Reconciliation of Local and Global Symmetries for a Class of Crystals with Defects

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Received: 26 November 2010 / Published online: 5 May 2011
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Abstract We consider the symmetry of discrete and continuous crystal structures which are compatible with a given choice of dislocation density tensor. By introducing the notion of a ‘defective point group’ (determined by the dislocation density tensor), we generalize the notion of Ericksen–Pitteri neighborhoods to this context.

Keywords Crystals · Defects · Lie groups

Mathematics Subject Classification (2000) 74A20 · 74E25

1 Introduction

The purpose of this paper is to generalize, to the case of crystals with certain uniform distributions of defects, symmetry considerations which are well known in the case of perfect crystals. In a perfect crystal, geometrical considerations begin with the specification of basis vectors \( e_1, e_2, e_3 \in \mathbb{R}^3 \) of a perfect lattice

\[
L = \{ x : x = n_i e_i, \quad n_i \in \mathbb{Z}, \quad i = 1, 2, 3 \},
\]

– in a defective crystal, if one is given a set of three linearly independent vectors \( e_1, e_2, e_3 \in \mathbb{R}^3 \) and a dislocation density tensor \( S \) (and this is what we shall be given), the first question is what set of points should be taken in generalization of the perfect lattice \( L \).

Then, it is well known that the geometrical ‘symmetries’ of a perfect crystal structure relate to the various changes of basis that preserve the lattice \( L \), and this leads to the requirement that, if \( w(\cdot) \) is the continuum strain energy density function per unit current volume, then \( w([e_i]) = w([e'_i]) \) if \( e_1, e_2, e_3 \) and \( e'_1, e'_2, e'_3 \) are different bases of the lattice \( L \).
we discuss this type of issue for defective crystals (of a certain class), having decided that the appropriate generalization of the defective lattices is a set of points $G_{\ell}$. We will require that $w(\{e_{l}\},S) = w(\{e'_{l}\},S')$ in the case that $(\{e_{l}\},S)$ and $(\{e'_{l}\},S')$ generate the same set of points $G_{\ell}$. So, having recalled from Cermelli and Parry [5], Parry [14, 15] how to determine this set, the paper will be concerned with deriving the set of all geometrical quantities $(\{e'_{l}\},S')$ which lead to a given $G_{\ell}$. This will end with a generalization, to crystals with defects, of the well known fact that $\{e_{l}\}$ and $\{e'_{l}\}$ are bases of the same lattice $L$ if and only if $e_{l} = \gamma_{ij} e'_{j}$ where $\gamma_{ij}$ are the integer components of a matrix $\gamma \in GL_{3}(\mathbb{Z})$.

We shall be concerned, also, with a generalization of the following result for a perfect crystal: let $C$ be a symmetric matrix with entries $e_{i} \cdot e_{j}$, $i, j = 1, 2, 3$, then a frame indifferent strain energy function has the symmetry $w(C) = w(\gamma C \gamma^{T})$, where $\gamma^{T}$ is the transpose of $\gamma$. Pitteri [19] has discussed the distribution of the points $\gamma C \gamma^{T}$ in the space of strictly positive definite symmetric matrices by showing that:

(i) the set $P(C)$ of matrices $\gamma \in GL_{3}(\mathbb{Z})$ such that $\gamma C \gamma^{T} = C$ is finite;
(ii) if $C_{0}$ is prescribed, then there is a neighborhood $N(C_{0})$ of $C_{0}$ such that if $C \in N(C_{0})$ then $\gamma C \gamma^{T} \in N(C_{0})$ if and only if $\gamma \in P(C_{0})$.

This result allows one to confine attention to a finite set of symmetries of the strain energy function, if one is concerned only with small but finite changes in the crystal configuration that is specified by $C_{0}$—we shall provide a similar result for crystals with defects (in a given class).

The context of the paper is a continuum model of defective crystals proposed by Davini [6]. In that model the geometrical structure of the defective crystalline continuum is given by the prescription of three smooth linearly independent lattice vector fields $\ell_{1}(\cdot), \ell_{2}(\cdot), \ell_{3}(\cdot)$, defined at all points of a region $\Omega$ (in this paper we shall take $\Omega \equiv \mathbb{R}^{3}$ throughout). These lattice vector fields have duals $d_{1}(\cdot), d_{2}(\cdot), d_{3}(\cdot)$, so that $d_{a}(x) \cdot \ell_{b}(x) = \delta_{ab}$, $a, b = 1, 2, 3$, $(\delta_{ab})$ the Krönecker delta, $x \in \mathbb{R}^{3}$, and the corresponding dislocation density tensor (ddt) $S$ is defined by

$$S = (S_{ab}) = \frac{\nabla \wedge d_{a} \cdot d_{b}}{d_{1} \cdot d_{2} \wedge d_{3}}, \quad a, b = 1, 2, 3. \tag{1}$$

The ddt, $S$, is related to the Lie bracket of pairs of lattice vector fields, Parry and Šilhavý [13], and if $S \neq 0$ the vector fields are not commutative.

Note that in a perfect crystal there is a natural concept of the ‘neighbor’ of a given point: both $x + e_{a}$ and $x - e_{a}$ may be called neighbors of a given point $x \in L$ relative to the vector field $\ell_{a}(\cdot)$ defined by $\ell_{a}(p) = e_{a}$, $p \in \mathbb{R}^{3}$. Said differently, if $x(t)$ is the solution of $\dot{x} = \ell_{a}(x(t))$, where the dot represents differentiation with respect to $t \in \mathbb{R}$, then $y$ is called a neighbor of $x$ (relative to the vector field $\ell_{a}(\cdot)$) if either $(x(0) = x$ and $x(1) = y$) or $(x(0) = y$ and $x(1) = x$). The lattice $L$ is the set of points which consists of the origin, the neighbors of the origin (relative to each of the vector fields $\ell_{1}(\cdot), \ell_{2}(\cdot), \ell_{3}(\cdot)$), the neighbors of those neighbors, and so forth. The ‘neighbor’ idea extends to arbitrary vector fields $\ell_{a}(\cdot)$, $a = 1, 2, 3$, in the obvious way, irrespective of whether or not the ddt is zero, and the sets of points $G_{\ell}$ that we will adopt as generalizations of the perfect lattices will be precisely those sets of points which consist of the origin, its neighbors, the neighbors of those neighbors, etc., relative to prescribed lattice vector fields $\ell_{1}(\cdot), \ell_{2}(\cdot), \ell_{3}(\cdot)$.

One aim of the paper is to discuss properties of energy functions of the form $w(\{e_{l}\},S)$ by associating a structure (i.e. a set of points in $\mathbb{R}^{3}$) $G_{\ell}$ with the prescribed values of the geometrical variables $\{e_{l}\},S$. In constructing $G_{\ell}$, then, one has only the single prescribed
value of $S$ (so far as the distribution of values of $S(\cdot)$ defined by (1) is concerned). To proceed, we assume that $S(\cdot)$ (defined by (1)) is constant in $\mathbb{R}^3$, with value equal to that prescribed as the second argument of $w$. (This would not be an appropriate assumption if $w$ were given to depend on gradients of $S$ also). Since $S$ involves derivatives of $d_a(\cdot)$ (or $\ell_a(\cdot)$), one cannot make analogous assumptions regarding $\ell_a(\cdot)$, if $S \neq 0$. It is a main result in Lie theory (phrased rather differently to the following), that if $S(\cdot)$ is constant, then the neighbors of the origin are elements of a Lie group, and the subgroup of that Lie group which is generated by the neighbors of the origin is the set $G_\ell$, which consists of the origin, its neighbors, the neighbors of those neighbors, and so on. These facts are recalled in more detail in Parry [14, 15], and recalled briefly in Sect. 2.1. One has also that:

(iii) Once it is assumed that $S(\cdot)$ is constant, there is defined a Lie group composition function $\psi(\cdot, \cdot): \mathbb{R}^3 \times \mathbb{R}^3 \rightarrow \mathbb{R}^3$ such that

$$\ell_a (\psi(x, y)) = \nabla_1 \psi(x, y) \ell_a(x), \quad a = 1, 2, 3. \quad (2)$$

When (2) holds, $\ell_a(\cdot)$ is called a right invariant field with respect to the group multiplication function $\psi(\cdot, \cdot)$. Putting $u(x) \equiv \psi(x, y)$ in (2), that equation can be rewritten as

$$\ell_a(u(x)) = \nabla u(x) \ell_a(x), \quad a = 1, 2, 3, \quad (3)$$

which expresses an (elastic) self–similarity of the geometrical crystal configuration defined by the lattice vector fields. (In the case $S = 0$, the elastic deformation $u(\cdot)$ can be chosen to be a translation, and the fields become translation invariant);

(iv) It is shown in Davini [6] that $S$ is an elastic invariant, which leads to a certain arbitrariness in the choice of the corresponding Lie group (e.g., if $S = 0$, then $d_a(\cdot)$ may be any fields of the form $d_a(x) = \nabla \psi_a(x)$, for potentials $\psi_1, \psi_2, \psi_3$ such that $\nabla \psi_1 \wedge \nabla \psi_2 \cdot \nabla \psi_3 \neq 0$. A certain elastic deformation of the fields ‘straightens’ them out to $d_a(\cdot) \equiv e_a$). It is shown in Mal’cev [12], Parry [16, 17], that this freedom allows one to choose the Lie group, in a canonical way, so that the integral curves through the origin of the lattice vector fields are straight lines (even when $S \neq 0$);

(v) The structures $G_\ell$ that are generated when the Lie group is chosen in this canonical way are generally not discrete sets of points. According to Auslander, Green and Hahn [1], there are three classes of Lie group (in three dimensions) which give rise to discrete structures $G_\ell$. Thurston [20] highlights a particular one of these classes (see remark above (19) below), and that is the case that we deal with exclusively in this paper. For this case, Mal’cev [12], Cermelli and Parry [5] show that one can provide sufficient conditions on $S$ in order that these sets of points are discrete. (These are rationality conditions on a form of $S$);

(vi) Mal’cev [12] provides a canonical form for the discrete set of points $G_\ell$, and shows that the automorphisms of $G_\ell$ (which are ‘symmetries’ of $G_\ell$) extend to automorphisms of the ambient Lie group;

(vii) Adopting the rationality conditions above, Cermelli and Parry [5] have investigated the nature of the structures $G_\ell$, and shown that they are multilattices in the sense of Ericksen [7] and Pitteri and Zanzotto [19].

The plan of the paper is as follows. In the next section we recall basic definitions and facts regarding Lie groups and algebras which will be useful later. These facts give information about $G_\ell$ as discrete subgroups of certain Lie groups—we generalize the relation $e'_i = \gamma_{ij} e_j$ (which connects bases of a perfect lattice) to connect different (multiplicative) generators.
of the discrete subgroups $G_\ell$ via some linear transformation. The canonical choice of Lie groups helps here because it ensures that the one parameter subgroups of the canonical group are straight lines through the origin. To get at this connection, we also introduce the translation subgroup $T_\ell$ of $G_\ell$—this is the set of vectors $t \in \mathbb{R}^3$ such that $g + t \in G_\ell$ if $g \in G_\ell$. $T_\ell$ has the structure of a perfect lattice, and one can introduce the linear transformations which map to $T_\ell$ to itself as a step on the way to describing the mappings from one set of (multiplicative) generators of $G_\ell$ to another. We also account for different descriptions of the cosets $G_\ell/T_\ell$ (represented by the ‘shift’ vectors in this particular example of a multilattice, in Ericksen’s [7] and Pitteri and Zanzotto’s [19] terminology).

We give, in Theorem 7, necessary and sufficient conditions that different generators \{e'_{\alpha}\}, \{e_{\alpha}\} give the same structure $G_\ell$, within the given canonical Lie group. It turns out that this canonical group is parameterized by an integer $k$ (which is related to the ddt, $S$), so we ask if the set of points corresponding to $G_\ell$ can be the same in different canonical groups (corresponding to different values of $k$, different values of $S$). We accept that $w(\{e'_{\alpha}\}, S') = w(\{e_{\alpha}\}, S)$ whenever the set of points generated by $\{e'_{\alpha}\}, S'$ is the same as the set of points generated by $\{e_{\alpha}\}, S$ (irrespective of the group structure), and calculate $(\{e'_{\alpha}\}, S')$ in terms of $(\{e_{\alpha}\}, S)$. Finally we discuss whether or not there is a result analogous to that of Pitteri [18], in this case, to facilitate the analysis of small but finite changes of geometrical configuration in this class of discrete defective crystals.

