On symmetries of crystals with defects related to a class of solvable groups (S_1)

Rachel Nicks[1] and Gareth P. Parry[2]
School of Mathematical Sciences,
University of Nottingham, Nottingham NG7 2RD, UK

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Abstract

We consider distributions of dislocations in continuum models of crystals which are such that the corresponding dislocation density tensor relates to a particular class of solvable Lie group, and discrete structures which are embedded in these crystals. We provide a canonical form of these structures and, by finding the set of all generators of a corresponding discrete subgroup, we determine the 'material' symmetries that constrain appropriate strain energy functions.

Keywords Crystals · Defects · Lie Groups

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1 Introduction

We consider solid crystals with uniform distributions of defects and extend previous treatments of the symmetry properties of such crystals to include the case where the distribution of defects corresponds to a certain class of solvable groups. The particular three dimensional class of solvable groups that we choose to consider is one of two that Auslander, Green and Hahn [1] highlight as the non–nilpotent Lie groups which contain discrete subgroups, and they call this particular group S_1. This distinguishing property, that S_1 contains discrete subgroups, gives the prospect of an explicit description of the connection between the symmetries of continuous and discrete models of crystals with corresponding uniform distributions of defects, where the dislocation density relates to the structure constants of the Lie group S_1, though in this paper we focus just on the discrete structure and its symmetries.

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[1] née Sigrist

[2] **Corresponding author:** G.P. Parry, School of Mathematical Sciences, University of Nottingham, Nottingham NG7 2RD, UK. email: gareth.parry@nottingham.ac.uk

To make these ideas definite, the reader may refer to Parry [2], [3], [4], where the motivation for the work is laid out, and the case of nilpotent groups is treated in detail (the nilpotent case appears to be the simplest non–trivial instance where continuous and discrete symmetries of a crystal with defects are related in a transparent way). But we also summarize this work briefly in points (i)–(vii) below, so that one may readily compare the main results of existing work with those obtained in this paper.

(i) First, we work with Davini's model of solid crystals, [5], [6], [7], where the kinematical state of the crystal corresponds to the prescription of three smooth linearly independent vector fields $\boldsymbol{\ell}_1(\cdot), \boldsymbol{\ell}_2(\cdot), \boldsymbol{\ell}_3(\cdot)$ in a domain which we may take to be $\mathbb{R}^3$. Then the dislocation density is defined by

$$\mathcal{S} = (\mathcal{S}_{ab}) = \left(\frac{\nabla \wedge \boldsymbol{d}_a \cdot \boldsymbol{d}_b}{\boldsymbol{d}_1 \cdot \boldsymbol{d}_2 \wedge \boldsymbol{d}_3} \right), \quad a, b = 1, 2, 3, \tag{1.1}$$

where the fields $\boldsymbol{d}_1(\cdot), \boldsymbol{d}_2(\cdot), \boldsymbol{d}_3(\cdot)$, are dual to the 'lattice vector fields' $\boldsymbol{\ell}_1(\cdot), \boldsymbol{\ell}_2(\cdot), \boldsymbol{\ell}_3(\cdot)$. We deal with configurations (i.e., distributions of lattice vector fields in $\mathbb{R}^3$) such that the tensor $\mathcal{S}$ is constant (in $\mathbb{R}^3$), and note that the motivation for this is given in [2]. This condition, that $\mathcal{S}$ is constant, is an integrability condition which guarantees that, if the lattice vector fields are given, the partial differential system

$$\boldsymbol{\ell}_a \left(\boldsymbol{\psi} \left(\boldsymbol{x}, \boldsymbol{y} \right) \right) = \nabla_1 \boldsymbol{\psi} \left(\boldsymbol{x}, \boldsymbol{y} \right) \boldsymbol{\ell}_a(\boldsymbol{x}), \quad a = 1, 2, 3, \tag{1.2}$$

where $\nabla_1 \boldsymbol{\psi}(\cdot, \cdot)$ denotes the gradient of $\boldsymbol{\psi}$ with respect to its first argument, has a solution for the unknown function $\boldsymbol{\psi}$. Moreover, the function $\boldsymbol{\psi} : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^3$ can be taken to satisfy the properties required for it to be a Lie group composition function, with identity element $\mathbf{0} \in \mathbb{R}^3$. Thus, given a value of dislocation density tensor $\mathcal{S}$ (consistent with the requirement that $\mathcal{S}$ is constant) one may arrive at a particular Lie group by constructing fields $\boldsymbol{\ell}_a(\cdot)$, $a = 1, 2, 3$ such that the dual fields satisfy (1.1), and then solving (1.2) for the group composition function $\boldsymbol{\psi}$.

(ii) The dislocation density tensor is an elastic invariant, in that if $\boldsymbol{u} : \mathbb{R}^3 \to \mathbb{R}^3$ is an elastic deformation, fields $\tilde{\boldsymbol{\ell}}_a(\cdot)$, $a = 1, 2, 3$ are defined by

$$\tilde{\boldsymbol{\ell}}_a \left(\boldsymbol{u}(\boldsymbol{x}) \right) = \nabla \boldsymbol{u}(\boldsymbol{x}) \boldsymbol{\ell}_a(\boldsymbol{x}), \ x \in \mathbb{R}^3, \quad a = 1, 2, 3 \tag{1.3}$$

and $\tilde{\mathcal{S}}$ is calculated by the analogue of (1.1), then

$$\tilde{\mathcal{S}} \left(\boldsymbol{u}(\boldsymbol{x}) \right) = \mathcal{S}(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{R}^{\ni}. \tag{1.4}$$

In particular, if $\mathcal{S}$ is constant, so is $\tilde{\mathcal{S}}$. So one sees that the composition function $\boldsymbol{\psi}$ obtained from (1.2) is just one amongst the infinite number of those which may be found by making different choices of the lattice vector fields, given a value of $\mathcal{S}$.

(iii) Discrete subgroups of a group corresponding to a particular choice of $\boldsymbol{\psi}$, given a value $\mathcal{S}$ of the dislocation density tensor, are constructed as follows. Let $\boldsymbol{\ell}_a(\cdot)$, $a = 1, 2, 3$, satisfy (1.2), let ν_1, ν_2, ν_3 be given real numbers and define the integral curve through $\boldsymbol{x}_0$ of the field $\nu_a \boldsymbol{\ell}_a(\cdot)$ to be the solution $\{\boldsymbol{x}(t);\ t \in \mathbb{R}\}$ of the ordinary differential equation

$$\frac{d\boldsymbol{x}}{dt}(t) = \nu_a \boldsymbol{\ell}_a\left(\boldsymbol{x}(t)\right), \quad \boldsymbol{x}(0) = \boldsymbol{x}_0. \tag{1.5}$$

(The summation convention operates). Note that $\boldsymbol{\nu} \equiv \nu_a \boldsymbol{\ell}_a(\mathbf{0})$ determines the field $\nu_a \boldsymbol{\ell}_a(\cdot)$, by (1.2), recalling that $\boldsymbol{\psi}(\mathbf{0}, \boldsymbol{y}) = \boldsymbol{y}$ by the properties of Lie group composition, with group identity $\mathbf{0}$. Define the *exponential mapping* $\exp(\boldsymbol{\nu}) : \mathbb{R}^3 \to \mathbb{R}^3$ by

$$\left(\exp(\boldsymbol{\nu})\right)(\boldsymbol{x}_0) = \boldsymbol{x}(1), \tag{1.6}$$

and the *group element* $e^{(\boldsymbol{\nu})}$ by

$$e^{(\boldsymbol{\nu})} = \left(\exp(\boldsymbol{\nu})\right)(\mathbf{0}). \tag{1.7}$$

It is an important standard result of Lie group theory that

$$\left(\exp(\boldsymbol{\nu})\right)(\boldsymbol{x}) = \boldsymbol{\psi}\left(e^{(\boldsymbol{\nu})}, \boldsymbol{x}\right). \tag{1.8}$$

This equation states that the flow along the integral curves of the lattice vector fields, which leads to the definition of the mapping $\exp(\boldsymbol{\nu})$, corresponds to group multiplication by the group element $e^{(\boldsymbol{\nu})}$.

