\ \boldsymbol{l}_2'(t, y) = (e^{-t}, \nu(t, y)),$$
$$[\boldsymbol{l}_1', \boldsymbol{l}_2'] = e^{-t}\boldsymbol{l}_1', \tag{90}$$

for some functions $\tau, \nu : \mathbb{R}^2 \to \mathbb{R}$. Next the single equation that derives from $(90)_3$ is an integrability condition that guarantees the existence of a mapping $\boldsymbol{v} : \mathbb{R}^2 \to \mathbb{R}^2$, with $\boldsymbol{v}(t, y) \equiv (t, v(t, y))$, such that $\boldsymbol{l}_i''(\cdot)$ defined by

$$\boldsymbol{l}_i''(\boldsymbol{v}(t, y)) = \nabla\boldsymbol{v}(t, y)\boldsymbol{l}_i'(t, y), \quad i = 1, 2, \tag{91}$$

have the form

$$\boldsymbol{l}_1''(t, v) = (0, e^t), \boldsymbol{l}_2''(t, v) = (e^{-t}, 0), [\boldsymbol{l}_1'', \boldsymbol{l}_2''](t, v) = (0, 1). \tag{92}$$

Finally, $\boldsymbol{w} : \mathbb{R}^2 \to \mathbb{R}^2$ defined by $\boldsymbol{w}(t,v) = (w,v)$, where $w \equiv e^t$, gives vector fields $'\boldsymbol{l}_i(\cdot)$ of the form

$$'\boldsymbol{l}_1(w,v) = (0,w), '\boldsymbol{l}_2(w,v) = (1,0), [\,'\boldsymbol{l}_1, '\boldsymbol{l}_2](w,v) = (0,1), \tag{93}$$

via $'\boldsymbol{l}_i(\boldsymbol{w}(t,v)) = \nabla \boldsymbol{w}(t,v)\boldsymbol{l}_i''(t,v)$, $i = 1,2$. In summary, when $\alpha > 0$ the solutions of (82) can be put into the form (93) modulo elastic deformation and the change of basis $\boldsymbol{l}_1 \to \boldsymbol{l}_1 + \lambda \boldsymbol{l}_2, \boldsymbol{l}_2 \to \boldsymbol{l}_2$. Note that if $\alpha < 0$ and we let $\boldsymbol{l}_1 \to \boldsymbol{l}_1, \boldsymbol{l}_2 \to -\boldsymbol{l}_2, \boldsymbol{l}_3 \to -\boldsymbol{l}_3$, then (82) holds for $\bar{\boldsymbol{l}}_1 \equiv \boldsymbol{l}_1, \bar{\boldsymbol{l}}_2 \equiv -\boldsymbol{l}_2, \bar{\boldsymbol{l}}_3 \equiv -\boldsymbol{l}_3$ and the coefficient of $\bar{\boldsymbol{l}}_1(\cdot)$ in the analogue of (83) is positive. Similar remarks apply in the case that $\beta(\cdot)$ is not identically zero in Ω. Also, note that whenever $\boldsymbol{l}_1(\cdot), \boldsymbol{l}_2(\cdot), \boldsymbol{l}_3(\cdot)$ solve (82), so also do

$$r\boldsymbol{l}_1(\cdot) + s\boldsymbol{l}_2(\cdot) + t\boldsymbol{l}_3(\cdot), \bar{r}\boldsymbol{l}_1(\cdot) + \bar{\boldsymbol{s}}l_2(\cdot) + \bar{\boldsymbol{t}}\bar{l}_3, (r\bar{s} - s\bar{r})[\boldsymbol{l}_1, \boldsymbol{l}_2](\cdot), \tag{94}$$

provided $r\bar{s} - s\bar{r} \neq 0$, $r, s, t, \bar{r}, \bar{s}, \bar{t} \in \mathbb{R}$. Since the particular changes of basis used to derive (93) have the form (94), for specific choices of $r, s, t, \bar{r}, \bar{s}, \bar{t}$, it follows that the (analytic) vector fields which solve (82) can be expressed as

$$\boldsymbol{l}_1(x,y) = (0,x), \quad \boldsymbol{l}_2(x,y) = (1,0), \quad \boldsymbol{l}_3(x,y) = (0,1), \tag{95}$$

modulo elastic deformation and change of basis (of the form (94)). (This is case 22 in Table 1 of González-López et al. [19], with $\eta_1(x), \eta_2(x)$ a basis of solutions of $\eta''(x) = 0$).