2 Definitions and Preliminary Results

Here we recall relevant definitions and facts to do with Lie groups and Lie algebras, and make a particular choice of Lie group (given the value of the elastic invariant dislocation density tensor $S$). The discrete structures with which we shall be concerned are discrete subgroups of the chosen ‘canonical’ group $J$, and we prove a few preliminary results regarding the translation group associated with such a discrete subgroup in order to facilitate the discussion of symmetries of the subgroup in terms of linear transformations of $\mathbb{R}^3$ to itself, in the next section.

2.1 Definitions

A Lie group $G$ is a group with the structure of a manifold where the group multiplication function $\psi : G \times G \rightarrow G$ is smooth. Group multiplication of elements $x, y \in G$ will be denoted here by $xy \equiv \psi(x, y)$. It will be sufficient for our purposes to identify elements of the group with points of $\mathbb{R}^3$, so that one may associate coordinates $x_1, x_2, x_3 \in \mathbb{R}$ with a group element $x = x_i e_i$, by introducing a basis $e_1, e_2, e_3$ of $\mathbb{R}^3$. Note that summation convention operates throughout, except when a summation is explicit. The group identity will be $0 \in \mathbb{R}^3$, and so

$$0x = x0 = x, \quad (xy)z = x(yz), \quad xx^{-1} = x^{-1}x = 0,$$  \hspace{1cm} (4)

for all $x, y, z \in G$, and where the inverse element $x^{-1}$ of $x$ exists for all $x \in G$.

The structure constants are defined to be the quantities

$$C_{ijk} = \frac{\partial^2 \psi_i}{\partial x_j \partial y_k}(0, 0) - \frac{\partial^2 \psi_i}{\partial x_k \partial y_j}(0, 0),$$  \hspace{1cm} (5)
where $\Psi(x, y) = \psi_t(x, y)e_t$, and the Lie bracket operation $[\cdot, \cdot]: \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^3$ is defined by

$$[x, y] = C_{ijk}x_jy_ke_k, \quad x, y \in \mathbb{R}^3. \quad (6)$$

Here, the vector space $\mathbb{R}^3$ and the operation $[\cdot, \cdot]$ make up the Lie algebra which corresponds to the group $G$. Note that

$$[e_i, e_j] = C_{kl}e_k. \quad (7)$$

Suppose that lattice vector fields $\ell_a(\cdot)$, $a = 1, 2, 3$, have duals $d_a(\cdot)$, $a = 1, 2, 3$, and define the dislocation density tensor $S = (S_{ab})$ by

$$S_{ab}(x) = \frac{\nabla \wedge d_a(x) \cdot d_b(x)}{d_1(x) \cdot d_2(x) \wedge d_3(x)}. \quad (8)$$

Then if $S_{ab}(\cdot)$ is constant for each $a, b = 1, 2, 3$, there exists a Lie group $G$ such that $(S_{ab})$ is related to the structure constants of $G$ with respect to $e_1 \equiv \ell_1(0), e_2 \equiv \ell_2(0), e_3 \equiv \ell_3(0)$ as basis via

$$C_{kl} = \varepsilon_{rij} S_{jr}, \quad (9)$$

where $\varepsilon_{rij}$ is the permutation symbol. It follows, when $S = (S_{ab}(\cdot))$ is constant, that the lattice vector fields $\ell_a(\cdot)$, $a = 1, 2, 3$, are right invariant with respect to the composition function $\Psi$, in the sense that

$$\ell_a(\Psi(x, y)) = \nabla_1 \Psi(x, y)\ell_a(x), \quad a = 1, 2, 3, \quad (10)$$

where

$$\nabla_1 \Psi(x, y) \equiv \frac{\partial \Psi}{\partial x}(x, y).$$

This is a self similarity property of lattice vector fields with constant $S$ (a generalization of the translational invariance of lattice vector fields when $S = 0, \Psi(x, y) \equiv x + y$). If $\lambda(\cdot)$ is any right invariant field, satisfying

$$\lambda(\Psi(x, y)) = \nabla_1 \Psi(x, y)\lambda(x), \quad (11)$$

then

$$\lambda(x) = \nabla_1 \Psi(0, x)\lambda(0), \quad (12)$$

so that the field $\lambda(\cdot)$ is determined by its value at the origin (once $\Psi$ is given). The integral curve through $x_0$, $\{x(t); t \in \mathbb{R}\}$, of the right invariant field $\lambda(\cdot)$ is defined to be the solution of

$$\frac{dx}{dt}(t) = \lambda(x(t)), \quad x(0) = x_0, \quad t \in \mathbb{R}. \quad (13)$$

Integral curves through the origin are one parameter subgroups of $G$, that is, the solutions of (13) satisfy $x(t)x(s) = x(t+s)$, $s, t \in \mathbb{R}$. The exponential mapping $\exp(t\lambda): \mathbb{R}^3 \to \mathbb{R}^3$, $t \in \mathbb{R}, \lambda \in \mathbb{R}^3$, is defined by constructing the right invariant field $\lambda(\cdot)$ from (12) and (13) by putting $\lambda(0) = \lambda$, setting

$$\exp(t\lambda)(x_0) = x(t). \quad (14)$$
and noting that \( \exp(t\lambda) = \exp(t\lambda') \), if \( t\lambda = t\lambda' \). Group elements \( e^{(t\lambda)} \) are defined by

\[
e^{(t\lambda)} = \exp(t\lambda)(0),
\]

and it is a fact that

\[
\psi(e^{(t\lambda)}, x) = e^{(t\lambda)} x = \exp(t\lambda)(x).
\]  

This, (16), is an important result which relates group multiplication to flow along the right invariant field. Let \( x_0 \in G \) be given, and say that \( y \) is a neighbor of \( x_0 \) if there is an index \( a \in \{1, 2, 3\} \) such that either \( \dot{x} = \ell_a(x), x(0) = x_0, x(1) = y \) or \( \dot{x} = \ell_a(x), x(0) = y, x(1) = x_0 \). Then, from (16), the subgroup \( G_\ell \) of \( G \) that is generated by the three elements \( e^{(\ell_1)}, e^{(\ell_2)}, e^{(\ell_3)} \), where \( \ell_1 = \ell(0), \) etc., is the set which consists of the origin, the neighbors of the origin, the neighbors of those neighbors, and so on. To be definite,

\[
G_\ell := \{ x \in G; x = a_1^{\varepsilon_1} \cdots a_n^{\varepsilon_n}, a_i \text{ is one of } e^{(\ell_1)}, e^{(\ell_2)}, e^{(\ell_3)}, \\
\varepsilon_i = \pm 1, \; i = 1 \ldots n, \; n \in \mathbb{Z} \}.
\]  

An automorphism of the Lie algebra determined by the Lie bracket \([\cdot, \cdot]\) is here an invertible linear transformation \( L : \mathbb{R}^3 \to \mathbb{R}^3 \) such that \([Lx, Ly] = L[x, y], x, y \in \mathbb{R}^3 \) and the corresponding structure constants satisfy \( C_{ijk} L_{lp} L_{kq} = L_{ir} C_{rqp} \). An automorphism of the Lie group \( G \) is an invertible mapping \( \phi : G \to G \) such that \( \phi(x)\phi(y) = \phi(x y) \). If \( L \) is a Lie algebra automorphism, then there exists a Lie group automorphism \( \phi \) such that \( L = \nabla \phi(0) \), and vice versa. Moreover,

\[
\phi(e^{(\lambda)}) = e^{(\lambda \nabla \phi(0))}.
\]  

According to Thurston [20], if the subgroup \( G_\ell \) of \( G \) is to be discrete (that is, if the elements of \( G_\ell \) are to be isolated, as points of \( \mathbb{R}^3 \)) in the case that the generators \( e^{(\ell_1)}, e^{(\ell_2)}, e^{(\ell_3)} \) of \( G_\ell \) are sufficiently small, then \( G \) must be a nilpotent group and this implies, in this case, that the structure constants can be put in the form

\[
C_{ijk} = \varepsilon_{ijp} \lambda \nu \nu \nu, \; \lambda \in \mathbb{Q}, \; \nu \nu \nu \in \mathbb{Z}, \; r = 1, 2, 3,
\]  

where \( \nu_1, \nu_2, \nu_3 \) are relatively prime integers, Parry [14], Cermelli and Parry [5]. It follows that

\[
[x, y] = \lambda (\varepsilon_{ijp} x_i y_j \nu p \nu k), \; \begin{bmatrix} x, [y, z] \end{bmatrix} = 0, \; x, y, z \in \mathbb{R}^3.
\]  

We shall assume henceforward that the structure constants are such that (19) holds, for some choice of the rational number \( \lambda \), some choice of the relatively prime integers \( \nu_1, \nu_2, \nu_3 \).

Now we recall the particular choice of the Lie group (equivalently, choice of composition function \( \psi \)) that was made in [12], compatible with the given structure constants (equivalently, Lie bracket). Let \( x, y \in \mathbb{R}^3 \), then according to the Campbell Baker Hausdorff theorem, there exists a function \( c = c(x, y) \) such that

\[
c(e) = c(x) c(y).
\]  

It is a fact that the function \( c \) has the properties required to be a Lie group composition function, and in the case that (19) holds we have \( c \equiv x + y + \frac{1}{2}[x, y] \). With Lie bracket given by (20), we choose

\[
\psi(x, y) = x + y + \frac{1}{2}[x, y]
\]  

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and call the corresponding $G$ the canonical Lie group $J$ associated with the Lie bracket (20), cf. Mal’cev [12]. This choice of composition function gives that

(i) the one-parameter subgroups of $J$ are straight lines through the origin,
(ii) $e^{(x)} \equiv \exp(x)(0) = x$,
(iii) from (18), $\phi(x) = \nabla\phi(0)x$.

According to the second of these facts, elements of the group $J$ may be identified with elements of the Lie algebra (here, $\mathbb{R}^3$). The third fact asserts that the automorphisms of $J$ can be written as linear transformations of $\mathbb{R}^3$ to itself. (From the point of view of continuum mechanics, this will allow us to interpret some symmetries of various structures as ‘homogeneous elastic deformations’.)

2.2 The Translation Group $T_\ell$

The translation group $T_\ell$ of the discrete subgroup $G_\ell \subset J$ is defined by

$$T_\ell := \{ t \in J; \text{ if } g \in G_\ell, g + t \in G_\ell \}.$$  

(23)

Note that, since $0 \in G_\ell, T_\ell \subseteq G_\ell$. Let $Z(G_\ell)$ be the center of $G_\ell$, so

$$Z(G_\ell) := \{ x \in G_\ell; \text{ if } y \in G_\ell, (x, y) = 0 \},$$  

(24)

where $(x, y) := x^{-1}y^{-1}xy, x, y \in G_\ell$. According to Cermelli and Parry [5]

$$t \in T_\ell \text{ if and only if } 1/2[t, g] \in Z(G_\ell) \text{ for all } g \in G_\ell.$$  

(25)

It follows from this and Hall’s identities [9] (see also (28) below) that $T_\ell$ is a normal subgroup of $G_\ell$. Also, $T_\ell$ is an additive subgroup of $\mathbb{R}^3$, and $Z(G_\ell) \subseteq T_\ell$.