(In the case $\mathcal{S} = 0$, choose $\boldsymbol{\ell}_a(\cdot) \equiv \boldsymbol{\ell}_a(\mathbf{0}) \equiv \boldsymbol{e}_a$ as solution of (1.1), where $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3\}$ is a basis of $\mathbb{R}^3$. Then $\boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{x} + \boldsymbol{y}$ is a solution of (1.2) which has the properties of a Lie group composition function. Solving (1.5) gives $\boldsymbol{x}(t) = \boldsymbol{\nu} t + \boldsymbol{x}_0$, where $\boldsymbol{\nu} = (\nu_1, \nu_2, \nu_3) \equiv \nu_a \boldsymbol{e}_a$, so $\left(\exp(\nu)\right)(\boldsymbol{x}) = \boldsymbol{\nu} + \boldsymbol{x} = \boldsymbol{\psi}(\boldsymbol{\nu}, \boldsymbol{x})$. Noting that $e^{\boldsymbol{\nu}} = \boldsymbol{\nu}$, one sees that (1.8) holds. Flow along the lattice vector fields themselves (where $\boldsymbol{\nu} = \boldsymbol{e}_1$ etc.) corresponds to group multiplication by $\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3$, which in this case represents translation by $\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3$. Successive translations produce the lattice $L = \{\boldsymbol{p} : \boldsymbol{p} = n_a \boldsymbol{e}_a,\ n_a \in \mathbb{Z},\ a = 1, 2, 3\}$, whose symmetries are the province of traditional crystallography.)

Consider the set of group elements produced by iterating the flow (from $t = 0$ to $t = 1$) along the lattice vector fields, starting at the origin, by analogy with what is done in the case $\mathcal{S} = 0$. By (1.8), one obtains the subgroup that is generated by the group elements $e^{\boldsymbol{\ell}_1}, e^{\boldsymbol{\ell}_2}, e^{\boldsymbol{\ell}_3}$, if one writes $\boldsymbol{\ell}_a = \boldsymbol{\ell}_a(\mathbf{0}),\ a = 1, 2, 3$.

(iv) According to Thurston [8], if the set of points generated in the procedure outlined in (iii) is discrete (i.e. there is a non-zero minimum separation between the elements), and if one further condition that we do not make explicit is satisfied, then the corresponding Lie group must be nilpotent. Parry [2] shows that this implies that $\mathcal{S}$ has the form

$$\mathcal{S} = (\lambda p_a p_b), \quad \lambda \in \mathbb{Q}, p_a \in \mathbb{Z}, a = 1, 2, 3, \tag{1.9}$$

and Cermelli and Parry [9] have shown that the flexibility afforded by the elastic invariance of $\mathcal{S}$ allows one to show that, in an appropriately chosen configuration, the corresponding discrete group is either a simple lattice or a 4-lattice, in Pitteri and Zanzotto's terminology [10] (even though the corresponding composition function is not additive).

(v) Mal'cev [11] has studied the structure of discrete subgroups of nilpotent Lie groups, and in particular obtained the following results (which are far reaching generalizations of the results for a perfect lattice):

(a) There are elements $\boldsymbol{\ell}_1, \boldsymbol{\ell}_2, \boldsymbol{\ell}_2$ of the discrete subgroup (call that subgroup D) such that

$$D = \{g : g = \boldsymbol{\ell}_1^{m_1} \boldsymbol{\ell}_2^{m_2} \boldsymbol{\ell}_3^{m_3}, \quad m_1, m_2, m_3 \in \mathbb{Z}\} \tag{1.10}$$

(In the expression $\boldsymbol{\ell}_1^{m_1} \boldsymbol{\ell}_2^{m_2} \boldsymbol{\ell}_3^{m_3}$, products of group elements are written as, for example, $\boldsymbol{\psi}(\boldsymbol{\ell}_1, \boldsymbol{\ell}_1) = \boldsymbol{\ell}_1^2$, $\boldsymbol{\psi}(\boldsymbol{\ell}_1, \boldsymbol{\ell}_2) = \boldsymbol{\ell}_1 \boldsymbol{\ell}_2$).

(b) The automorphisms of D, which are the invertible mappings of D to itself which preserve the group structure, extend uniquely to automorphisms of the corresponding continuous (nilpotent) group.

(c) The flexibility that comes from the elastic invariance of $\mathcal{S}$ allows one to choose the integral curves of the lattice vector fields through the origin to be straight lines, the automorphisms of the continuous group to be linear mappings, and (by (b)) the automorphisms of D to be (restrictions of) linear mappings.

(vi) In a three dimensional Lie group G, with group multiplication $\boldsymbol{\psi}$, write (as in (v)(a))

$$\boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{x}\boldsymbol{y}, \tag{1.11}$$

as an alternative notation. Let $(\boldsymbol{x}, \boldsymbol{y})$ denote the commutator of two group elements $\boldsymbol{x}, \boldsymbol{y} \in G$, so

$$(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{x}^{-1} \boldsymbol{y}^{-1} \boldsymbol{x} \boldsymbol{y}, \tag{1.12}$$

where $\boldsymbol{x}^{-1}$ is the inverse of $\boldsymbol{x}$, so

$$\boldsymbol{\psi}(\boldsymbol{x}^{-1},\boldsymbol{x})=\psi(\boldsymbol{x},\boldsymbol{x}^{-1})=\mathbf{0}, \tag{1.13}$$

or $\boldsymbol{x}^{-1}\boldsymbol{x}=\boldsymbol{x}\boldsymbol{x}^{-1}=\mathbf{0}$, recalling that $\mathbf{0}$ is the group identity. For a Lie group G where the underlying manifold is $\mathbb{R}^3$, let the components of a group element $\boldsymbol{x}$ be real numbers x_1, x_2, x_3 relative to a basis $\{\boldsymbol{e}_1,\boldsymbol{e}_2,\boldsymbol{e}_3\}$ of $\mathbb{R}^3$. Let the quadratic terms in the Taylor expansion of the commutator $(\boldsymbol{x},\boldsymbol{y})$ about $\mathbf{0}$ be denoted, temporarily, by

$$\gamma(\boldsymbol{x},\boldsymbol{y})\equiv C_{ijk}x_jy_k\boldsymbol{e}_i, \tag{1.14}$$

where $\boldsymbol{x}=x_i\boldsymbol{e}_i, \boldsymbol{y}=y_j\boldsymbol{e}_j$. Then the constants C_{ijk} are the structure constants of the Lie algebra $\mathfrak{g}$ of the group G. The function $\boldsymbol{\gamma}:\mathbb{R}^3\times\mathbb{R}^3\to\mathbb{R}^3$ is an antisymmetric bilinear form on the Lie algebra (here identified with $\mathbb{R}^3$) called the Lie bracket of $\mathfrak{g}$, and we introduce further notation

$$\gamma(\boldsymbol{x},\boldsymbol{y})=[\boldsymbol{x},\boldsymbol{y}]. \tag{1.15}$$

Vector fields $\boldsymbol{\zeta}(\cdot)$ which satisfy

$$\boldsymbol{\zeta}\left(\boldsymbol{\psi}(\boldsymbol{x},\boldsymbol{y})\right)=\nabla_1\boldsymbol{\psi}(\boldsymbol{x},\boldsymbol{y})\boldsymbol{\zeta}(\boldsymbol{x}),\quad \boldsymbol{x}\in\mathbb{R}^3, \tag{1.16}$$

are said to be right invariant on G, so from (1.2) the lattice vector fields $\boldsymbol{\ell}_1(\cdot),\boldsymbol{\ell}_2(\cdot),\boldsymbol{\ell}_3(\cdot)$ are right invariant – in fact these fields provide a basis for the vector space of all right invariant fields on G.

The connection between the dislocation density tensor $\mathcal{S}$, defined via (1.1), and the structure constants is

$$C_{ijk}\ell_{rj}(\mathbf{0})\ell_{sk}(\mathbf{0})=\varepsilon_{prs}\mathcal{S}_{kp}\ell_{ki}(\mathbf{0}), \tag{1.17}$$

where ε_{prs} is the permutation symbol and $\boldsymbol{\ell}_r(\mathbf{0})=\ell_{rj}(\mathbf{0})\boldsymbol{e}_j$, see Elzanowski and Parry [12]. Mal'cev [11] shows that a condition necessary and sufficient that G has non trivial discrete subgroups is that the structure constants of $\mathfrak{g}$ be rational with respect to an appropriate basis, in the case that G is nilpotent, and this translates to the requirement that $\mathcal{S}$ has the form given in (1.9) above.