3.2 Homogeneous space (J, Ω)

Recall from section 3.2 that the one dimensional subgroups of J have the form $H_{\boldsymbol{v}}$ given by (59) — one thinks of them as 'straight lines' through the origin, in J. They are closed subgroups (the complement is open), and there are two inequivalent subgroups modulo automorphisms of J. Let us calculate the group action corresponding to the subgroup $H_{\boldsymbol{v}_1}$ (the composition in J has components (52) with respect to a basis $\boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3 \in \mathbb{R}^3$). The projection mapping $\boldsymbol{\pi} : J \to J/H_{\boldsymbol{v}_1}$ is given by:

$$\begin{aligned} \boldsymbol{\pi}(\boldsymbol{g}) = gH_{\boldsymbol{v}_1} &= \big\{\boldsymbol{\psi}(\boldsymbol{g}, t\boldsymbol{v}_1); t \in \mathbb{R}\big\} \\ &= \big\{(g_1 + t, g_2, g_3 + \tfrac{1}{2}(-g_2 t)) : t \in \mathbb{R}\big\}. \end{aligned} \tag{96}$$

There is precisely one element of this coset with first component zero (that element with $t = -g_1$), so we may parameterize $gH_{\boldsymbol{v}_1}$ by $(g_2, g_3 + \frac{1}{2}g_1g_2)$. Let $g_2, g_3 + \frac{1}{2}g_1g_2$ be the two components x_1, x_2 of a point $\boldsymbol{x} = x_i\boldsymbol{\gamma}_i, \quad i = 1,2$, of $\mathbb{R}^2$, where $\boldsymbol{\gamma}_1, \boldsymbol{\gamma}_2$ is a basis of $\mathbb{R}^2$. This choice of basis allows us to identify $J/H_{\boldsymbol{v}_1}$ with $\mathbb{R}^2$. We may also choose

$$\boldsymbol{\sigma}(\boldsymbol{g}H_{\boldsymbol{v}_1}) = \boldsymbol{\sigma}\big((g_2, g_3 + \tfrac{1}{2}g_1g_2)\big) = (0, g_2, g_3 + \tfrac{1}{2}g_1g_2), \tag{97}$$

so

$$\boldsymbol{\sigma}\big((x,y)\big) = (0,x,y), \quad (x,y) \in \mathbb{R}^2. \tag{98}$$

Therefore the group action $\boldsymbol{\lambda} : J \times \mathbb{R}^2 \to \mathbb{R}^2$ (regarding $G/H_{\boldsymbol{v}_1}$ as $\mathbb{R}^2$) corresponding to this projection is

$$\begin{aligned}\boldsymbol{\lambda}(\boldsymbol{p},(x,y)) &= \boldsymbol{\pi}(\boldsymbol{p}\boldsymbol{\sigma}(x,y)) = \boldsymbol{\pi}(\boldsymbol{\psi}(\boldsymbol{p},(0,x,y)) \\ &= \pi(p_1, p_2 + x, p_3 + y + \tfrac{1}{2}p, x) \\ &= (p_2 + x, p_3 + y + p_1 x + \tfrac{1}{2}p_1 p_2). \end{aligned} \tag{99}$$