**Proposition 1** If $g \in G_\ell$, then $g^2 = 2g \in T_\ell$.

**Proof** Let $G'_\ell$ be the commutator subgroup of $G_\ell$, so $G'_\ell$ is generated by all elements of the form $(x, y), x, y \in G_\ell$. Thus

$$G'_\ell := \{ x \in G; x = b_1^{\epsilon_1} \ldots b_i^{\epsilon_i} \ldots b_n^{\epsilon_n}, b_i = (x_i, y_i) \text{ for} \ x_i, y_i \in G, \epsilon_i = \pm 1, i = 1 \ldots n, n \in \mathbb{Z} \}.$$  

(26)

By Hall’s identities, if $g \in G_\ell$, $1/2[g^2, x] = [g, x] \in G'_\ell \subseteq Z(G_\ell)$ for all $x \in G_\ell$. So the result follows by (25). □

If $x_1, x_2 \ldots x_p \in \mathbb{R}^3, p$ an integer, let

$$(x_1, x_2, \ldots x_p) := \left\{ x \in \mathbb{R}^3; x = \sum_{i=1}^{p} n_i x_i, n_i \in \mathbb{Z}, i = 1, 2 \ldots p \right\},$$  

(27)

denote the integer linear span of the vectors $x_1, x_2 \ldots x_p$. Note that, since $T_\ell$ is a discrete additive subgroup of $\mathbb{R}^3$, it equals the integer linear span of a finite number of elements of the vector space $\mathbb{R}^3$, Bourbaki [3].
Proposition 2

(i) If \( \alpha \in G_\ell \), then \( \alpha + T_\ell = \alpha T_\ell \).

(ii) Let \( T_\ell = \langle x_1, x_2 \ldots x_p \rangle \) and suppose that one of \( x_1, x_2 \ldots x_p \) is a generator of \( \mathbb{Z}(G_\ell) \). Then each element of \( T_\ell \) is expressible as a product of the elements \( x_1, x_2 \ldots x_p \in G_\ell \) and their inverses.

Proof

(i) \( \alpha T_\ell \subseteq \alpha + T_\ell \) because, if \( t \in T_\ell \), then \( \alpha t = \alpha + t + \frac{1}{2}[\alpha, t] = \alpha + s \), where \( s \in T_\ell \) because \( s = t + \frac{1}{2}[\alpha, t] \in T_\ell \) and \( \frac{1}{2}[\alpha, t] \in \mathbb{Z}(G_\ell) \subseteq T_\ell \) by (25). The reverse inclusion is similar.

(ii) Let \( t, t' \in T_\ell \). Since \( tt' = t + t' + \frac{1}{2}[t, t'] \) and \( \frac{1}{2}[t, t'] \in \mathbb{Z}(G_\ell) \) by (25), it follows that

\[
\frac{1}{2}[t, t']^{-1} \equiv t + t' \mod 2
\]

and the result follows by induction.

Next we record some results from Cermelli and Parry [5], for later convenience. Recall that \( \mathbb{Z}(G_\ell) \) is the center of \( G_\ell \), \( G_\ell' \) is the commutator subgroup. Then in the case in hand \( G_\ell' \subseteq \mathbb{Z}(G_\ell) \) and \( \mathbb{Z}(G_\ell) \) has a single generator. The index of \( G_\ell' \) in \( \mathbb{Z}(G_\ell) \) is denoted \( k \) (so, if \( s \in G_\ell \) generates \( \mathbb{Z}(G_\ell) \), then \( s^k \) generates \( G_\ell' \)).

Theorem 3 Let \( J \) be the Lie group with composition function (22), where \([x, y]\) is given by (20) with \( \lambda = p/q \in \mathbb{Q} \), where \( p, q \in \mathbb{Z} \) have no common factors, and \( v_1, v_2, v_3 \) are relatively prime. Define \( \nu := v_1 v_2 v_3 \). Let \( G_\ell \) be the discrete subgroup of \( J \) generated by the three elements \( e^{(\ell)}_1, e^{(\ell)}_2, e^{(\ell)}_3 \) (so \( e^{(\ell)}_1 = \ell_1(0) \), etc., by the remark following (16)). Then:

(i) \( \mathbb{Z}(G_\ell) \) is generated by \( \lambda \nu, \ell_1(0)/k = \lambda \nu/k \) if we put \( e_\nu \equiv \ell_\nu(0), \nu \equiv v_1 e_1 \); 
(ii) \( G_\ell' \) is generated by \( \lambda \nu \); 
(iii) (a) \( k = p \) if \( \nu \) is even, or if \( (\nu \text{~odd} \text{~and} \text{~} p \in 4\mathbb{Z}) \), 
(b) \( k = \frac{1}{2} p \) if \( \nu \text{~odd} \text{~and} \text{~} p \in 2\mathbb{Z}, \text{~} p \notin 4\mathbb{Z} \), 
(c) \( k = 2p \) if \( \nu \text{~odd} \text{~and} \text{~} p \notin 2\mathbb{Z} \); 
(iv) If \( k \) is even, \( T_\ell = G_\ell \), and \( T_\ell \) consists of (all) integer linear combinations of \( e_1, e_2, e_3, \lambda \nu/k \); 
(v) If \( k \) is odd, \( T_\ell \) consists of (all) integer linear combinations of \( 2e_1, 2e_2, 2e_3, \lambda \nu/k \). \( G_\ell/T_\ell \) has four elements which may be written as \( T_\ell, \alpha T_\ell, \beta T_\ell, \alpha \beta T_\ell \), for some \( \alpha, \beta \in G_\ell \).

Proof (i) and (ii) are Proposition 2, [5]. (iii) is Proposition 3, [5]. (iv) comes from remarks following (89), [5]. The first sentence of (v) is Proposition 6, [5]. Regarding the second sentence of (v), let \( \alpha = e^{n_1}_1 e^{n_2}_2 e^{n_3}_3 \), \( \beta = e^{n'_1}_1 e^{n'_2}_2 e^{n'_3}_3 \), modulo \( G_\ell' \) (putting \( e^{1}_1 = \ell_1(0) = e_1 \), etc.). Then according to (98), [5], \( \alpha \) and \( \beta \) are equivalent modulo \( T_\ell \) if and only if \( n_a - n'_a = v_a \mod 2, a = 1, 2, 3 \). So if \( T_\ell, \alpha T_\ell \) and \( \beta T_\ell \) are distinct cosets in \( G_\ell \), then each of \( (n_a = v_a \mod 2), (n'_a - v_a = v_a \mod 2) \) is false for some choice of \( a = 1, 2, 3 \). Since \( \alpha \beta = e^{n_1+n'_1}_1 e^{n_2+n'_2}_2 e^{n_3+n'_3}_3 \), modulo \( G_\ell' \), it follows that \( \alpha \beta T_\ell \) is distinct from each of \( T_\ell, \alpha T_\ell, \beta T_\ell \) (since, for example, it is false that \( n_a + n'_a = v_a \mod 2, a = 1, 2, 3 \), so \( \alpha \beta T_\ell \neq T_\ell \)). It is shown in [5] that \( G_\ell/T_\ell \) has four elements.
Note that according to (iv), if \( k \) is even, the points of \( G_\ell \) form a three dimensional lattice (since \( T_\ell \) is an additive discrete subgroup of \( \mathbb{R}^3 \)), and according to (v), if \( k \) is odd, \( G_\ell \) is a 4-lattice.

### 2.3 Canonical Coordinates for \( G_\ell \)

\( G_\ell \) is generated by three elements \( e^{(\ell_1)}, e^{(\ell_2)}, e^{(\ell_3)} \). Thus if \( g \in G_\ell \), \( g \) is expressible as a product of the three generators and their inverses. According to Mal’cev [12], in a nilpotent group (in particular, in a three dimensional nilpotent group, where the structure constants have the form (19)) one may choose the three generators in such a way that the Lie bracket has a particular simple form: there are generators of \( G_\ell \subset J \) and corresponding Lie algebra elements \( e_1, e_2, e_3 \in \mathbb{R}^3 \) such that for some integer \( k \),

\[
[c_1, c_2] = kc_3, \quad [c_1, c_3] = [c_2, c_3] = 0, \quad k \in \mathbb{Z}. \tag{29}
\]

Recalling that group and algebra elements may be identified in \( J \), Mal’cev shows further that any \( g \in G_\ell \subset J \) may be written in the form

\[
g = e_\alpha^\beta e_2^{\beta} e_3^{\gamma}, \quad \alpha, \beta, \gamma \in \mathbb{Z}. \tag{30}
\]

(Note that this relation (30) is a generalization of the expression of a point \( x \) of a perfect lattice with basis \( e_1, e_2, e_3 \) as \( x = \alpha e_1 + \beta e_2 + \gamma e_3, \alpha, \beta, \gamma \in \mathbb{Z} \).)

Let \( G'_\ell \) be the commutator subgroup of \( G_\ell \) and recall the following identities, due to Hall [9],

\[
(x, yz) = (x, z)(x, y) ((x, y), z), \quad (xy, z) = (x, z)((x, y), y, z). \tag{31}
\]

In the nilpotent case, one has \((x, y, z) = 0\) for all \( x, y, z \in G_\ell \), so that \((x, yz) = (x, z)(x, y), (xy, z) = (x, z)(y, z)\). It follows that if \( x = c_1^{n_1} c_2^{m_2} c_3^{m_3}, y = c_1^{m_1} c_2^{m_2} c_3^{m_3} \) for integers \( n_i, m_i, i = 1, 2, 3 \), then \((x, y)\) is a product of terms of the form \((e_i, e_j)\). Also, note that, for \( x, y \in J \), with \( x^{-1} = -x \), etc.,

\[
(x, y) = \left(-x - y + \frac{1}{2}[x, y]\right) \left(x + y + \frac{1}{2}[x, y]\right) = [x, y], \tag{32}
\]

using properties of \([\cdot, \cdot]\) given above. In particular, (29) may be rewritten as

\[
(c_1, c_2) = c_3^k, \quad (c_1, c_3) = (c_2, c_3) = 0. \tag{33}
\]

and it follows that \( G'_\ell \) is generated by \( c_3^k \).

Also, let \( \mathbb{Z}(G_\ell) \) be the center of \( G_\ell \). If \( x = c_1^{n_1} c_2^{m_2} c_3^{\gamma}, \) then \((x, c_1) = (c_2, c_1)^\beta\). Also, let \( e_3^k \) be the center of \( G_\ell \), then \( x = c_3^k \) for some integer \( \gamma \). Moreover \((c_3^k, y) = 0\) for all \( \gamma \in \mathbb{Z} \), so \( \mathbb{Z}(G_\ell) \) is generated by \( c_3 \) (this is consistent with Theorem 3).

Less formally, let us refer to the commutator \((e_1, e_2) = c_1^{c_2} c_2^{-c_1} e_1 e_2\) as the “discrete Burgers’ vector” which represents flow along the vector fields defined by the Lie algebra elements \( c_2, c_1, -c_2, -c_1 \), successively. So the discrete Burgers’ vector corresponding to this choice of vector fields equals \( c_3^n \in G_\ell \). Because group and algebra elements may be identified in this canonical representation of the discrete structure, \( c_3^n = kc_3 \), and one may picture this lack of commutativity (of the vector fields \( c_1, c_2 \)) as a “screw dislocation”, because the Burgers’ vector is an integer multiple of the third vector \( c_3 \).
3 Generators of $G_e$

Here we presume that a canonical basis $c_1, c_2, c_3$ of a discrete subgroup $G_e \subset J$ is given, and find necessary and sufficient conditions that elements $e_1, e_2, e_3 \in G_e$ also generate $G_e$.

3.1 Canonical Basis

Let $J = (\mathbb{R}^3, \cdot)$ be the canonical nilpotent Lie group with composition function (multiplication of group elements) defined by

$$xy = x + y + \frac{1}{2}[x, y], \quad x, y \in \mathbb{R}^3.$$  \hspace{1cm} (34)

Now let $c_1, c_2, c_3$ be a canonical basis of some discrete group $G_e \subset J$. Then there exists an integer $k_e$, which is the index of $G_e' \equiv [G_e, G_e]$ in $\mathbb{Z}(G_e)$, with the property that

$$[c_1, c_2] = k_e c_3, \quad [c_1, c_3] = [c_2, c_3] = 0.$$  \hspace{1cm} (35)

With respect to that particular basis, writing $x = x_i c_i$, $y = y_i c_i$, one has

$$[x, y] = x_i y_j \epsilon_{ijp} k_e \delta_{j3} \delta_{p3} (\delta_{r3} c_r),$$  \hspace{1cm} (36)

a particular form of (20) above.