(vii) For nilpotent Lie groups satisfying the rationality conditions of (vi), Parry and Sigrist [13] construct all sets of generators of a given discrete subgroup explicitly. The formulae that connect different sets of generators (of a given discrete subgroup) generalize the well–known formula for a perfect crystal, where bases $\{\boldsymbol{\ell}_1,\boldsymbol{\ell}_2,\boldsymbol{\ell}_3\}$, $\{\boldsymbol{\ell}'_1,\boldsymbol{\ell}'_2,\boldsymbol{\ell}'_3\}$ of $\mathbb{R}^3$ generate the same lattice if and only if $\boldsymbol{\ell}_i=\gamma_{ij}\boldsymbol{\ell}'_j$ where $(\gamma_{ij})\in GL_3(\mathbb{Z})$.

This paper is concerned with the extension of some of the above results, (i)–(vii), to defective crystals where the corresponding Lie group is solvable, and the group has non–trivial discrete subgroups. As stated above, and shown in [1], there are only three classes of three dimensional Lie groups which have non-trivial discrete subgroups – they are the nilpotent group and two classes of solvable group, which Auslander, Green and Hahn denote S_1 and S_2. We shall consider here the class S_1, and treat the remaining class elsewhere.

Recall the following facts regarding solvable Lie groups and algebras:

- In a solvable Lie algebra of dimension 3, it can be shown that there are basis vectors $\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{Z}$ of $\mathbb{R}^3$ such that

$$[\boldsymbol{X}, \boldsymbol{Y}] = \boldsymbol{0}, [\boldsymbol{X}, \boldsymbol{Z}] = \alpha\boldsymbol{X} + \beta\boldsymbol{Y}, [\boldsymbol{Y}, \boldsymbol{Z}] = \gamma\boldsymbol{X} + \delta\boldsymbol{Y}, \tag{1.18}$$

  where $\alpha, \beta, \gamma, \delta$ are real numbers such that $\alpha\delta - \beta\gamma \neq 0$;

- If $\mathfrak{g}$ is a Lie algebra, and one defines $\mathfrak{g}_1 = \mathfrak{g}, \mathfrak{g}_2 = [\mathfrak{g}_1, \mathfrak{g}_1] \ldots \mathfrak{g}_k = [\mathfrak{g}_{k-1}, \mathfrak{g}_{k-1}]$, then $\mathfrak{g}$ is called solvable if $\mathfrak{g}_k = \boldsymbol{0}$ for some k. It's clear that if (1.18) holds, then $\mathfrak{g}_3 = \boldsymbol{0}$;

- Let G be a connected Lie group, let (G, G) denote the subgroup generated by all commutators of G and define $G_1 = G$, $G_2 = (G_1, G_1), \ldots G_k = (G_{k-1}, G_{k-1})$. Then G is called solvable if $G_k = \boldsymbol{0}$ for some integer k.

- G is solvable if and only if $\mathfrak{g}$ is solvable.

In the case with which we shall be concerned $G = S_1$, and we shall write $\mathfrak{g} = \mathfrak{s}$. It will also be true that $G_3 = \boldsymbol{0}$, so that commutators of elements of S_1 commute, and this is an important fact that one should bear in mind throughout.

Note that group elements $\boldsymbol{x} \in S_1$ are parameterized by real numbers (x_1, x_2, x_3) and that we have chosen to identify the group elements with points of $\mathbb{R}^3$ (so that any discrete subgroup corresponds to a set of points in $\mathbb{R}^3$, for example). Auslander, Green and Hahn [1], on the other hand, represent group elements as 4×4 matrices (still parameterized by (x_1, x_2, x_3)), and in that representation the group composition is matrix multiplication – let S_m denote that representation of the group. Thus if $\boldsymbol{x} \in S_1$ and group composition in S_1 is denoted $\boldsymbol{\psi}$, then

$$r_m(\boldsymbol{x})r_m(\boldsymbol{y}) = r_m\left(\boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{y})\right), \quad \boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^3, \tag{1.19}$$

where $r_m : S_1 \to S_m$ is an isomorphism (which represents elements of S_1 as 4×4 matrices). In fact we calculate $\boldsymbol{\psi}$ from Auslander, Green and Hahn's representation of S_m using (1.19).

This enables us to calculate the basis right invariant fields and their duals, the corresponding dislocation density tensor, and the exponential in S_1. Auslander, Green and Hahn [1] assert that $r_m(\boldsymbol{e}_1), r_m(\boldsymbol{e}_2), r_m(\boldsymbol{e}_3)$ generate a canonical form of discrete subgroups $D_m \subset S_m$, and it follows that $\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3$ generate a canonical form of discrete subgroups $D \subset S_1$ where $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3\}$ is a basis of $\mathbb{R}^3$.

The isomorphism r_m involves a function $\phi : \mathbb{R} \to SL_2(\mathbb{R})$, with $\phi(1) \in SL_2(\mathbb{Z})$ and this is central to our calculations. In §2 we derive an expression for $\boldsymbol{\psi}$ in terms of ϕ, using the remark above. Also, it turns out the the 'structure' of the discrete subgroup D depends in essence on properties of the matrix

$$\theta \equiv \phi(1) \in SL_2(\mathbb{Z}), \tag{1.20}$$

cf. (3.1) below.

In §3, we discuss a canonical discrete subgroup $D_m \subset S_m$ and show that there exist elements of D_m (4×4 matrices), denoted A, B, C, such that a general element of D_m has the form $A^Q B^M C^N$, $Q, M, N \in \mathbb{Z}$. We also calculate the commutator subgroup $D'_m \equiv (D_m, D_m)$. Let D and D' be the subgroups of S_1 such that their matrix representations are D_m and D'_m respectively. We show that $D = (\mathbb{Z}^3, \boldsymbol{\psi})$, i.e., that the elements of $D \subset S_1$, are the points of $\mathbb{Z}^3$ (and the composition function is $\boldsymbol{\psi}$, of course), and that the points of D' can be identified with a proper two-dimensional sublattice of $\mathbb{Z}^3$.

The purpose of the calculations in §3 is to allow us, in due course, to calculate the 'symmetries' of the discrete subgroup D. More precisely, we find the set of all generators of D – that is we find all choices of three elements $\boldsymbol{g}_1, \boldsymbol{g}_2, \boldsymbol{g}_3 \in D$ such that the collection of all products of $\boldsymbol{g}_1, \boldsymbol{g}_2, \boldsymbol{g}_3$ and their inverses equals D. To do this, let G denote the subgroup of S_1 which consists of all products of $\boldsymbol{g}_1, \boldsymbol{g}_2, \boldsymbol{g}_3$ and their inverses (this subgroup G is unrelated to the connected Lie group of the third bullet point above). In Lemma 1 we construct a different set of generators for G which has a particular property that is useful for later calculations (the matrix representation of the new generators has the form (4.6)). Then we note that, in the case of interest where commutators commute, one can make sense of the symbol, $(\boldsymbol{x}, \boldsymbol{y})^P$, $\boldsymbol{x}, \boldsymbol{y} \in G$, where P is a polynomial in the generators of G and their inverses. This allows us to give a canonical expression for an arbitrary element $\boldsymbol{g} \in G$:

$$\boldsymbol{g} = \boldsymbol{g}_1^{\alpha} \boldsymbol{g}_2^{\beta} \boldsymbol{g}_3^{\gamma} (\boldsymbol{g}_1, \boldsymbol{g}_2)^{P_3} (\boldsymbol{g}_2, \boldsymbol{g}_3)^{P_1} (\boldsymbol{g}_3, \boldsymbol{g}_1)^{P_2}, \tag{1.21}$$

cf.(4.19) Lemma 2, where P_1, P_2, P_3, are polynomials of the stated form. This relation, (1.21), is a generalization of the expression $\boldsymbol{x} = m_1 \boldsymbol{\ell}_1 + m_2 \boldsymbol{\ell}_2 + m_3 \boldsymbol{\ell}_3$, $m_1, m_2, m_3 \in \mathbb{Z}$ for the general element $\boldsymbol{x}$ of a perfect lattice with basis $\boldsymbol{\ell}_1, \boldsymbol{\ell}_2, \boldsymbol{\ell}_3$ and a generalization of Mal'cev's expression $\boldsymbol{g} = \boldsymbol{g}_1^{m_1}\boldsymbol{g}_2^{m_2}\boldsymbol{g}_3^{m_3}, m_1, m_2, m_3 \in \mathbb{Z}$ for the elements of a discrete subgroup of a nilpotent Lie group in terms of a canonical basis $\boldsymbol{g}_1, \boldsymbol{g}_2, \boldsymbol{g}_3$, to the case at hand where the relevant Lie group is solvable. The statement that (1.22) holds may be found in Bachmuth [14], but we have not found a proof of the statement, so that is provided in Lemma 2.