The lattice vector fields deriving from this projection are, from (32),

$$\boldsymbol{l}_i(\boldsymbol{x}) = \nabla_1 \boldsymbol{\lambda}(\boldsymbol{e},\boldsymbol{x})\boldsymbol{v}_i = \frac{\partial \lambda r}{\partial p_i}(\boldsymbol{e},\boldsymbol{x})\boldsymbol{\gamma}_r, \quad i = 1,2,\ \boldsymbol{x} \in \mathbb{R}^2. \tag{100}$$

So from (100) the components of $\boldsymbol{l}_i(\cdot)$ with respect to the basis $\boldsymbol{\gamma}_1, \boldsymbol{\gamma}_2$, are $\left(\frac{\partial \lambda_r}{\partial p_i}(\boldsymbol{e},\boldsymbol{x})\right)$ and this gives

$$\boldsymbol{l}_1(\boldsymbol{x}) = (0,x), \quad \boldsymbol{l}_2(\boldsymbol{x}) = (1,0), \quad \boldsymbol{l}_3(x) = (0,1). \tag{101}$$

Note that these are the canonical forms (95) of the lattice vector fields. So we have an explicit construction of the objects whose existence is asserted in Theorem 1, namely we have a Lie group J, Lie algebra $\boldsymbol{j}$, basis $\boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3$ of $\boldsymbol{j}$ and group action $\boldsymbol{\lambda} : J \times \mathbb{R}^2 \to \mathbb{R}^2$ such that (32) holds, in this case.

Remark 2 – Regarding Theorem 1, if $\{G, \boldsymbol{g}, \boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3, \boldsymbol{\lambda}\}$ and $\{G', \boldsymbol{g}', \boldsymbol{v}'_1, \boldsymbol{v}'_2, \boldsymbol{v}'_3, \boldsymbol{\lambda}'\}$ are such that (32) holds, ie

$$\nabla_1 \boldsymbol{\lambda}(\boldsymbol{e},\boldsymbol{x})\boldsymbol{v}_i = \nabla_1 \boldsymbol{\lambda}'(\boldsymbol{e}',\boldsymbol{x})\boldsymbol{v}'_i\,(\equiv \boldsymbol{l}_i(\boldsymbol{x})), \quad i = 1,2,3, \tag{102}$$

where $\boldsymbol{e}, \boldsymbol{e}'$ are the identity elements in G, G' respectively, then G and G' are isomorphic, as are $\boldsymbol{g}$ and $\boldsymbol{g}'$. That is, given any one choice of group and corresponding group action, other choices preserving the infinitesimal generators are isomorphic to that chosen.

– Given a particular choice of $\{G, \boldsymbol{g}, \boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3, \boldsymbol{\lambda}\}$ the $\{\boldsymbol{v}_i\}$ and $\boldsymbol{\lambda}$ can be chosen modulo automorphisms of G and $\boldsymbol{g}$, when the infinitesimal generators are given. This implies that the isotropy group can be chosen modulo automorphisms of G, in that case, and the calculation above chose $H_{\boldsymbol{v}_1}$ as isotropy group. (The infinitesimal generators $\boldsymbol{l}_1(\cdot), \boldsymbol{l}_2(\cdot)$ would commute, were we to choose $H_{\boldsymbol{v}_3}$ as isotropy group, contradicting the starting assumption that $S \neq 0$.)

4 Sets of points obtained by discrete flow along the lattice vector fields

Given a two-dimensional crystal state Σ as in (27), with vector fields $\boldsymbol{l}_1(\cdot), \boldsymbol{l}_2(\cdot)$ generating a three-dimensional lattice algebra, we generate a set of points S_Σ in Ω by the following iterative process: choose a point $\boldsymbol{x}_0 \in \Omega \subseteq \mathbb{R}^2$ as initial point, construct two points $\boldsymbol{x}(1), \boldsymbol{x}(-1)$ by solving (41) in the form

$$\frac{d\boldsymbol{x}}{dt}(t) = \boldsymbol{l}_1(\boldsymbol{x}(t)), \quad \boldsymbol{x}(0) = \boldsymbol{x}_0, \quad t \in \mathbb{R}, \tag{103}$$

for $\boldsymbol{x}(t)$. Obtain two further points by solving the analogue of (103) with $\boldsymbol{l}_1(\cdot)$ replaced by $\boldsymbol{l}_2(\cdot)$. Iterate this process, using the four points so obtained as initial points in turn. Continuing, one obtains S_Σ.