Let $T_e$ be the translational group corresponding to $G_e$. According to remarks in Sect. 2.3, $G_e'$ is generated by $c_3^{k_e}$, the index of $G_e'$ in $\mathbb{Z}(G_e)$ is $k_e$, and $\mathbb{Z}(G_e)$ is generated by $c_3$. (These facts are evident from (35), directly.) From Cermelli and Parry [5], or Theorem 3 above, we have that

$$T_e = \begin{cases} \langle e_1, e_2, e_3 \rangle, & k_e \text{ even} \\ \langle 2e_1, 2e_2, e_3 \rangle, & k_e \text{ odd} \end{cases}$$  \hspace{1cm} (37)

3.2 Conditions Necessary and Sufficient that $e_1, e_2, e_3 \in G_e$ Generate $G_e$

In this section we find the set of all generators of the given discrete group $G_e$. Let $e_1, e_2, e_3 \in G_e$ and consider to begin with the subgroup of $G_e$ which consists of all products of the elements $e_1, e_2, e_3$ and their inverses, denoted $G_e$. We shall assume that $e_1, e_2, e_3$ provide a basis of $\mathbb{R}^3$.

**Proposition 4** With respect to the basis vectors $e_1, e_2, e_3$, the composition function $xy = x + y + \frac{1}{2}[x, y]$ with Lie bracket given by (36) has the form

$$xy = x + y + \frac{\theta k_e}{2\Gamma} \epsilon_{ijp} x_i y_j v_p(v, e_r).$$  \hspace{1cm} (38)
for some integers $\Gamma, \nu_i, i = 1, 2, 3$, where $\theta = 1$ if $k_c$ is even and $\theta = 2$ if $k_c$ is odd. Also $[e_i, e_j] = \frac{\delta_{ik}}{\Gamma} e_{ijp}v_p(v_i e_i)$.

**Proof**

(i) Suppose that $k_c$ is even. Then according to Cermelli and Parry [5], $G_c = T_c = \langle e_1, e_2, e_3 \rangle$. Since $e_i \in G_c, i = 1, 2, 3$, there exists a matrix $\gamma \equiv (\gamma_{ij})$ of integers, with determinant $\Gamma := \det(\gamma)$ such that

$$e_i = \gamma_{ij} e_j.$$  \hfill (39)

So $[e_i, e_j] = \gamma_{ip} \gamma_{jq} [e_p, e_q] = \varepsilon_{pq3} \gamma_{ip} \gamma_{jq} k_c e_3$. Define, and observe that,

$$p_{ik} := \pm \frac{1}{2} \varepsilon_{pq\ell} \varepsilon_{ijk} \gamma_{ip} \gamma_{jq}, \quad p_{ik} \in \mathbb{Z}, \ \ell, k = 1, 2, 3.$$  \hfill (40)

Then

$$p_{ik} \gamma_{km} = \pm \frac{1}{2} \varepsilon_{pq\ell} \varepsilon_{pqn} \Gamma = \pm \Gamma \delta_{\ell m}, \quad \gamma^{-1} = \pm \left( \frac{p_{ik}}{\Gamma} \right),$$  \hfill (41)

and so

$$e_j = \pm \frac{1}{\Gamma} p_{ji} e_i, \quad \Gamma, p_{ij} \in \mathbb{Z}, \ i, j = 1, 2, 3.$$  \hfill (42)

Thus,

$$[e_1, e_2] = \frac{1}{2} \varepsilon_{ij3} [e_i, e_j] = \frac{1}{2} \varepsilon_{ij3} \varepsilon_{pq3} \gamma_{ip} \gamma_{jq} k_c e_3$$

$$= \pm p_{33} k_c e_3 = p_{33} \frac{k_c}{\Gamma} (p_{3i} e_i).$$  \hfill (43)

Similarly one finds $[e_2, e_3] = \pm p_{31} k_c e_3, \ [e_3, e_1] = \pm p_{32} k_c e_3$.

Define $\nu_i := p_{3i},$ so $\nu_i \in \mathbb{Z}, \ i = 1, 2, 3$. Then

$$[x, y] = x_i y_j [e_i, e_j] = x_i y_j \varepsilon_{ijp} v_p \frac{k_c}{\Gamma} (v_i e_i),$$  \hfill (44)

noting that $[e_i, e_j] = \varepsilon_{ijp} v_p \frac{k_c}{\Gamma} (v_j e_j)$. This proves the result in the case that $k_c$ is even.

(ii) Suppose that $k_c$ is odd. From Cermelli and Parry [5], $T_c = \langle 2c_1, 2c_2, c_3 \rangle$ and $T_c$ is a normal subgroup of $G_c$. Note that if $g \in G_c$, then $g^2 \in T_c$, from Proposition 1 in Sect. 2.2. Hence, since $e_i \in G_c, i = 1, 2, 3$, there exists a matrix $\gamma \equiv (\gamma_{ij})$ of integers, with determinant $\Gamma := \det(\gamma) \in \mathbb{Z}$, such that

$$2e_i = \gamma_{ij} e'_j.$$  \hfill (45)

where one defines $e'_1 = 2c_1, \ e'_2 = 2c_2, \ e'_3 = c_3$. Note that $[e'_1, e'_2] = 4k_c e_3$, so $[e'_p, e'_q] = 4k_c \varepsilon_{pq3} e_3$. So from (45)

$$[e_i, e_j] = \frac{1}{4} \varepsilon_{ijp} \gamma_{jq} [e'_p, e'_q] = \varepsilon_{pq3} \varepsilon_{ijp} \gamma_{jq} k_c e_3,$$  \hfill (46)
which has the form shown above (40). Define $p_{jk}$ as in (40) above and note that, correspondingly, $\gamma^{-1} = \pm \frac{1}{\Gamma} p$. Hence $c'_1 = 2c_1 = \gamma_{ij}^{-1}(2e_j) = \pm \frac{2}{\Gamma} p_{ij} e_j$, etc. Thus

$$c_1 = \pm \frac{p_{1j} e_j}{\Gamma}, \quad c_2 = \pm \frac{p_{2j} e_j}{\Gamma}, \quad c_3 = \pm \frac{2p_{3j} e_j}{\Gamma}. \tag{47}$$

Let $v_i := p_{3i}$ as before, then we have

$$[e_1, e_2] = \pm v_3 k_c e_3, \quad [e_2, e_3] = \pm v_1 k_c e_3, \quad [e_3, e_1] = \pm v_2 k_c e_3, \tag{48}$$

from which the second assertion in the proposition follows, in this case, using (47). The form of the composition function follows from the expression for $[e_i, e_j]$. □

Now since $xy$ is expressed in terms of the basis $e_1, e_2, e_3$ in Proposition 4, Theorem 3 allows us to calculate $G'_e, \mathbb{Z}(G_e)$, and the index of $G'_e$ in $\mathbb{Z}(G_e)$, denoted $k_c$. First we have:

**Proposition 5** $G'_e = G'_e$ if and only if the integers $v_1, v_2, v_3$ are relatively prime. In that case, $G'_e$ is generated by $k_c e_3$ (as is $G'_e$).

**Proof** Let $v_i = dv_i', i = 1, 2, 3$, where $d := hcf(v_1, v_2, v_3)$, the highest common factor of $v_1, v_2, v_3$. Then the expression for $xy$, with respect to the basis $e_1, e_2, e_3$, is

$$xy = x + y + \frac{\theta d^2}{2\Gamma} \varepsilon_{ijp} v_{ij} v'_p k_c (v'_e) \tag{49}$$

It follows that $G'_e$ is generated by $\frac{\theta d^2 k_c}{\Gamma} (v'_e e_r) = \frac{\theta d k_c}{\Gamma} v_r e_r = d k_c e_3$ (as is evident from (48)). But $G'_e$ is generated by $k_c e_3$. Hence $d = \pm 1$ and the integers $v_1, v_2, v_3$ are relatively prime, in case $G'_e = G'_e$.

**Proposition 6** $G'_e = G'_e$ and $\mathbb{Z}(G_e) = \mathbb{Z}(G_e)$ if and only if the integers $v_1, v_2, v_3$ are relatively prime, and also (with $v := v_1 v_2 v_3$ and with $\Gamma := \det(\gamma)$, and $\gamma = (\gamma_{ij})$ such that (39) or (45) holds),

(i) if $k_c \in 4\mathbb{Z}$, $hcf(k_c, \Gamma) = 1$,
(ii) if $k_c \in 2\mathbb{Z}$, $k_c \notin 4\mathbb{Z}$, either ($v$ is even and $hcf(k_c, \Gamma) = 1$ or ($v$ is odd and $hcf(k_c, \Gamma) = 2$),
(iii) if $k_c \notin 2\mathbb{Z}$, $hcf(k_c, \Gamma) = 1$ and either ($v$, $\Gamma$ are both even) or ($v$, $\Gamma$ are both odd).

**Proof** Let $k_c$ be the index of $G'_e$ in $\mathbb{Z}(G_e)$. One only has to find the conditions that $k_c = k_e$, which may be found from Theorem 3.

Suppose that $k_c$ is even, so $\theta = 1$ in (38). Comparing (38) with (20) we see that in this case we have $\lambda = p/q = k/\Gamma$ where $hcf(p, q) = 1$ and so $p = k/d$ where $d := hcf(k_c, \Gamma)$. Then by Theorem 3:

(ai) $k_c = k_c/d$ if $v$ is even,
(aii) $k_c = k_c/d$ if $v$ is odd and $k_c/d \in 4\mathbb{Z}$,
(aiii) $k_c = 2k_c/d$ if $v$ is odd and $k_c/d \in 2\mathbb{Z}$, $k_c/d \notin 4\mathbb{Z}$ (this implies $k_c$ is odd),
(iv) $k_c = 2k_c/d$ if $v$ is odd and $k_c/d \notin 2\mathbb{Z}$.
From these observations, it follows that in the case where \( k_c \) is even, \( k_c = k_e \) if and only if

\[(b) \text{ if } \nu \text{ is even}, hcf(k_c, \Gamma) = 1,\]
\[(bii) \text{ if } \nu \text{ is odd}, hcf(k_c, \Gamma) = 1, k_e \in 4\mathbb{Z},\]
\[(biii) \text{ if } \nu \text{ is odd}, hcf(k_c, \Gamma) = 2, k_e/2 \notin 2\mathbb{Z},\]

noting that \( k_c \neq k_e \) in case (a(iii)). Then, (b) and (bii) give (i) in the proposition, (b) and (biii) give (ii) in the proposition.