From (1.21), a general element of the commutator subgroup $G' \equiv (G, G)$ has the form

$$(\boldsymbol{g}_1, \boldsymbol{g}_2)^{P_3}(\boldsymbol{g}_2, \boldsymbol{g}_3)^{P_1}(\boldsymbol{g}_3, \boldsymbol{g}_1)^{P_2}, \tag{1.22}$$

for appropriate polynomials P_1, P_2, P_3. This leads to an expression for basis elements of G', considered now as a two dimensional sublattice of $\mathbb{Z}^3$. In fact we know from §3.3 that a basis of D' can be given in terms of the columns of the matrix $\theta \equiv \phi(1) \in SL_2(\mathbb{Z})$. So, if $G' = D'$ (as is necessary if we require that $G = D$), then we have a connection between an arbitrary set of generators of D and the columns of θ. The algebraic conditions deriving from this connection are treated in §6 – there are other conditions which are (nominally) required in order that $G = D$, but we show in §6.2 and §6.3 that they are identically satisfied if $G' = D'$.

Note that (1.22) shows, in the language of continuum mechanics, that the Burgers vector corresponding to any choice of circuit can be decomposed as the product of three fundamental Burgers vectors, and that these three Burgers vectors generate a two dimensional lattice (additively).

The conditions which ensure that $G = D$ turn out to be divisibility conditions on integers that appear in the matrix representations of the group elements $\boldsymbol{g}_1, \boldsymbol{g}_2, \boldsymbol{g}_3$, and we summarize those condition in the conclusion to the paper. There we also discuss the symmetries of a continuum strain energy function that models a discrete solid crystal with local structure corresponding to the points of D – these symmetries derive from the infinite number of different choices of generators of D.

Finally we note that a particular symmetry of the strain energy, corresponding to a change in generators from $\boldsymbol{g}_1, \boldsymbol{g}_2, \boldsymbol{g}_3$ to $\boldsymbol{g}'_1, \boldsymbol{g}'_2, \boldsymbol{g}'_3$ may or may not correspond to an automorphism of D. Magnus, Karrass and Solitar [15] give a condition that is necessary and sufficient for such a change to correspond to an automorphism of D. When that condition holds, a result of Gorbatsevich [16] shows that the automorphisms (of D) extends uniquely to automorphisms of the continuous group S_1, so that in continuum mechanical terms, the discrete symmetries of D are (restrictions of) elastic deformations when Magnus, Karrass and Solitar's condition holds.

So, when that condition holds, the dislocation density is unchanged, because it is an elastic invariant. Thus the symmetries of the strain energy function may be divided into two classes, in the case at hand – there are the (self) mappings of the points of D which are restrictions of elastic deformations, and these are those which are not. One might call these the elastic, and the inelastic, symmetries of the crystal. We remark that in the case of the perfect crystal, where $\mathcal{S} = 0$, Magnus, Karrass and Solitar's condition is empty, so all self mappings of a perfect lattice corresponding to a change of generators are restrictions of elastic deformations.

2 Continuous groups

According to Auslander, Green and Hahn [1], if S is a connected, simply connected, non compact, three dimensional Lie group with a discrete subgroup D such that S/D is compact, and S is not nilpotent, then S is isomorphic to a matrix group S_m where the elements of S_m have the form

$$r_m(\boldsymbol{x}) \equiv \left(\begin{array}{cc|cc} \multicolumn{2}{c|}{\multirow{2}{*}{$\phi(x_3)$}} & 0 & x_1 \\ & & 0 & x_2 \\ \hline 0 & 0 & 1 & x_3 \\ 0 & 0 & 0 & 1 \end{array} \right), \quad \boldsymbol{x} \equiv \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \in \mathbb{R}^3. \tag{2.1}$$

In (2.1) , $\phi(x_3) \in SL_2(\mathbb{R}), \phi(1) \in SL_2(\mathbb{Z})$. Also, $\{\phi(x_3) : x_3 \in \mathbb{R}\}$ is a one parameter subgroup of the unimodular group, so

$$\phi(x)\phi(y) = \phi(x+y), \quad x, y \in \mathbb{R}. \tag{2.2}$$

It follows that

$$\phi(0) = \mathbb{I}_2 \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{2.3}$$

and by differentiating (2.2) with respect to y and putting $y = 0$, etc.,

$$\phi'(x) = \phi(x)\phi'(0) = \phi'(0)\phi(x), \tag{2.4}$$

where $'$ denotes $\dfrac{d}{dx}$. Let us write

$$\phi(x) = \begin{pmatrix} a(x) & b(x) \\ c(x) & d(x) \end{pmatrix}, \tag{2.5}$$

so

$$\phi'(0) \equiv \mathcal{A} = \begin{pmatrix} a'(0) & b'(0) \\ c'(0) & d'(0) \end{pmatrix}, \tag{2.6}$$

and

$$a(x)d(x) - b(x)c(x) = 1. \tag{2.7}$$

From (2.4)

$$\phi(x) = e^{\mathcal{A}x} \equiv \sum_{j=0}^{\infty} \mathcal{A}^j \frac{x^j}{j!}. \tag{2.8}$$

Since $\phi(0) = \mathbb{I}_2$, by differentiating (2.7) and putting $x = 0$ one obtains that $a'(0) + d'(0) = 0$, hence

$$\mathcal{A}^2 + \det(\mathcal{A})\mathbb{I}_2 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \tag{2.9}$$

where $\det(\mathcal{A})$ is the determinant of $\mathcal{A}$. It is then straightforward to show that, for arbitrary 2×2 matrices $\mathcal{B}$, satisfying (2.9),

$$e^{\mathcal{B}} = \begin{cases} (\cosh k)\mathbb{I}_2 + \left(\dfrac{\sinh k}{k}\right)\mathcal{B}, & \text{if } \det(\mathcal{B}) < 0, \quad k \equiv \sqrt{-\det(\mathcal{B})}; \\ (\cos k)\mathbb{I}_2 + \left(\dfrac{\sin k}{k}\right)\mathcal{B}, & \text{if } \det(\mathcal{B}) > 0, \quad k \equiv \sqrt{\det(\mathcal{B})}; \\ \mathbb{I}_2 + \mathcal{B}, & \text{if } \det(\mathcal{B}) = 0. \end{cases} \tag{2.10}$$

See Gallier [17], for example.