We use theorem 2 to calculate S_Σ, and choose $G = J$, the canonical group. So put $\boldsymbol{g} = \boldsymbol{e}$ in theorem 2 to obtain that $\boldsymbol{x}(t) = \boldsymbol{\lambda}(e^{t\boldsymbol{v}_1}, \boldsymbol{x}_0)$ solves (103). Let $\boldsymbol{\pi}, \boldsymbol{\sigma}$ be the projection and section mappings of section 3.2, so $\boldsymbol{\lambda}(\boldsymbol{g}, \boldsymbol{x}) = \boldsymbol{\pi}(\boldsymbol{g}\boldsymbol{\sigma}(\boldsymbol{x}))$. Then

$$\boldsymbol{x}(t) = \boldsymbol{\lambda}(e^{t\boldsymbol{v}_1}, \boldsymbol{x}_0) = \boldsymbol{\pi}(e^{t\boldsymbol{v}_1}\boldsymbol{\sigma}(\boldsymbol{x}_0)) = \boldsymbol{\pi}(e^{t\boldsymbol{v}_1}\boldsymbol{g}_0), \tag{104}$$

if we set

$$\boldsymbol{g}_0 = \boldsymbol{\sigma}(\boldsymbol{x}_0). \tag{105}$$

Hence $\boldsymbol{x}(1) = \boldsymbol{\pi}(e^{\boldsymbol{v}_1}\boldsymbol{g}_0)$, $\boldsymbol{x}(-1) = \boldsymbol{\pi}(e^{-\boldsymbol{v}_1}\boldsymbol{g}_0)$, and the two further points obtained are $\boldsymbol{\pi}(e^{\boldsymbol{v}_2}\boldsymbol{g}_0)$, $\boldsymbol{\pi}(e^{-\boldsymbol{v}_2}\boldsymbol{g}_0)$. It follows that

$$S_\Sigma = \boldsymbol{\pi}(D\boldsymbol{g}_0), \tag{106}$$

where D is the subgroup of J generated by $e^{\boldsymbol{v}_1}$ and $e^{\boldsymbol{v}_2}$.

Now, in J, group and algebra elements may be identified, $e^{\boldsymbol{x}} = \boldsymbol{x}$, and $(\boldsymbol{x}, \boldsymbol{y}) = [\boldsymbol{x}, \boldsymbol{y}]$, according to (53) and (54). Hence

$$(e^{\boldsymbol{x}}, e^{\boldsymbol{y}}) = (\boldsymbol{x}, \boldsymbol{y}) = [\boldsymbol{x}, \boldsymbol{y}] = e^{[\boldsymbol{x}, \boldsymbol{y}]}, \quad \boldsymbol{x}, \boldsymbol{y} \in J. \tag{107}$$

Since $\boldsymbol{v}_3 = [\boldsymbol{v}_1, \boldsymbol{v}_2]$, because the structure constants in $\boldsymbol{j}$ correspond to those in the lattice algebra, we have

$$(e^{\boldsymbol{v}_1}, e^{\boldsymbol{v}_2}) = e^{\boldsymbol{v}_3}, \text{ so } e^{\boldsymbol{v}_2}e^{\boldsymbol{v}_1} = e^{\boldsymbol{v}_1}e^{\boldsymbol{v}_2}(e^{\boldsymbol{v}_2}, e^{\boldsymbol{v}_1}) = e^{\boldsymbol{v}_1}e^{\boldsymbol{v}_2}e^{-\boldsymbol{v}_3}. \tag{108}$$