Next, if \( k_e \) is odd, so \( \theta = 2 \) in (38), we have from Theorem 3, again with \( d := hcf(k_c, \Gamma) \) (noting that if \( 2k_c/\Gamma = p/q \) and \( p, q \in \mathbb{Z} \) have no common factors, then \( p = k_c/d, q = \Gamma/2d \) if \( \Gamma \) is even, and \( p = 2k_e/d, q = \Gamma/d \) if \( \Gamma \) is odd):

\[(c) \text{ if } \nu \text{ is even, } \Gamma \text{ is even, } k_e = k_c/d,\]
\[(cii) \text{ if } \nu \text{ is odd, } \Gamma \text{ is odd, } k_e = 2k_c/d \text{ (this implies } k_e \text{ is even),}\]
\[(ciii) \text{ if } \nu \text{ is odd, } \Gamma \text{ is even, } k_e/2 \in 2\mathbb{Z}, k_e \in 4\mathbb{Z}, \text{ (this implies } k_e \in 4\mathbb{Z}),\]
\[(civ) \text{ if } \nu \text{ is odd, } \Gamma \text{ is odd, } 2k_e/d \in 4\mathbb{Z}, k_e = k_c/2d \text{ (this implies } k_e < k_c),\]
\[(cv) \text{ if } \nu \text{ is odd, } \Gamma \text{ is odd, } 2k_e/d \notin 4\mathbb{Z}, k_e = k_c/2d, \text{ (this implies } k_e = k_c/d,\]
\[(cvii) \text{ if } \nu \text{ is odd, } \Gamma \text{ is even, } k_e = 2k_c/d \text{ (this implies } k_e \text{ is even),}\]
\[(cviii) \text{ if } \nu \text{ is odd, } \Gamma \text{ is odd, } 2k_e/d \notin 2\mathbb{Z}, k_e = 4k_c/d \text{ (this case is empty).}\]

Only cases (c) and (cvi) survive, if \( k_e = k_c \notin 2\mathbb{Z} \), and they give statement (iii) of the proposition. □

**Theorem 7** \( G_c = G_e \) if and only if there exist integers \( l_0, m_0, \Gamma \), a matrix \( A \in GL_3(\mathbb{Z}) \) with third row \( v_1, v_2, v_3 \), such that the conditions of Proposition 6 are satisfied, and

\[(i) \text{ if } k_c \text{ is even,}\]
\[
\begin{pmatrix}
 1 & 0 & -l_0 \\
 0 & 1 & -m_0 \\
 0 & 0 & \pm \Gamma
\end{pmatrix}
\begin{pmatrix}
 c_1 \\
 c_2 \\
 c_3
\end{pmatrix}
= A
\begin{pmatrix}
 e_1 \\
 e_2 \\
 e_3
\end{pmatrix},
\]

(50)

\[(ii) \text{ if } k_c \text{ is odd,}\]
\[
\begin{pmatrix}
 1 & 0 & -(2l_0 + \theta(l)) \\
 0 & 1 & -(2m_0 + \theta(m)) \\
 0 & 0 & \pm \Gamma
\end{pmatrix}
\begin{pmatrix}
 c_1 \\
 c_2 \\
 1/2 c_3
\end{pmatrix}
= A
\begin{pmatrix}
 e_1 \\
 e_2 \\
 e_3
\end{pmatrix},
\]

(51)

where
\[
A = \begin{pmatrix}
 l_1 & l_2 & l_3 \\
 m_1 & m_2 & m_3 \\
 v_1 & v_2 & v_3
\end{pmatrix},
\]
\[
\theta(l) = v_1l_2l_3 - v_2l_3l_1 + v_3l_1l_2 \mod 2,
\]
\[
\theta(m) = v_1m_2m_3 - v_2m_3m_1 + v_3m_1m_2 \mod 2
\]

and \( \Gamma \det\{e_i\} = \det\{e_i\}. \)

**Proof**

(i) Suppose that \( G_c = G_e \) and \( k_c = k_e \) is even. Then the conditions of Proposition 6 hold and also \( T_e = T_e, T_e = G_e \) regarding \( T_e \) as a (normal) subgroup of \( G_e \). Thus

\[
\langle e_1, e_2, e_3 \rangle = \langle e_1, e_2, e_3, \frac{v_i e_1}{\Gamma} \rangle,
\]

(52)
with \( e_3 = \pm v_i e_i / \Gamma \). Hence there exist integers \( l_0, l_1, l_2, l_3, m_0, m_1, m_2, m_3 \) such that

\[
\begin{align*}
  c_1 &= \ell_1 e_1 + \ell_2 e_2 + \ell_3 e_3 + \ell_0 \frac{v_i e_i}{\Gamma}, \\
  c_2 &= m_1 e_1 + m_2 e_2 + m_3 e_3 + m_0 \frac{v_i e_i}{\Gamma}, \\
  c_3 &= v_1 e_1 + v_2 e_2 + v_3 e_3.
\end{align*}
\]

If \( A \) is the matrix with rows \( (l_1, l_2, l_3) \), \( (m_1, m_2, m_3) \), \( (v_1, v_2, v_3) \), it follows that (50) holds with \( A \) an integral matrix, but as yet no information regarding \( \det A \) is known. Taking the determinant of (50), \( \pm \Gamma c_1 \cap c_2 \cdot c_3 = \det A e_1 \cap e_2 \cdot e_3 \). From \( e_i = \gamma_{ij} e_j \), we have \( \det \{ e_i \} = \Gamma \det \{ e_i \} \), and comparing with (50) we get \( A \in GL_3(\mathbb{Z}) \).

Conversely if (50) holds with \( A \in GL_3(\mathbb{Z}) \), then \( e_i = \gamma_{ij} e_j \) where

\[
\gamma = A^{-1} \begin{pmatrix} 1 & 0 & -l_0 \\ 0 & 1 & -m_0 \\ 0 & 0 & \pm \Gamma \end{pmatrix}.
\]

Also \( \det \gamma = \Gamma \) (since \( \Gamma \det \{ e_i \} = \det \{ e_i \} \)). Since

\[
c_1 - l_0 e_3 = l_1 e_i, \quad c_2 - m_0 e_3 = m_1 e_i, \quad \pm \Gamma c_3 = v_i e_i,
\]

we have

\[
T_e = \{ e_1, e_2, e_3, l_1 e_e \} = \{ l, m, v, \Gamma \} = \langle c_1, c_2, c_3 \rangle = T_e
\]

(writing \( l = l_1 e_i \), etc.).

The conditions of Proposition 6 ensure that \( k_e = k_e \), so that \( c_3 = \pm v_i e_i / \Gamma \) is a generator of \( \mathbb{Z}(G_e) \). Hence by Proposition 2, \( e_1, e_2, e_3 \) generate \( T_e = G_e \) (multiplicatively), since \( v_i e_i / \Gamma \in \mathcal{Z}(G_e) \) implies that \( \Gamma e_i / \Gamma \) is a product of \( e_1, e_2, e_3 \) and their inverses. Hence, \( e_1, e_2, e_3 \) is a (multiplicative) set of generators of \( G_e = T_e = T_e = G_e \).

(ii) Next suppose that \( G_e = G_e \) and \( k_e = k_e \) is odd. Then the conditions of the previous proposition hold and \( T_e = T_e \). We have that

\[
G_e = T_e \cup e_1 T_e \cup e_2 T_e \cup e_1 e_2 T_e,
\]

from Cermelli and Parry [5]. Let the four cosets in \( G_e/T_e \) be \( T_e, \alpha T_e, \beta T_e, \gamma T_e \) for some \( \alpha, \beta, \gamma \in G_e \). It is necessary, then, that \( T_e = T_e \) and that \( c_1 T_e, c_2 T_e \) and \( c_1 c_2 T_e \) are the same as \( \alpha T_e, \beta T_e, \gamma T_e \), in some order. Note that if \( c_1 T_e, c_2 T_e \) are some two of \( \alpha T_e, \beta T_e, \gamma T_e \), then \( c_1 c_2 T_e \) is the one remaining coset of those three.

Notice that \( T_e = T_e \) if and only if

\[
(2c_1, 2c_2, c_3) = \left\langle 2e_1, 2e_2, 2e_3, \frac{2v_i e_i}{\Gamma} \right\rangle.
\]

Consider first the constraints on representatives \( 0, \alpha, \beta, \gamma \) of the four distinct cosets in \( G_e/T_e \). According to Cermelli and Parry [5] and Parry [16], all elements \( \alpha \in G_e \) have the form \( \alpha = e_1^{l_1} e_2^{l_2} e_3^{l_3} c_3^{l_0} \), for some integers \( l_0, l_1, l_2, l_3 \) (writing \( c_3 \) for a generator}
of $\mathbb{Z}(G_e) = \mathbb{Z}(G_e)$. If $\alpha$ has this form, and correspondingly $\beta = e_1^{m_1} e_2^{m_2} e_3^{m_3} e_0^{m_0}$, for integers $m_0, m_1, m_2, m_3$, then from [5], $\alpha$ and $\beta$ are in the same coset if and only if

$$l_i - m_i = \tau v_i \mod 2, \quad i = 1, 2, 3,$$

(58)

for some integer $\tau$. Let $\bar{l} = 0$ if $l$ is even, $\bar{l} = 1$ if $l$ is odd. Then (58) is equivalent to

$$\bar{l}_i - \bar{m}_i = \bar{\tau} \bar{v}_i = \bar{\tau} \bar{v}_i = 0 \text{ or } \bar{v}_i \mod 2.$$

(59)

Note that (59) is also equivalent to the condition that

$$rl_i + sm_i = \tau v_i \mod 2,$$

(60)

for some integers $r, s, \tau$, as this also reduces to the requirement that either two of $\bar{l}_i, \bar{m}_i, \bar{v}_i$ are the same (for all $i = 1, 2, 3$), or that any one of $\bar{l}_i, \bar{m}_i, \bar{v}_i$ is the sum (or difference) of the other two, for all $i = 1, 2, 3$. Bearing in mind that $e_1^{l_1} e_2^{l_2} e_3^{l_3} e_0^{l_0} \in \mathbb{Z}(G_e) \subset T_e$, it follows that $T_e, \alpha T_e, \beta T_e$ are different cosets, in $G_e/T_e$, if and only if the rows, $\bar{l} = (l_1, l_2, l_3), \bar{m} = (m_1, m_2, m_3), v = (v_1, v_2, v_3)$, of the matrix $A$ are linearly independent, mod 2.

It follows that, if $G_e = G_e$, then $c_1 \in \alpha T_e, c_2 \in \beta T_e$ for $\alpha, \beta \in G_e$ corresponding to triples $l, m$ such that $A$ is an integer matrix whose rows are linearly independent mod 2. Since

$$\alpha T_e = \alpha + T_e = e_1^{l_1} e_2^{l_2} e_3^{l_3} e_0^{l_0} + T_e$$

$$= \bar{l}_1 e_1 + \bar{l}_2 e_2 + \bar{l}_3 e_3 + \frac{1}{2} \theta(\bar{l}) e_3 + T_e,$$

(61)

where the definition of $\theta(\bar{l})$ is given in the statement of the theorem, it follows that there are integers $L_1, L_2, L_3$ with the same parity as $\ell_1, \ell_2, \ell_3$, respectively, such that

$$c_1 = L_1 e_1 + L_2 e_2 + L_3 e_3 + \frac{1}{2} \theta(\bar{L}) e_3 + l_0 e_3.$$

(62)

Without loss of generality, we write $l_1, l_2, l_3$ for $L_1, L_2, L_3$, etc., and have:

$$c_1 = l_1 e_1 + l_2 e_2 + l_3 e_3 + \frac{1}{2} \theta(\bar{l}) e_3 + l_0 e_3,$$

$$c_2 = m_1 e_1 + m_2 e_2 + m_3 e_3 + \frac{1}{2} \theta(\bar{m}) e_3 + m_0 e_3,$$

(63)

$$\pm \frac{1}{2} c_3 = v_1 e_1 + v_2 e_2 + v_3 e_3.$$

This gives (51) in the statement of the theorem, except that we have no information regarding $\det A$ yet. From (63), comparing with $2e_i = \gamma_i e_i'$, we get

$$\gamma = A^{-1} \begin{pmatrix} 1 & 0 & -(2l_0 + \theta(l)) \\ 0 & 1 & -(2m_0 + \theta(m)) \\ 0 & 0 & \pm \Gamma \end{pmatrix}$$

(64)

and it follows that $\det \gamma = \det A^{-1}(\pm \Gamma) = \Gamma$, so $\det A = \pm 1$ and $A \in GL_3(\mathbb{Z})$. This condition is itself sufficient that the rows of $A$ as linearly independent, mod 2 (for if one
adds two to a single element of $A$, then $\det A$ is changed by an even number). So the necessity of (51) is proven.

Conversely, if (51) holds, then the group elements corresponding to the rows $l, m, v$ of $A$ are in different cosets, in $G_e/T_e$. Multiplying the first two equations of (63), or (51), by two, one sees that (51) implies that $T_e = T_e$ (via (57)). The first equation of (63) gives $c_1 \in aT_e$, so $c_1$ is a product of $\alpha \in G_e$ with an integer linear combination of $2e_1, 2e_1, 2e_3, 2v_i e_i / \Gamma$. But $2v_i e_i / \Gamma$ generates $Z(G_e)$ (by the conditions which appear in Proposition 6), for they guarantee that $Z(G_e) = Z(G_e)$, and $Z(G_e)$ is generated by $c_1 = 2v_i e_i / \Gamma$, and so is a product of $e_1, e_2, e_3$ and their inverses. Hence $c_1$ is expressible as a product of $e_1, e_2, e_3$ and their inverses. Likewise for $c_2$. This proves that $e_1, e_2, e_3$ is a (multiplicative) set of generators for $G_e$.

\[ \square \]

4 Generalization of Ericksen–Pitteri Neighborhoods

Let $e_1, e_2, e_3$ be a canonical basis of a discrete subgroup $G_e \subset J$ such that (33) holds for some $k \in \mathbb{Z}$. With respect to this basis the Lie bracket associated with this subgroup is given by (36) and hence the corresponding structure constants are $C_{ijk} = \varepsilon_{3jk} k \delta_{i3}$ and by (9) the components of the dislocation density tensor, $S$, with respect to this basis are $S_{pr} = k \delta_{p3} \delta_{r3}$.