We shall be concerned, in this paper, with the particular case where

$$a(1) + d(1) > 2, \tag{2.11}$$

which is the condition that guarantees that the integer matrix

$$\phi(1) \equiv \begin{pmatrix} a(1) & b(1) \\ c(1) & d(1) \end{pmatrix} \tag{2.12}$$

has (real) positive eigenvalues. We call corresponding group S_1, rather than S, for definiteness, as noted above. Now, with tr denoting trace, so $tr\ \mathcal{A} = 0$,

$$a(1) + d(1) = tr\ e^{\mathcal{A}} = \begin{cases} 2\cosh k, & \text{if } \det(\mathcal{A}) < 0; \\ 2\cos k, & \text{if } \det(\mathcal{A}) > 0; \\ 2, & \text{if } \det(\mathcal{A}) = 0, \end{cases} \tag{2.13}$$

where k denotes $\sqrt{|\det(\mathcal{A})|}$ here and henceforward. Hence, according to (2.11) above, we shall be concerned here with the case that $\det(\mathcal{A}) < 0$, $k = \sqrt{-\det(\mathcal{A})}$, where $\phi : \mathbb{R} \to SL_2(\mathbb{R})$ is given explicitly by

$$\phi(x) = e^{\mathcal{A}x} = (\cosh kx)\,\mathbb{I}_2 + \left(\frac{\sinh kx}{k}\right)\mathcal{A}. \tag{2.14}$$

Note also that

$$\phi(1) = (\cosh k)\mathbb{I}_2 + \left(\frac{\sinh k}{k}\right)\mathcal{A}, \tag{2.15}$$

so

$$tr\ \phi(1) = 2(\cosh k). \tag{2.16}$$

Hence if we define

$$\phi(1) = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \tag{2.17}$$

so $a = a(1)$, etc., then

$$a + d = 2\cosh k, \tag{2.18}$$

and we have

$$\phi(1) \equiv \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \frac{1}{2}(a+d)\mathbb{I}_2 + \frac{(\sinh k)}{k}\begin{pmatrix} a'(0) & b'(0) \\ c'(0) & d'(0) \end{pmatrix} \tag{2.19}$$

and

$$\frac{(\sinh k)}{k}\mathcal{A} = \begin{pmatrix} \frac{1}{2}(a-d) & b \\ c & \frac{1}{2}(d-a) \end{pmatrix}. \tag{2.20}$$

Let $\boldsymbol{\psi} : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^3$ be the group operation in S_1, then since the group operation in S_m is matrix multiplication we have

$$r_m(\boldsymbol{x})r_m(\boldsymbol{y}) = r_m\left(\boldsymbol{\psi}(\boldsymbol{x},\boldsymbol{y})\right), \quad \boldsymbol{x},\boldsymbol{y} \in \mathbb{R}^3, \tag{2.21}$$

and one calculates that

$$\boldsymbol{\psi}(\boldsymbol{x},\boldsymbol{y}) = \boldsymbol{x} + \left(a\left(x_3\right)y_1 + b\left(x_3\right)y_2\right)\boldsymbol{e}_1 + \left(c\left(x_3\right)y_1 + d\left(x_3\right)y_2\right)\boldsymbol{e}_2 + y_3\boldsymbol{e}_3, \tag{2.22}$$

where $\boldsymbol{x} = x_i\boldsymbol{e}_i \equiv (x_1, x_2, x_3)^T$, $\boldsymbol{y} = y_i\boldsymbol{e}_i \equiv (y_1, y_2, y_3)^T$, where T denotes transpose, where $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3\}$ is a basis of $\mathbb{R}^3$ and the summation convention operates.

Thus S_1 is the Lie group $(\mathbb{R}^3, \boldsymbol{\psi})$, isomorphic (via r_m) to the matrix group S_m. Let $\mathfrak{s}$ be the Lie algebra corresponding to S_1, and let $[\cdot,\cdot]$ denote the corresponding Lie bracket, so

$$[\boldsymbol{x}, \boldsymbol{y}] = C_{ijk} x_j y_k \boldsymbol{e}_i, \tag{2.23}$$

where

$$C_{ijk} \equiv \frac{\partial^2 \psi_i}{\partial x_j \partial y_k}(\mathbf{0}, \mathbf{0}) - \frac{\partial^2 \psi_i}{\partial x_k \partial y_j}(\mathbf{0}, \mathbf{0}), \tag{2.24}$$

and $\boldsymbol{\psi} \equiv \psi_i \boldsymbol{e}_i$. One calculates from (2.22) and this last definition that

$$\frac{\partial^2 \psi_i}{\partial x_j \partial y_k}(\mathbf{0}, \mathbf{0}) = \begin{cases} a'(0), & \text{if } i = 1,\ j = 3,\ k = 1; \\ b'(0), & \text{if } i = 1,\ j = 3,\ k = 2; \\ c'(0), & \text{if } i = 2,\ j = 3,\ k = 1; \\ d'(0), & \text{if } i = 2,\ j = 3,\ k = 2; \\ 0, & \text{otherwise,} \end{cases} \tag{2.25}$$

and from this one obtains

$$[\boldsymbol{x}, \boldsymbol{y}] = \left(a'(0)\boldsymbol{x} \wedge \boldsymbol{y} \cdot \boldsymbol{e}_2 - b'(0)\boldsymbol{x} \wedge \boldsymbol{y} \cdot \boldsymbol{e}_1\right) \boldsymbol{e}_1 + \left(c'(0)\boldsymbol{x} \wedge \boldsymbol{y} \cdot \boldsymbol{e}_2 - d'(0)\boldsymbol{x} \wedge \boldsymbol{y} \cdot \boldsymbol{e}_1\right) \boldsymbol{e}_2. \tag{2.26}$$

In particular

$$[\boldsymbol{e}_1, \boldsymbol{e}_2] = \mathbf{0}, \quad [\boldsymbol{e}_1, \boldsymbol{e}_3] = -a'(0)\boldsymbol{e}_1 - c'(0)\boldsymbol{e}_2, \quad [\boldsymbol{e}_2, \boldsymbol{e}_3] = -b'(0)\boldsymbol{e}_1 - d'(0)\boldsymbol{e}_2. \tag{2.27}$$

Next we calculate the dislocation density tensor corresponding to this choice of Lie group. First

$$\nabla_1 \boldsymbol{\psi}(\mathbf{0}, \boldsymbol{x}) = \begin{pmatrix} \begin{matrix} 1 & 0 \\ 0 & 1 \end{matrix} & \left(\phi'(0) \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}\right) \\ \begin{matrix} 0 & 0 \end{matrix} & 1 \end{pmatrix}, \tag{2.28}$$

and this gives that the right invariant lattice vector fields $\boldsymbol{\ell}_a(\boldsymbol{x}) \equiv \nabla_1 \boldsymbol{\psi}(\mathbf{0}, \boldsymbol{x}) \boldsymbol{e}_a$ are given by

$$\boldsymbol{\ell}_1(\boldsymbol{x}) = \boldsymbol{e}_1,\ \boldsymbol{\ell}_2(\boldsymbol{x}) = \boldsymbol{e}_2,\ \boldsymbol{\ell}_3(\boldsymbol{x}) = \left(a'(0)x_1 + b'(0)x_2\right) \boldsymbol{e}_1 + \left(c'(0)x_1 + d'(0)x_2\right) \boldsymbol{e}_2 + \boldsymbol{e}_3. \tag{2.29}$$

The dual lattice fields $\boldsymbol{d}_a(\boldsymbol{x})$ are

$$\boldsymbol{d}_1(\boldsymbol{x}) = \boldsymbol{e}_1 - \left(a'(0)x_1 + b'(0)x_2\right) \boldsymbol{e}_3,\ \boldsymbol{d}_2(\boldsymbol{x}) = \boldsymbol{e}_2 - \left(c'(0)x_1 + d'(0)x_2\right) \boldsymbol{e}_3,\ \boldsymbol{d}_3(\boldsymbol{x}) = \boldsymbol{e}_3. \tag{2.30}$$

Hence the lattice components of the dislocation density tensor are

$$\left(\frac{\nabla \wedge \boldsymbol{d}_a \cdot \boldsymbol{d}_b}{\boldsymbol{d}_1 \cdot \boldsymbol{d}_2 \wedge \boldsymbol{d}_3}\right) = \begin{pmatrix} -b'(0) & -d'(0) & 0 \\ a'(0) & c'(0) & 0 \\ 0 & 0 & 0 \end{pmatrix} = \frac{k}{\sinh(k)} \begin{pmatrix} -b & \frac{1}{2}(a-d) & 0 \\ \frac{1}{2}(a-d) & c & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{2.31}$$

from (2.20). In particular the dislocation density tensor is symmetric. Note that, from (2.11) and (2.13), $e^k + e^{-k}$ is an integer greater than 2. Also, if the dislocation density tensor is known, so is $\phi'(0) \equiv \mathcal{A}$ via (2.6), so is $\phi(0)$ via (2.8), and vice versa.