It follows that any element of D can be written in the form

$$\boldsymbol{d} \equiv e^{n_1\boldsymbol{v}_1}e^{n_2\boldsymbol{v}_2}e^{n_3\boldsymbol{v}_3}, \quad n_1, n_2, n_3 \in \mathbb{Z}, \tag{109}$$

cf. (55). Then results of Cermelli and Parry [13] gives that $\boldsymbol{d} = d_i\boldsymbol{v}_i$ where

$$(d_i) = (n_1, n_2, n_3 + \tfrac{1}{2}n_1n_2), \quad n_1, n_2, n_3 \in \mathbb{Z}. \tag{110}$$

From (106), we need to calculate $\pi(\boldsymbol{d}\boldsymbol{g}_0)$,where $\boldsymbol{g}_0 = \boldsymbol{\sigma}(\boldsymbol{x}_0)$. So put $\boldsymbol{x}_0 = (x_1^0, x_2^0), \boldsymbol{\sigma}(\boldsymbol{x}_0) = (0, x_1^0, x_2^0)$ to find:

$$\begin{aligned}\boldsymbol{\pi}(\boldsymbol{d}\boldsymbol{\sigma}(\boldsymbol{x}_0)) &= \boldsymbol{\pi}(\boldsymbol{\psi}((n_1, n_2, n_3 + \tfrac{1}{2}n_1n_2), (0, x_1^0, x_2^0)) \\ &= \boldsymbol{\pi}((n_1, n_2 + x_1^0, n_3 + \tfrac{1}{2}n_1n_2 + x_2^0 + \tfrac{1}{2}n_1n_1^0) \\ &= (n_2 + x_1^0, n_3 + x_2^0 + n_1n_2 + n_1x_1^0) \\ &= (x_1^0, x_2^0) + n_1(0, x_1^0) + (n_2, n_3 + n_1n_2), \quad n_1, n_2, n_3 \in \mathbb{Z}. \end{aligned} \tag{111}$$

Let $K \equiv \{n_1(0, x_1^0); n_1 \in \mathbb{Z}\}$ be the set of integer multiples of $(0, x_1^0)$, and note that for fixed n_1,

$$\{(n_2, n_3 + n_1n_2); n_2, n_3 \in \mathbb{Z}\} = \mathbb{Z}^2. \tag{112}$$

Then

$$\begin{aligned} S_\Sigma &= \pi(D\sigma(\boldsymbol{x}_0)) \\ &= \boldsymbol{x}_0 + K + \mathbb{Z}^2. \end{aligned} \tag{113}$$

Notice that:

1. If x_1^0 is irrational, S_Σ contains $\{\boldsymbol{x}_0 + (n_2, n_1 x_1^0 + k); n_1, n_2, k \in \mathbb{Z}\}$, so S_Σ is dense on an infinite set of parallel lines;
2. If $x_1^0 = p/q$, with $p, q \in \mathbb{Z}$ relatively prime, then there exist $k, l \in \mathbb{Z}$ such that $kp + lq = 1$, so $\frac{1}{q} = k\left(\frac{p}{q}\right) + l$, and $\left\{n_1 x_1^0 + k; n_1, k \in \mathbb{Z}\right\}$ is the set of all integer multiples of $\frac{1}{q}$. Hence S_Σ is a simple lattice, containing $\boldsymbol{x}_0$, with basis $(1, 0), (0, 1/q)$.

5 Conclusion

The purpose of the paper was to lay out the apparatus needed to construct low-dimensional discrete crystal structures associated with continua that have non-constant dislocation density tensor systematically, and to illustrate the construction in what appears to be the simplest non-trivial case. We intend to catalogue other low-dimensional discrete structures in future work, and will try to correlate the results obtained with those that feature in current applications (quasicrystals, graphene ...) with a view to analysing corresponding variational problems, to begin with.

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