Let $e_1, e_2, e_3$ be a basis of $\mathbb{R}^3$ which satisfies the conditions of Theorem 7 so that $G_e = G_e$ where $G_e$ is the group generated by $e_1, e_2, e_3$. By Proposition 4, with respect to the basis $e_1, e_2, e_3$, the Lie bracket has the form (38) and hence the components of the dislocation density tensor with respect to this basis are $S_{pr} = \theta(T) \nu_p \nu_r$ where the integers $k, \Gamma, \nu_p, p = 1, 2, 3$ satisfy the conditions of Proposition 6.

Since $G_e$ and $G_e$ are the same group they correspond to the same set of points in $\mathbb{R}^3$ and hence if $w$ is a strain energy function then that depends only on the positions of these points, then

\[ w\left(\{e_i\}, S_{pr} = \frac{\theta k}{\Gamma} \nu_p \nu_r\right) = w\left(\{e_i\}, S_{pr} = k \delta_{p3} \delta_{r3}\right) \tag{65} \]

where the $e_i, i = 1, 2, 3$ can be expressed in terms of the $c_i, i = 1, 2, 3$ and vice versa via (50) or (51) depending on the parity of $k$.

Suppose now that $e_1^*, e_2^*, e_3^* \in \mathbb{R}^3$ is a canonical basis of another discrete subgroup $G_{e^*} \subset J$ and that $G_{e^*} = G_{e^*}$ where $G_{e^*}$ is generated by $e_1^*, e_2^*, e_3^* \in G_{e^*}$. Then we also have

\[ w\left(\{e_i^*\}, S_{pr}^* = \frac{\theta^* k^*}{\Gamma^*} \nu_p^* \nu_r^*\right) = w\left(\{e_i^*\}, S_{pr}^* = k^* \delta_{p3} \delta_{r3}\right), \tag{66} \]

where the integers $k^*, \Gamma^*, \nu_p^*, p = 1, 2, 3$ also satisfy the conditions of Proposition 6 and the $e_j^*, i = 1, 2, 3$ can be expressed in terms of the $e_j^*, j = 1, 2, 3$ and vice versa via (50) or (51) depending on the parity of $k^*$.

Equations (65), (66) express some global symmetries of a strain energy function that depends only on the positions of points that correspond to the elements of a given discrete subgroup. In what follows we shall see that a given set of points may correspond to different subgroups $G_e, G_{e^*}$, with $k \neq k^*$, so that (65) and (66) must be supplemented by further conditions so as to reflect the fact that the energy density is to be independent of the description of the given set of points in terms of any particular choice of group, and any particular choice of generators within a group. However to begin with we deal with the simplest case where $G_e = G_{e^*}, k = k^*$ and the relevant symmetries derive just from (65) and (66), and prove an analogue of the Ericksen–Pitteri result (cf. (i) and (ii) in Introduction).
Specifically, in Sect. 4.1 we first write down the symmetries of the strain energy function which derive from (65), first of all expressing those symmetries in terms of the group generators $e_a$, then using the frame indifference of the energy to express the symmetries in terms of $C = (C_{ij}) \equiv (e_i, e_j)$. Then, to ‘localize’ these symmetries, we define a neighborhood $N_{\varepsilon}$ of the descriptors $S = (S_{pr})$ of the discrete subgroups $G_e$. Generally, changes in the generators $\{e_a\}$ cannot be extended to elastic deformations of the continuous structure in which $G_e$ is embedded, but we show that those changes of generators which lie in $N_{\varepsilon}$, for $\varepsilon$ sufficiently small, can indeed be so extended. Moreover, extending the reach of Ball and James’ [2] treatment of the perfect crystal case, we find that those elastic deformations are precisely the rotations that preserve the discrete defective structure $G_e$.

In Sect. 4.2, we show that these results also extend to the case where $k \neq k^*$. 

### 4.1 $k = k^*$, $G_e = G_{e^*}$

Suppose that $k = k^*$ with $\{e_i\} = \{e^*_i\}$ a canonical basis of $J$ such that $(e_1, e_2) = e^*_1$, $(e_2, e_3) = (e_1, e_3) = 0$. We then have from (65) and (66), since $k = k^*$ and since $\theta$ depends only on the parity of $k$, $\theta = \theta^*$,

$$w(\{e_i\}, S_{pr} = \frac{\theta k}{\Gamma} v_p v_r) = w(\{e^*_i\}, S_{pr}^* = \frac{\theta k}{\Gamma^*} v^*_p v^*_r).$$  \hfill (67)

Then from (50) and (51), since $e_1, e_2, e_3$ and $e^*_1, e^*_2, e^*_3$ are two different sets of generators of the group $G_e = G_e = G_{e^*} = G_{e^*}$, we have for $k$ even

$$\begin{pmatrix} e^*_1 \\ e^*_2 \\ e^*_3 \end{pmatrix} = (A^*)^{-1} \begin{pmatrix} 1 & 0 & -l_0^* \\ 0 & 1 & -m_0^* \\ 0 & 0 & \pm \Gamma^* \end{pmatrix} \begin{pmatrix} e_1^* \\ e_2^* \\ e_3^* \end{pmatrix} = (A^*)^{-1} \begin{pmatrix} 1 & 0 & -l_0^* \\ 0 & 1 & -m_0^* \\ 0 & 0 & \pm \Gamma^* \end{pmatrix} \begin{pmatrix} e_1 \\ e_2 \\ e_3 \end{pmatrix}. \hfill (68)$$

and for $k$ odd,

$$\begin{pmatrix} e^*_1 \\ e^*_2 \\ e^*_3 \end{pmatrix} = (A^*)^{-1} \begin{pmatrix} 1 & 0 & -(2l_0^* + \theta(I^*)) \\ 0 & 1 & -(2m_0^* + \theta(m^*)) \\ 0 & 0 & \pm \Gamma^* \end{pmatrix} \begin{pmatrix} e^*_1 \\ e^*_2 \\ e^*_3 \end{pmatrix} = (A^*)^{-1} \begin{pmatrix} 1 & 0 & -(2l_0^* + \theta(I^*)) \\ 0 & 1 & -(2m_0^* + \theta(m^*)) \\ 0 & 0 & \pm \Gamma^* \end{pmatrix} \begin{pmatrix} e_1 \\ e_2 \\ e_3 \end{pmatrix}, \hfill (69)$$

where $A, A^* \in GL_3(\mathbb{Z})$ and

$$\det(e^*_i) = \Gamma^* \det(e^*_i) = \frac{\Gamma^*}{\Gamma} \det(e_i) = \frac{\Gamma^*}{\Gamma} \det(e_i).$$  \hfill (70)

In (68) and (69), let

$$e^*_i = M_{ij} e_j, \quad i, j = 1, 2, 3.$$  \hfill (71)
Let the third row of $A$ be $(v_1, v_2, v_3)$, and let the third row of $A^*$ be $(v_1^*, v_2^*, v_3^*)$, with the elements of each row consisting of relatively prime integers (as $A^*, A \in GL_3(\mathbb{Z})$). We have from (68)–(71),

$$\det M = \frac{\Gamma^*}{\Gamma}, \quad M_{ij} = \frac{m_{ij}}{\Gamma} \quad \text{for some } m_{ij} \in \mathbb{Z}, \ i, j = 1, 2, 3. \quad (72)$$

From Theorem 7, (68)–(71), we get

$$M_{ij} v_i^* = \tau \frac{\Gamma^*}{\Gamma} v_j, \quad \text{where } \tau \equiv \text{sign}(\det A^*) \text{sign}(\det A). \quad (73)$$

Now define

$$\mathcal{H}(k, \Gamma, \{v_i\}) \equiv \left\{ M \in GL_3(\mathbb{Q}) : \{e_i^* = M_{ij} e_j\} \text{ generates } G_e \right\}$$

$$= \left\{ M \in GL_3(\mathbb{Q}) : M \text{ is as in (68), (69)} \right\} \quad (74)$$

Notice that if $M, M' \in \mathcal{H}(k, \Gamma, \{v_i\})$, and $M \neq M'$, then there exist indices $i, j \in \{1, 2, 3\}$ such that (with $M' = (M'_{ij}) \equiv (m'_{ij}/\Gamma)$)

$$|M'_{ij} - M_{ij}| \geq 1/|\Gamma|. \quad (75)$$

Now any frame indifferent strain energy function $w$ must satisfy $w([e_i], S) = w([Re_i], S)$ for any rotation $R$ (see Parry [16], Sect. 4, for a discussion of this point). So $w([e_i], S) = \tilde{w}(C, S)$ where $C$ is the positive definite symmetric matrix with entries $C_{ij} = e_i \cdot e_j$. $C$ is the metric of the basis $e_1, e_2, e_3$ and $C = E^T E$ where $E$ is the matrix with columns $e_1, e_2, e_3$. Defining the metric $C^*$ similarly, from (67) we have $\tilde{w}(C, S) = \tilde{w}(C^*, S^*)$. Note that since $e_i^* = M_{ij} e_j$, if $E^*$ is the matrix with columns $e_1^*, e_2^*, e_3^*$, $(E^*)^T = M E^T$ and thus

$$C^* = (E^*)^T C^* E^* = M E^T (M E^*)^T = M E^T E M^T = M C M^T. \quad (76)$$

We want to determine, in part, whether or not if $(C, S)$ is given, the quantities $(C^*, S^*)$ may accumulate at $(C, S)$. To proceed, we adapt Ball and James [2] a little and introduce a neighborhood $N_\varepsilon, \varepsilon > 0$, of the point $([e_i], S)$ via the following definitions:

$$N_\varepsilon ([e_i], k, \Gamma, \{v_i\}) \equiv \left\{ \left( e_i^*, \frac{k^*}{\Gamma^*} v_i^* v_j^* \right) : \|C^* - C\|_{[e_i]} < \varepsilon, \left\| \left( \frac{k^*}{\Gamma^*} v_i^* v_j^* - \frac{k}{\Gamma} v_i v_j \right) \right\| < \varepsilon \right\}. \quad (77)$$

where if $A$ is the matrix with components $A_{ij}, \|A\| \equiv \|(A_{ij})\| \geq 0$ is defined by

$$\|A\|^2 \equiv tr(A^T A), \quad (78)$$

and

$$\|A\|_{[e_i]} = \|DAD^T\|, \quad (79)$$

where $E$ is the matrix with columns $e_1, e_2, e_3$ and $D \equiv E^{-T}$.

**Proposition 8** If $\varepsilon$ is small enough, $k \neq 0$ and some $v_i \neq 0$, then $([e_i^*], \{\frac{k^*}{\Gamma^*} v_i^* v_j^*\}) \in N_\varepsilon ([e_i], k, \Gamma, \{v_i\})$ only if $\Gamma = \Gamma^*, v_i^* = \pm v_i$ for $i = 1, 2, 3$ (with the choice of sign independent of the index $i$).
Proof First, if \( \| C^* - C \|_{(1)} = \| DC^* D^T - DCD^T \| \) is sufficiently small, then \( \text{det} \, DC^* D^T \) can be made arbitrarily close to \( \text{det} \, DCD^T \). Hence, as \( \text{det} \, D \neq 0 \) is fixed, \( \text{det} \, C^* = \text{det} \, C(\text{det} \, M)^2 \) is arbitrarily close to \( \text{det} \, C \), and so from (72), \( (\Gamma^*)^2 = \Gamma^2 \), since both \( \Gamma^* \), \( \Gamma \) are integers.