Let $\mathfrak{s}_m$ be the Lie algebra corresponding to the matrix Lie group $\mathcal{S}_m$, then the following diagram is commutative, see for example Warner [18], Varadarajan [19]

$$\begin{tikzcd} \mathfrak{s} \arrow[r, "\nabla r_m(\mathbf{0})"] \arrow[d, "e^{(\cdot)}"'] & \mathfrak{s}_m \arrow[d, "\text{matrix exponential}"] \\ S_1 \arrow[r, "r_m"'] & S_m \end{tikzcd}$$

Fig 1: Mappings between Lie algebras $\mathfrak{s}, \mathfrak{s}_m$ and Lie groups S_1, S_m.

In the figure, $e^{(\bullet)} : \mathfrak{s} \to S_1$ is the exponential calculated in the manner that was outlined in the introduction. Thus

$$r_m\left(e^{(\boldsymbol{x})}\right) = e^{\nabla r_m(\mathbf{0})\boldsymbol{x}}, \tag{2.32}$$

where the exponential on the right hand side is the matrix exponential. From (2.1),

$$\nabla r_m(\mathbf{0})\boldsymbol{x} = \left(\begin{array}{cc|cc} \multicolumn{2}{c|}{\multirow{2}{*}{$\phi'(0)x_3$}} & 0 & x_1 \\ & & 0 & x_2 \\ \hline 0 & 0 & 0 & x_3 \\ 0 & 0 & 0 & 0 \end{array}\right), \tag{2.33}$$

and one calculates that

$$e^{\nabla r_m(\mathbf{0})\boldsymbol{x}} = \left(\begin{array}{cc|cc} \multicolumn{2}{c|}{\multirow{2}{*}{$e^{\phi'(0)x_3}$}} & 0 & \multirow{2}{*}{$\left(f(\phi'(0)x_3)\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}\right)$} \\ & & 0 & \\ \hline 0 & 0 & 1 & x_3 \\ 0 & 0 & 0 & 1 \end{array}\right), \tag{2.34}$$

where we define $f : GL_2(\mathbb{R}) \to GL_2(\mathbb{R})$ by

$$f(A) \equiv \sum_{j=0}^{\infty} \frac{A^j}{(j+1)!}. \tag{2.35}$$

(So $f(A) = \dfrac{e^A - \mathbb{I}_2}{A}$ if $\det A \neq 0$).

Recall that from (2.6) and (2.8)

$$e^{\phi'(0)x_3} = \phi(x_3). \tag{2.36}$$

Since $r_m : \mathbb{R}^3 \to S_m$ is invertible, from (2.1), (2.34) and (2.32) we obtain

$$e^{(\boldsymbol{x})} = \begin{pmatrix} f(\phi'(0)x_3)\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \\ x_3 \end{pmatrix}. \tag{2.37}$$

This formula gives the explicit form of the exponentiation which is involved in the iteration process described in the introduction (derived differently to the method given there).

3 Discrete groups

3.1 $D = (\mathbb{Z}^3, \boldsymbol{\psi})$

According to Auslander, Green and Hahn [1] once again, one can assume that the discrete subgroup $D \subset S_1$ is isomorphic, via r_m, to a discrete subgroup $D_m \subset S_m$ and that D_m is generated by three elements $r_m(\boldsymbol{e}_1), r_m(\boldsymbol{e}_2), r_m(\boldsymbol{e}_3)$ of S_m. Set

$$A \equiv r_m(\boldsymbol{e}_3) = \left(\begin{array}{cc|cc} \multicolumn{2}{c|}{\multirow{2}{*}{$\phi(1)$}} & 0 & 0 \\ & & 0 & 0 \\ \hline 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 \end{array}\right), B \equiv r_m(\boldsymbol{e}_1) = \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, C \equiv r_m(\boldsymbol{e}_2) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{3.1}$$

Let $(\boldsymbol{x}, \boldsymbol{y}) \equiv \boldsymbol{x}^{-1}\boldsymbol{y}^{-1}\boldsymbol{x}\boldsymbol{y}$, denote the commutator of elements $\boldsymbol{x}, \boldsymbol{y} \in D$ and similarly let $(X, Y) \equiv X^{-1}Y^{-1}XY$ denote the commutator of elements $X, Y \in D_m$.

Recalling (2.17) one finds that

$$(A, B) = B^{1-d}C^c, \ (A, C) = B^bC^{1-a}, \ (B, C) = 0. \tag{3.2}$$

Now any element of D_m can be expressed as a product of the form

$$d_m = A^{\alpha_1}B^{\beta_1}C^{\gamma_1}A^{\alpha_2}B^{\beta_2}C^{\gamma_2}\dots A^{\alpha_r}B^{\beta_r}C^{\gamma_r} \tag{3.3}$$

with $\alpha_i, \beta_i, \gamma_i \in \{0, \pm 1\}, \ i = 1, 2 \dots r$. Noting that $BC = CB$, and computing that

$$(B^\beta C^\gamma, A^\alpha) = B^{m-\beta}C^{n-\gamma}, \quad \text{where} \quad \begin{pmatrix} m \\ n \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}^{-\alpha} \begin{pmatrix} \beta \\ \gamma \end{pmatrix}, \tag{3.4}$$

we have

$$B^\beta C^\gamma A^\alpha = A^\alpha B^\beta C^\gamma B^{m-\beta}C^{n-\gamma} = A^\alpha B^m C^n.$$

Using this we can rewrite (3.3) as

$$d_m = A^{\alpha_1+\alpha_2+\dots\alpha_r} B^M C^N$$

for some $M, N \in \mathbb{Z}$.

Notice then that D_m contains $d_m = A^Q B^M C^N$ for any $Q, M, N, \in \mathbb{Z}$. So a general element $d_m = A^Q B^M C^N \in D_m \subset S_m$ has the representation

$$\left(\begin{array}{c|c} \begin{pmatrix} a & b \\ c & d \end{pmatrix}^Q & \begin{matrix} 0 \\ 0 \end{matrix} \quad \begin{pmatrix} a & b \\ c & d \end{pmatrix}^Q \begin{pmatrix} M \\ N \end{pmatrix} \\ \hline \begin{matrix} 0 & 0 \\ 0 & 0 \end{matrix} & \begin{matrix} 1 & \quad Q \\ 0 & \quad 1 \end{matrix} \end{array} \right). \tag{3.5}$$

One calculates that

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^Q = U_Q \begin{pmatrix} a & b \\ c & d \end{pmatrix} - U_{Q-1} \mathbb{I}_2, \tag{3.6}$$

where

$$U_Q := \frac{e^{kQ} - e^{-kQ}}{e^k - e^{-k}} \tag{3.7}$$

are the Chebyshev polynomials of the second kind, defined alternatively by the recurrence relation

$$U_{Q+1} = nU_Q - U_{Q-1}, \tag{3.8}$$

where $U_0 = 0, U_1 = 1$ and $n \equiv a + d$.

Henceforward we write

$$\theta \equiv \phi(1) \equiv \begin{pmatrix} a & b \\ c & d \end{pmatrix} \equiv \begin{pmatrix} a(1) & b(1) \\ c(1) & d(1) \end{pmatrix}, \tag{3.9}$$

and recall that the condition $tr\ \theta \equiv a + d > 2$ implies that θ has (real) positive eigenvalues. In fact, since the eigenvalues of $\mathcal{A}$ are $\pm\sqrt{|\det \mathcal{A}|} \equiv \pm k$, by (2.9) and Cayley–Hamilton, the eigenvalues of $\theta \equiv e^{\mathcal{A}}$ are $e^{\pm k} > 0$.

Let $\boldsymbol{x} \in \mathbb{R}^3$ be such that

$$r_m(\boldsymbol{x}) = A^Q B^M C^N, \quad Q, M, N \in \mathbb{Z}. \tag{3.10}$$

Then

$$\boldsymbol{x} = \begin{pmatrix} \theta^{Q} \begin{pmatrix} M \\ N \end{pmatrix} \\ Q \end{pmatrix}. \tag{3.11}$$

Since $\theta \in SL_2(\mathbb{Z})$, it is clear that $r_m^{-1}(D_m) \equiv D = (\mathbb{Z}^3, \boldsymbol{\psi})$, i.e. that the discrete subgroup of S_1 with which we are concerned is the cubic lattice $\mathbb{Z}^3$ with group multiplication given by(2.22).

3.2 Composition in D_m

Suppose that $d_1 = A^{x_3}B^{x_1}C^{x_2}$ and $d_2 = A^{y_3}B^{y_1}C^{y_2}$ are elements of D_m (i.e. $x_i, y_i \in \mathbb{Z}, i = 1,2,3$). Then

$$\begin{aligned} d_1 d_2 &= \left(\begin{array}{cc|cc} \multicolumn{2}{c|}{\theta^{x_3}} & \begin{matrix} 0 \\ 0 \end{matrix} & \theta^{x_3}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \\ \hline 0 & 0 & 1 & x_3 \\ 0 & 0 & 0 & 1 \end{array}\right) \left(\begin{array}{cc|cc} \multicolumn{2}{c|}{\theta^{y_3}} & \begin{matrix} 0 \\ 0 \end{matrix} & \theta^{y_3}\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \\ \hline 0 & 0 & 1 & y_3 \\ 0 & 0 & 0 & 1 \end{array}\right) \\ &= \left(\begin{array}{cc|cc} \multicolumn{2}{c|}{\theta^{x_3+y_3}} & \begin{matrix} 0 \\ 0 \end{matrix} & \theta^{x_3+y_3}\left(\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} + \theta^{-y_3}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}\right) \\ \hline 0 & 0 & 1 & x_3+y_3 \\ 0 & 0 & 0 & 1 \end{array}\right) \\ &= A^{z_3}B^{z_1}C^{z_2}, \end{aligned} \tag{3.12}$$

and so

$$\begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix} = \begin{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} + \theta^{-y_3}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \\ x_3 + y_3 \end{pmatrix} = \begin{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} + (\theta^{-y_3} - \mathbb{I})\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \\ x_3 + y_3 \end{pmatrix}. \tag{3.13}$$

Now

$$\begin{aligned} (\theta^{-y_3} - \mathbb{I}) &= \left(\theta^{-1} - \mathbb{I}\right)\left(\mathbb{I} + \theta^{-1} + \theta^{-2} + \cdots + \theta^{-y_3+1}\right) \\ &= \begin{pmatrix} d-1 & -b \\ -c & a-1 \end{pmatrix}\begin{pmatrix} p & q \\ r & s \end{pmatrix} \end{aligned} \tag{3.14}$$

for some $p, q, r, s \in \mathbb{Z}$ which depend on y_3. Thus

$$d_1 d_2 = A^{x_3+y_3}B^{x_1+y_1}C^{x_2+y_2}\left(B^{d-1}C^{-c}\right)^{px_1+qx_2}\left(B^{-b}C^{a-1}\right)^{rx_1+sx_2}. \tag{3.15}$$

3.3 The commutator subgroup D'_m

The commutator (or derived) subgroup D'_m of D_m is the subgroup generated by all commutators $(d_1, d_2) = d_1^{-1} d_2^{-1} d_1 d_2$, $d_1, d_2 \in D_m$. From the previous section we can see that

$$d_1^{-1} = \left(\begin{array}{cc|cc} \multicolumn{2}{c|}{\multirow{2}{*}{θ^{-x_3}}} & 0 & -x_1 \\ & & 0 & -x_2 \\ \hline 0 & 0 & 1 & -x_3 \\ 0 & 0 & 0 & 1 \end{array}\right) = A^{-x_3} B^{U_{x_3-1}x_1 - U_{x_3}(ax_1+bx_2)} C^{U_{x_3-1}x_2 - U_{x_3}(cx_1+dx_2)} \tag{3.16}$$

and then

$$\begin{aligned}(d_1, d_2) &= \left(\begin{array}{cc|cc} \multicolumn{2}{c|}{\theta^{-x_3-y_3}} & \begin{matrix}0\\0\end{matrix} & -\theta^{-x_3}\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} - \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \\ \hline 0 & 0 & 1 & -x_3-y_3 \\ 0 & 0 & 0 & 1 \end{array}\right)\left(\begin{array}{cc|cc} \multicolumn{2}{c|}{\theta^{x_3+y_3}} & \begin{matrix}0\\0\end{matrix} & \theta^{x_3+y_3}\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} + \theta^{-y_3}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \\ \hline 0 & 0 & 1 & x_3+y_3 \\ 0 & 0 & 0 & 1 \end{array}\right) \\ &= \left(\begin{array}{cc|cc} \begin{matrix}1 & 0\\0 & 1\end{matrix} & & \begin{matrix}0\\0\end{matrix} & (\theta^{-y_3} - \mathbb{I})\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} - (\theta^{-x_3} - \mathbb{I})\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \\ \hline 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{array}\right) \\ &= (B^{d-1}C^{-c})^{px_1+qx_2-ty_1-uy_2}(B^{-b}C^{a-1})^{rx_1+sx_2-vy_1-wy_2}\end{aligned} \tag{3.17}$$

where

$$\begin{pmatrix} p & q \\ r & s \end{pmatrix} = \mathbb{I}_2 + \theta^{-1} + \cdots + \theta^{-y_3+1} \qquad \begin{pmatrix} t & u \\ v & w \end{pmatrix} = \mathbb{I}_2 + \theta^{-1} + \cdots + \theta^{-x_3+1}. \tag{3.18}$$

Thus every commutator in D_m can be written as a product of $B^{d-1}C^{-c} = (B, A)$ and $B^{-b}C^{a-1} = (C, A)$. Let $r_m(\boldsymbol{u}) = (B, A), r_m(\boldsymbol{v}) = (C, A)$. Since, from (2.22), $\boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{x} + \boldsymbol{y}$ if $x_3 = y_3 = 0$, and all commutators have third components equal to zero, it follows that $r_m(\alpha\boldsymbol{u} + \beta\boldsymbol{v}) = (B, A)^\alpha (C, A)^\beta, \alpha, \beta \in \mathbb{Z}$. So if $D'_m \equiv r_m(D')$, then the points of D' coincide with the sublattice of $\mathbb{Z}^3$ generated (additively) by $\boldsymbol{u}$ and $\boldsymbol{v}$. Let $\langle \boldsymbol{u}, \boldsymbol{v} \rangle$ denote the integer linear span of the vectors $\boldsymbol{u}, \boldsymbol{v} \in \mathbb{Z}^3$.

For convenience, we write $\boldsymbol{u} = \begin{pmatrix} d-1 \\ -c \end{pmatrix}$ instead of $\boldsymbol{u} = \begin{pmatrix} d-1 \\ -c \\ 0 \end{pmatrix}$. Let $\{\boldsymbol{u}, \boldsymbol{v}\}$ denote the 2×2 matrix with columns $\boldsymbol{u}, \boldsymbol{v}$, so

$$\{\boldsymbol{u}, \boldsymbol{v}\} = \begin{pmatrix} d-1 & -b \\ -c & a-1 \end{pmatrix} = (\theta^{-1} - \mathbb{I}_2) \equiv (\theta^{-1} - \mathbb{I}_2)\{\boldsymbol{e}_1, \boldsymbol{e}_2\}. \tag{3.19}$$

Note

$$\det(\theta^{-1} - \mathbb{I}_2) = 2 - (a+d) < 0. \tag{3.20}$$

So in the case that $a+d=3$, the points of D' are just $\mathbb{Z}^2 \equiv \{(a,b,c) \in \mathbb{Z}^3;\ c=0\}$. In the case that $a+d>3$, the points of D' coincide with those of a proper sublattice of $\mathbb{Z}^2$ (with unit cell of area $(a+d-2)$).

3.4 Maximal normal nilpotent subgroup N

According to Auslander, Green and Hahn, [1], S_1 has an unique maximal normal connected nilpotent subgroup N, which is abelian in this case. Thus $N = \left(\left\{(x,y,z) \in \mathbb{R}^3; z=0\right\}, \boldsymbol{\psi}\right)$ and $\boldsymbol{\psi}(\boldsymbol{x},\boldsymbol{y}) = \boldsymbol{x}+\boldsymbol{y}, \boldsymbol{x},\boldsymbol{y} \in N$. Moreover, $D \cap N = (\mathbb{Z}^2, \boldsymbol{\psi}) = (\mathbb{Z}^2, +)$, and $D' \cap N = (\langle \boldsymbol{u}, \boldsymbol{v}\rangle, +)$ according to the previous section.