Next, if \( \| \frac{k}{|\Gamma|} v_i^* v_j^* - \frac{1}{|\Gamma|} v_i v_j \| = \| \frac{k}{|\Gamma|} || v_i^* v_j^* \pm v_i v_j \| \) is sufficiently small (recall \( k = k^* \) in this section), then \( v_i^* = \pm v_i, \) \( i = 1, 2, 3 \), with the choice of sign possibly dependent on the index \( i \). (For if this were not so, \( v_i^* \neq v_i \) for some index \( i \) and this would contradict the fact that \( \| \frac{k}{|\Gamma|} || v_i^2 \pm v_i^2 \| \geq |\frac{k}{|\Gamma|} | \) is sufficiently small).

Then, if for example \( v_1^* = v_1, v_2^* = -v_2 \) with \( v_1 v_2 \neq 0 \), in the case \( \Gamma = \Gamma^* \) we get \( \frac{k}{|\Gamma|} || v_i^* v_j^* - v_i v_j || \geq \frac{1}{|\Gamma|} || 2v_i v_2 || \geq \frac{1}{|\Gamma|} || \), whereas in the case \( \Gamma = -\Gamma^* \) one has \( \frac{k}{|\Gamma|} || v_i^* v_j^* + v_i v_j || \geq \frac{1}{|\Gamma|} || 2v_i v_2 || \geq \frac{1}{|\Gamma|} || \). In either case we get a contradiction, so that \( v_i^* = \pm v_i, \), with sign independent of the index. Finally, with this information, \( \| \frac{k}{|\Gamma|} v_i^* v_j^* - \frac{1}{|\Gamma|} v_i v_j \| = \| \frac{k}{|\Gamma|} \text{sign} \frac{\Gamma}{\Gamma^*} - 1 \| v_i v_j \| \) leads to a contradiction unless \( \Gamma = \Gamma^* \). This proves the proposition.

\[ \square \]

Definition

\[ \mathcal{L}(k, \Gamma, \{ v_i \}) \equiv \{ M \in \mathcal{H}(k, \Gamma, \{ v_i \}) : \Gamma^* = \Gamma \text{ and } v_i^* = \pm v_i, \, i = 1, 2, 3, \} \tag{80} \]

when the sign in the expression \( \pm v_i \) is independent of the index \( i \). We remark that \( \mathcal{L}(k, \Gamma, \{ v_i \}) \) is a subgroup of \( GL_3(\mathbb{Q}) \).

Recall that the dislocation density tensor \( S \), defined via the duals \( d_a(\cdot) \) of the lattice vector fields \( \ell_a(\cdot) \) (cf. (1)), is an elastic invariant, so that if fields \( \ell_a(\cdot) \) are defined via a mapping \( u : \mathbb{R}^3 \to \mathbb{R}^3 \) by \( \tilde{\ell}_a(u(x)) = \nabla u(x) \ell_a(x) \), and a dislocation density tensor \( \tilde{S} \) is calculated from \( \tilde{\ell}_a(\cdot) \), then \( \tilde{S}(u(x)) = S(x) \). In the case at hand, then, \( \tilde{S}(\cdot) = S(\cdot) = \text{constant} \). The following proposition gives the analogue of this result in the discrete case, where instead of the elastic deformations one has the changes of generators of the discrete set of points which make up \( G_e \), and instead of \( S \) one has (a priori) the structure constants \( \frac{k}{|\Gamma|} v_i v_j \). The proposition is phrased, more precisely, in terms of the free substitutions of \( G_e \), which represent the replacement of one set of generators by another, and the corresponding replacement of any element of \( G_e \), expressed as a product of elements of the original set of generators by the corresponding product of elements of the new set of generators [see Magnus, Karrass, Solitar [11], Johnson [10] for a discussion].

Proposition 9 Free substitutions of \( G_e \) which take generators \( \{ e_i \} \) to generators \( \{ e_i^* \} \) (corresponding to \( e_i^* = M_{ij} e_j \), with \( M_{ij} \) the matrices that appear in (68) and (69)) extend to elastic deformations of \( J \) if and only if \( \frac{k}{|\Gamma|} v_i^* v_j^* = \frac{1}{|\Gamma|} v_i v_j \).

Proof Let \( \psi : G_e \to G_e \) be a free substitution defined by \( \psi(e_i) = e_i^* \), \( i = 1, 2, 3 \), where \( e_i^* = M_{ij} e_j \) in line with (68), (69). Then according to Auslander [1], Parry [14], \( \psi \) extends to an elastic deformation (automorphism) of \( J \) if and only if the defining relations of \( G_e \) are invariant under that substitution and its inverse, i.e., if and only if

\[ (\psi(e_i), \psi(e_j)) = \psi(e_{ijp} k_{vp} c_3), \quad (\psi^{-1}(e_i), \psi^{-1}(e_j)) = \psi^{-1}(e_{ijp} k_{vp} c_3), \tag{81} \]

where, in (81), \( c_3 \) is a product of the elements \( e_1, e_2, e_3 \) that generates \( \mathbb{Z}(G_e) \). Note that \( \psi^{-1} \) is the substitution that maps \( \psi(e_i) \) to \( e_i, \, i = 1, 2, 3 \). Thus we have to show just that (81) is equivalent to \( \Gamma = \Gamma^* \), \( v_i^* \pm v_i \) (bearing in mind that \( \frac{k}{|\Gamma|} v_i^* v_j^* = \frac{1}{|\Gamma|} v_i v_j \) is equivalent to \( \Gamma = \Gamma^* \), \( v_i^* \pm v_i \), when \( \{ v_i^* \}, \{ v_i \} \) are triples of relatively prime integers).
First suppose that (81)\(_1\) holds. Then

\[
(\psi(e_i), \psi(e_j)) = [M_{ip} e_p, M_{jq} e_q] = M_{ip} M_{jq} \varepsilon_{pqr} k v_r c_3
\]

\[
= \varepsilon_{ij\ell} M^{-1}_{\ell} \text{det}(M) k v_c c_3 = \varepsilon_{ij\ell} \tau v^\ast_\ell k c_3,
\]

(82)

from (73) and (74). Since \(\varepsilon_{ijp} k v_p\) is an integer,

\[
\psi(\varepsilon_{ijp} k v_p c_3) = \varepsilon_{ijp} k v_p \psi(c_3).
\]

(83)

Since \(\psi\) is an automorphism, \(\psi(c_3)\) generates \(\mathbb{Z}(G_e)\), as does \(c_3\), so

\[
\psi(c_3) = c_3^{\pm 1} = \varepsilon c_3, \quad \text{say, where} \ \varepsilon = \pm 1.
\]

(84)

So from (82), (83), (84)

\[
\tau v^\ast_\ell = \varepsilon v_\ell.
\]

(85)

From Parry [14], following Mal’cev [12], as \(\psi : G_e \to G_e\) is an automorphism, it extends uniquely to a linear automorphism \(\phi : J \to J\). In the case \(k\) even, from (42), \(c_3 = \pi /\Gamma \nu_k e_k\), where \(\pi = \pm 1\), so

\[
\varepsilon c_3 = \psi(c_3) = \psi\left(\frac{\pi}{\Gamma} v_k e_k\right) = \phi\left(\frac{\pi}{\Gamma} v_k e_k\right) = \frac{\pi}{\Gamma} v_k \phi(e_k) = \frac{\pi}{\Gamma} v_k e^*_k
\]

\[
= \frac{\pi}{\Gamma} v_k M_{kj} e_j = \frac{\varepsilon \pi}{\Gamma} v^*_k M_{kj} e_j = \varepsilon \pi \Gamma^* v^*_j e_j,
\]

(86)

via (73). Hence

\[
\varepsilon c_3 \equiv \varepsilon \left(\frac{\pi}{\Gamma} v_k e_k\right) = \varepsilon \pi \Gamma^* v^*_j e_j, \quad \text{so} \ \Gamma = \Gamma^*.
\]

(87)

Equations (85) and (87) show that \(v^*_\ell = \pm v_\ell, \ \Gamma^* = \Gamma\).

Since \(\psi^{-1}\) is also an automorphism, it also extends to a (linear) automorphism of \(J\) and so corresponds to the linear transformation \(M^{-1}\). One checks that (81)\(_2\) provides no further information, in this case. The case where \(k\) is odd is similar, and we leave it to the reader to check that if \(v^*_\ell = \pm v_\ell, \ \Gamma^* = \Gamma\), then (81) holds. \(\square\)

Propositions 8 and 9, taken together, imply that the symmetries of this class of defective crystals which are sufficiently small (in the sense of (77)) extend to elastic deformations. In particular, if \(\varepsilon\) is sufficiently small then (cf. (77))

\[
N_\varepsilon(\{e_i\}, k, \Gamma, \{v_i\}) = \left\{ \left(\{e^*_i\}, \frac{k}{\Gamma} v_i v_j \right) : \|C^* - C\|_{\{e_j\}} < \varepsilon \right\}.
\]

(88)

As a matter of notation, define \(M[N_\varepsilon]\) for sufficiently small \(\varepsilon\) by

\[
M[N_\varepsilon] = \left\{ \left(\{M_{ij} e^*_j\}, \frac{k}{\Gamma} v_i v_j \right) : (M_{ij}) \in \mathcal{H}(k, \Gamma, \{v_i\}), \right.
\]

\[
\left. \left(\{e^*_i\}, \frac{k}{\Gamma} v_i v_j \right) \in N_\varepsilon(\{e_i\}, k, \Gamma, \{v_i\}) \right\}
\]

(89)
Now one can follow Ball and James [2], Cermelli and Mazzucco [4], Fosdick and Hertog [8] to prove (in particular) that if \( \varepsilon \) is sufficiently small:

- either \( M[N_\varepsilon] = N_\varepsilon \), in which case \( M_{ij} e_j = Q e_i \), with \( Q \) orthogonal,
- or \( M[N_\varepsilon] \cap N_\varepsilon = \emptyset \). (90)

For the proof of (90), it suffices to remark that Ball and James’ proof [2] of their Theorem 2.4 applies with the replacement of \( (\mu^i_\varepsilon) \in GL_3(\mathbb{Z}) \) by \( M = (M_{ij}) = \frac{1}{\varepsilon} (m_{ij}) \in \mathcal{H}(k, \Gamma, \{v_i\}) \) — this relies on the fact that if \( \{M_r\}, r = 1, 2, \ldots \), is a convergent sequence of elements of \( \mathcal{H}(k, \Gamma, \{v_i\}) \), then \( M_r = M_0 \) if \( r \geq r_0 \), for some \( r_0 \in \mathbb{Z} \).

**Definition** Define \( P(\{e_i\}, k, \Gamma, \{v_i\}) \) by

\[
P(\{e_i\}, k, \Gamma, \{v_i\}) \equiv \{ Q \in O(3) : Q e_i = M_{ij} e_j \text{ for some } (M_{ij}) = M \in \mathcal{L}(k, \Gamma, \{v_i\}) \},
\]

and call it the **defective point group** of the discrete structure defined by the parameters \( (\{e_i\}, k, \Gamma, \{v_i\}) \).

**Proposition 10** If \( (\{e_i\}, k, \Gamma, \{v_i\}) \) and \( (\{e_i^*\}, k, \Gamma, \{v_i\}) \) define the same discrete structure, then the corresponding defective point groups are identical.

**Proof** The hypotheses imply that, from (68)–(73),

\[
e_i^* = M_{ij} e_j, \quad \text{where } (M_{ij}) = M \in \mathcal{L}(k, \Gamma, \{v_i\}).
\]

Let \( Q \in P(\{e_i\}, k, \Gamma, \{v_i\}) \), then \( Q e_i = \gamma_{ij} e_j \) for some \( (\gamma_{ij}) = \gamma \in \mathcal{L}(k, \Gamma, \{v_i\}) \). It follows that \( Q e_i^* = (M \gamma M^{-1})_{ij} e_j^* \). Since \( \mathcal{L}(k, \Gamma, \{v_i\}) \) is a matrix group, one obtains that \( Q \in P(\{e_i^*\}, k, \Gamma, \{v_i\}) \) and this leads to the result. \[ \square \]

Note that, if one is to examine the defective point group \( P(\{e_i\}, k, \Gamma, \{v_i\}) \) relating to a set of generators \( \{e_i\} \) which satisfy (50), one may first of all (say in the case \( k \) even) construct \( G_c = T_c = \langle c_1, c_2, c_3 \rangle \), noting that \( T_c \) is a perfect lattice, and that the (standard) point group of \( T_c \) is found straightforwardly (one may also calculate the corresponding standard lattice group). The defective point group corresponds to particular matrices \( M \) in (68), or (69), which are such that \( \Gamma = \Gamma^* = 1 \), \( M \in GL_3(\mathbb{Z}) \) via (68), or (69), so \( M \) is in the lattice group corresponding to \( \{e_i\} \) because it represents an orthogonal transformation, via (90)\(_1\). Hence \( P(\{e_i\}, k, \Gamma, \{v_i\}) \) is contained in the standard point group, in this case. This is a strict inclusion, in general. For example, if \( k = k_c = 2 \) in (35), \( c_1 = e_1, c_2 = e_1 + e_2, c_3 = e_3 \), where \( \{e_i\} \) is an orthonormal basis of \( \mathbb{R}^3 \), in (50), so \( \ell_0 = m_0 = 0, \Gamma = 1 \), and \( v_1 \equiv p_{31} = 0, v_2 = p_{32} = 0, v_3 = p_{33} = 1 \) from (39) and (41)\(_2\), then \( T_c \) is a perfect cubic lattice. The general expression for \( M \) is obtained from (68) in terms of \( \ell_0^*, m_0^* \), and the integral elements of the first two rows of \( A^* \). Since \( M \in GL_3(\mathbb{Z}) \) in this case, one may pick out the matrices \( M \) which have the appropriate form from the standard cubic lattice group. Let \( R_p^w \) represent rotation by angle \( w \) about the direction \( p \). It turns out that \( P(\{e_i\}, 2, 1, \{0, 0, 1\}) = \{ \pm I, \pm R_3^x, \pm R_3^y, \pm R_3^z, \pm R_k^{3x/2}, \pm R_k^{3y/2}, \pm R_k^{3z/2}, \pm R_{k+1}^x, \pm R_{k-1}^y \} \), which is strictly included in the cubic point group.
4.2 $k \neq k^*$, $G_c \neq G_{c^*}$

Suppose now that $k \neq k^*$ so that the canonical bases $e_1, e_2, e_3$ and $c_1^*, c_2^*, c_3^*$ generate different groups $G_e$ and $G_{e^*}$ with $G_c \neq G_{c^*}$. Suppose however that $\{(e_i), S_{pr} = k\delta_3\delta_{13}\}$ and $\{(e_i^*), S_{pr} = k^*\delta_3\delta_{13}\}$ define the same set of points so that

$$w\left(\{e_i\}, S_{pr} = \theta k \frac{v_r}{\Gamma} \right) = w\left(\{e_i\}, S_{pr} = k\delta_3\delta_{13}\right) = w\left(\{e_i^*\}, S_{pr}^* = k^*\delta_3\delta_{13}\right) = w\left(\{e_i^*\}, S_{pr}^* = \frac{\theta^* k^* v_r^*}{\Gamma^*} \right). \quad (92)$$

For this to occur it must be the case that $k$ and $k^*$ have the same parity (so $\theta = \theta^*$) since the structure associated with $\{(e_i), k\delta_3\delta_{13}\}$ is a lattice for $k$ even or a multilattice for $k$ odd. In either case, $k$ and $k^*$ both even or both odd, the translation groups $T_e$ and $T_{e^*}$, given by (37), are lattices. If these lattices are to consist of the same points of $\mathbb{R}^3$, then if $k$ and $k^*$ are even,

$$\begin{pmatrix} c_1^* \\ c_2^* \\ e_3^* \end{pmatrix} = B \begin{pmatrix} c_1 \\ c_2 \\ e_3 \end{pmatrix} \quad (93)$$

where $B \in GL_3(\mathbb{Z})$ and if $k$ and $k^*$ are odd then

$$\begin{pmatrix} e_1^* \\ c_2^* \\ \frac{1}{2} e_3^* \end{pmatrix} = B \begin{pmatrix} c_1 \\ c_2 \\ \frac{1}{2} e_3 \end{pmatrix} \quad (94)$$

where $B \in GL_3(\mathbb{Z})$. Then the generators $e_1, e_2, e_3$ of $G_e$ and $e_1^*, e_2^*, e_3^*$ of $G_{e^*}$ are related in the following way. If $k$ is even then

$$\begin{pmatrix} e_1^* \\ e_2^* \\ e_3^* \end{pmatrix} = (A^*)^{-1} \begin{pmatrix} 1 & 0 & -l_0^* \\ 0 & 1 & -m_0^* \\ 0 & 0 & \pm \Gamma^* \end{pmatrix} B \begin{pmatrix} 1 & 0 & -l_0 \\ 0 & 1 & -m_0 \\ 0 & 0 & \pm \Gamma \end{pmatrix}^{-1} A \begin{pmatrix} e_1 \\ e_2 \\ e_3 \end{pmatrix} \quad (95)$$

or for $k$ odd,

$$\begin{pmatrix} e_1^* \\ e_2^* \\ e_3^* \end{pmatrix} = (A^*)^{-1} \begin{pmatrix} 1 & 0 & -(2l_0^* + \theta(l^*)) \\ 0 & 1 & -(2m_0^* + \theta(m^*)) \\ 0 & 0 & \pm \Gamma^* \end{pmatrix} B \begin{pmatrix} 1 & 0 & -(2l_0 + \theta(l)) \\ 0 & 1 & -(2m_0 + \theta(m)) \\ 0 & 0 & \pm \Gamma \end{pmatrix}^{-1} A \begin{pmatrix} e_1 \\ e_2 \\ e_3 \end{pmatrix} \quad (96)$$

where $A, A^*, B \in GL_3(\mathbb{Z})$.

Then (92) is to hold when $\{e_i^*\}$ and $\{e_i\}$ are related by (95), in the case $k$ and $k^*$ even, since (93) is sufficient that the points of $G_e = T_e = T_e$ coincide with those of $G_{e^*} = T_{e^*} = T_{e^*}$. However, (94) is not evidently sufficient to guarantee that the points of $G_e$ coincide with those of $G_{e^*}$ in the case where $\{e_i^*\}$ and $\{e_i\}$ are related by (96) and $k$ and $k^*$ odd, since one also requires that the cosets of $T_e$ in $G_e$ coincide with those of $T_{e^*}$ in $G_{e^*}$ (as sets of points in $\mathbb{R}^3$).
Proposition 11  In the case that \( k \) and \( k^* \) are both odd with \( k \neq k^* \), the sets of points determined by the groups \( G_e, G_e^* \) coincide provided that (94) holds and that certain conditions on the parity of the elements of \( B \) are satisfied.

Proof  Relation (94) gives that the points of \( T_e \) and \( T_e^* \) coincide. Recall from (56) that the cosets of \( G_e \) are \( T_e, e_1 T_e, e_2 T_e, e_1 e_2 T_e \) and similarly for \( G_e^* \). So we have to find the conditions that \( \{e_1, e_2, e_1 e_2\} \) are equivalent to \( \{e_1^*, e_2^*, e_1^* e_2^*\} \) mod \( T_e \) (recall Proposition 2(ii)). So, as points of \( \mathbb{R}^3, e_1^* = e_1^1 e_2^1 e_3^1 = \bar{e}_e c_1 + \ell_2 c_2 + (2\ell_3 + k\ell_1 \ell_2) c_3 \) for some integers \( \ell_1, \ell_2, \ell_3 \).

Note that \( c_1^1 e_2^1 \ell_1^2 \ell_3^3 = c_1^1 e_2^1 \ell_3^2 \ell_1^3 \mod T_e = (2e_1, 2e_2, e_3) \) provided that \( \bar{e}_e = \bar{L}_1, \ell_2 = \bar{L}_2 \), where \( \bar{e}_e = 1 \) if \( e \) is odd, \( \bar{e}_e = 0 \) if \( e \) is even. Hence \( c_1^1 = e_1^1 e_2^1 \ell_1^2 \ell_3^3 = e_1^\bar{m}_1 e_2^\bar{m}_2 \mod T_e \), for some integers \( \bar{m}_1, \bar{m}_2 \). So \( (\bar{e}_e, \bar{L}_2, (\bar{m}_1, \bar{m}_2)) \) must be some two of \( (1, 0), (0, 1), (1, 1) \), and so \( c_1^1 = \bar{e}_e e_1 + \ell_2 c_2 + k\ell_1 \ell_2 (\frac{1}{2} c_3) = \bar{e}_e e_1 + \ell_2 c_2 + \ell_1 \ell_2 (\frac{1}{2} c_3) \mod T_e \), as \( k \) is odd, and similarly for \( c_2^1 \). Since \( T_e = (2e_1, 2e_2, 2(\frac{1}{2} c_3)) \), these relations are constraints on the parity of elements in the first two rows of \( B \) in (94). Next \( e_1^1 c_2^* = e_1^1 + e_2^1 + \frac{1}{2} k^* e_3^* = e_1^1 + e_2^1 + \frac{1}{2} e_3^* \), mod \( T_e^* \), as \( k^* \) is odd, and there is a similar expression for \( e_1 c_2 \). Since the elements of \( \{e_1^1, e_2^1, e_1^1 e_2^1\} \) are just \( \{e_1, e_2, e_1 e_2\} \), mod \( T_e \), it follows that

\[
\frac{1}{2} e_3^1 = e_1^1 e_2^1 - e_1^1 = e_2^1 = e_2^1 e_3^1 + e_1^1 + e_2^1
\]

\[
= e_1 c_2 + e_1 + e_2 = e_1 c_2 - e_1 - e_2 = \frac{1}{2} e_3 \mod T_e = T_e^*.
\]

Hence \( \frac{1}{2} e_3^1 = \frac{1}{2} e_3 \), mod \( T_e \), and this is a constraint on the parity of elements in the third row of \( B \) in (94).

Finally, an argument which is in all essential details identical to that presented above in the case \( k = k^* \) leads to an analysis of the Ericksen–Pitteri result (cf. (90)) in the case \( k \neq k^* \). (For in the proof of the analogue of Proposition 8, one may note first of all that \( \Gamma^* = \Gamma \) is obtained as before.) The second paragraph of the proof may be replaced by the following:

Next, since \( \|v_i^* v_j^* - \frac{1}{k} v_j v_i\| \geq \frac{1}{|k|} \) if \( k^* v_i^* v_j^* \neq k v_j v_i \) for any choice of indices \( i, j \), it follows that if \( \|v_i^* v_j^* - \frac{1}{k} v_j v_i\| \) is sufficiently small, then \( k^* = k \) and \( v_i^* = \pm v_i, i = 1, 2, 3, \) with the choice of sign possibly dependent on the index \( i \). The proof of Proposition 8 then proceeds as before, with the additional information that \( k = k^* \). The calculations that follow Proposition 8 are taken across effectively unchanged (in this case \( \mu_i^j \) is replaced by \( M \) from (95), (96)).

5 Summary  

In the given class of defective crystals, when the dislocation density tensor \( S \) has a given form, we have calculated the symmetries of energy density functions based on the assumptions that: (i) such functions depend only on the location of points in \( \mathbb{R}^3 \) which correspond to a certain discrete structure \( G_e \), and (ii) such functions are frame indifferent. The structures \( G_e \) are determined by \( S \) and a choice of three vectors \( e_1, e_2, e_3 \in \mathbb{R}^3 \), and we have accounted for the fact that different choices of \( \{e_i\}, S \) may lead to the same set of points in \( \mathbb{R}^3 \).

The symmetries that are sufficiently small (in the sense of (77)) preserve the dislocation density tensor and extend uniquely to elastic deformations of a continuum in which the points of the crystal may be embedded. Indeed those ‘elastic’ (discrete) symmetries are
conjugate to rotations which map the discrete structure to itself. The ‘defective point group’ which consists of those rotations that are conjugate to the elastic symmetries is an invariant of the discrete structures, once the dislocation density is chosen (cf. Proposition 10).

Acknowledgements We thank the Engineering and Physical Sciences Research Council for support in the form of grant no EP/G047162/1.

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