4 Generators of D

Let $\boldsymbol{g}_1, \boldsymbol{g}_2, \boldsymbol{g}_3$ be elements of D. We wish to determine conditions on the choice of those three elements which are necessary and sufficient that the group generated by $\boldsymbol{g}_1, \boldsymbol{g}_2, \boldsymbol{g}_3$, with composition function (2.22) denoted

$$G = gp(\boldsymbol{g}_1, \boldsymbol{g}_2, \boldsymbol{g}_3), \tag{4.1}$$

equals D.

Let $\boldsymbol{g}_{im} \equiv r_m(\boldsymbol{g}_i)$. Then, via (3.10), we may write

$$\begin{aligned} \boldsymbol{g}_{1m} &= A^{\alpha_1} B^{\beta_1} C^{\gamma_1}, \\ \boldsymbol{g}_{2m} &= A^{\alpha_2} B^{\beta_2} C^{\gamma_2}, \\ \boldsymbol{g}_{3m} &= A^{\alpha_3} B^{\beta_3} C^{\gamma_3}, \qquad \alpha_i, \beta_i, \gamma_i \in \mathbb{Z},\ i=1,2,3. \end{aligned} \tag{4.2}$$

If $G=D$, then $G_m \equiv gp(\boldsymbol{g}_{1m}, \boldsymbol{g}_{2m}, \boldsymbol{g}_{3m})$, with matrix multiplication as group operation, equals D_m. But if $\boldsymbol{g}_m \in G_m$, then

$$\boldsymbol{g}_m = \boldsymbol{g}_{1m}^{\varepsilon_1} \boldsymbol{g}_{2m}^{\nu_1} \boldsymbol{g}_{3m}^{\mu_1} \boldsymbol{g}_{1m}^{\varepsilon_2} \boldsymbol{g}_{2m}^{\nu_2} \boldsymbol{g}_{3m}^{\mu_2} \cdots \boldsymbol{g}_{1m}^{\varepsilon_r} \boldsymbol{g}_{2m}^{\nu_r} \boldsymbol{g}_{3m}^{\mu_r}, \tag{4.3}$$

where $\varepsilon_i, \nu_i, \mu_i \in \{0, \pm 1\},\ i = 1 \ldots r$. This expression may be rewritten, via (3.2), (3.4), (4.2), as

$$\boldsymbol{g}_m = A^{\alpha_1(\varepsilon_1+\cdots+\varepsilon_r)+\alpha_2(\nu_1+\cdots+\nu_r)+\alpha_3(\mu_1\cdots+\mu_r)} B^M C^N, \tag{4.4}$$

for some $M, N \in \mathbb{Z}$ whose values depend on $\alpha_i, \beta_i, \gamma_i, \varepsilon_i, \nu_i, \mu_i$ for $i = 1, 2, 3$. Since $A \in G_m$ and $A^\ell \neq B^m C^n$ for any $\ell, m, n, \in \mathbb{Z}\backslash\{0\}$, it follows that there are integers $\varepsilon \equiv \varepsilon_1 + \cdots + \varepsilon_r,\ \nu \equiv \nu_1 + \cdots + \nu_r,\ \mu \equiv \mu_1 + \cdots + \mu_r$, such that $\alpha_1\varepsilon + \alpha_2\nu + \alpha_3\mu = 1$. Therefore $\alpha_1, \alpha_2, \alpha_3$ are relatively prime integers. Let $hcf(a, b \ldots c)$ denote the positive highest common factor of the set of integers $\{a, b \ldots c\}$. Then

$$hcf(\alpha_1, \alpha_2, \alpha_3) = 1. \tag{4.5}$$

Lemma 1. *Let $\boldsymbol{g}_{1m}, \boldsymbol{g}_{2m}, \boldsymbol{g}_{3m}$ be given by* (4.2)*, let $G_m = gp(\boldsymbol{g}_{1m}, \boldsymbol{g}_{2m}, \boldsymbol{g}_{3m})$ and suppose that $hcf(\alpha_1, \alpha_2, \alpha_3) = 1$. Then there is a set of generators of G_m, denoted $\boldsymbol{g}'_{1m}, \boldsymbol{g}'_{2m}, \boldsymbol{g}'_{3m}$, such that*

$$\boldsymbol{g}'_{1m} = AB^{\beta'_1}C^{\gamma'_1}, \boldsymbol{g}'_{2m} = B^{\beta'_2}C^{\gamma'_2}, \boldsymbol{g}'_{3m} = B^{\beta'_3}C^{\gamma'_3}, \quad \beta'_i, \gamma'_i \in \mathbb{Z}, \quad i = 1, 2, 3. \tag{4.6}$$

Proof

Given $\boldsymbol{g}_m = A^\alpha B^\beta C^\gamma$, note that $\boldsymbol{g}_m^A \equiv \alpha$ is well defined because $A^\ell \neq B^m C^n$ for any $\ell, m, n \in \mathbb{Z}\backslash\{0\}$. Note that if $P \in SL_3(\mathbb{Z})$ with

$$P = (P_{ij}) \equiv \begin{pmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{pmatrix}, \quad i, j = 1, 2, 3, \tag{4.7}$$

and $\{\boldsymbol{g}_{1m}, \boldsymbol{g}_{2m}, \boldsymbol{g}_{3m}\}P$ is defined to be the set of elements

$$\left\{\boldsymbol{g}_{1m}^{a_1}\boldsymbol{g}_{2m}^{b_1}\boldsymbol{g}_{3m}^{c_1}, \boldsymbol{g}_{1m}^{a_2}\boldsymbol{g}_{2m}^{b_2}\boldsymbol{g}_{3m}^{c_2}, \boldsymbol{g}_{1m}^{a_3}\boldsymbol{g}_{2m}^{b_3}\boldsymbol{g}_{3m}^{c_3}\right\} \equiv \{\boldsymbol{g}'_{1m}, \boldsymbol{g}'_{2m}, \boldsymbol{g}'_{3m}\} \tag{4.8}$$

of G_m, then

$$\boldsymbol{g}'^A_{1m} = \boldsymbol{g}^A_{1m}a_1 + \boldsymbol{g}^A_{2m}b_1 + \boldsymbol{g}^A_{3m}c_1, \text{etc.}, \tag{4.9}$$

so

$$\boldsymbol{g}'^A_{im} = \boldsymbol{g}^A_{jm}P_{ji}, \quad i = 1, 2, 3. \tag{4.10}$$

Also note that, according to Coxeter and Moser [20], p92, any element $P \in SL_3(\mathbb{Z})$ is expressible as a product of the following matrices:

$$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{4.11}$$

For each matrix P' in the above list (4.11). $\{\boldsymbol{g}_{1m}, \boldsymbol{g}_{2m}, \boldsymbol{g}_{3m}\}\, P'$ generates G_m, since $\{\boldsymbol{g}_{1m}, \boldsymbol{g}_{2m}, \boldsymbol{g}_{3m}\} \to \{\boldsymbol{g}_{1m}, \boldsymbol{g}_{2m}, \boldsymbol{g}_{3m}\}\, P'$ is a free substitution, in Magnus, Karrass and Solitar's terminology [15]. It follows that $\{\boldsymbol{g}_{1m}, \boldsymbol{g}_{2m}, \boldsymbol{g}_{3m}\}\, P$ generates G_m whenever $P \in SL_3(\mathbb{Z})$.

Now let $\{\boldsymbol{g}_{1m}, \boldsymbol{g}_{2m}, \boldsymbol{g}_{3m}\}$ be given as in (4.2) above, so that $\boldsymbol{g}^A_{im} = \alpha_i,\ i = 1,2,3$. Since $hcf(\alpha_1, \alpha_2, \alpha_3) = 1$ by (4.5), one may choose $Q \in SL_3(\mathbb{Z})$ with first row $(\alpha_1, \alpha_2, \alpha_3)$, so that $(\alpha_1, \alpha_2, \alpha_3)Q^{-1} = (1,0,0)$. Let $P = Q^{-1}$, so that $P \in SL_3(\mathbb{Z})$ and $\{\boldsymbol{g}_{1m}, \boldsymbol{g}_{2m}, \boldsymbol{g}_{3m}\}\, P \equiv \{\boldsymbol{g}'_{1m}, \boldsymbol{g}'_{2m}, \boldsymbol{g}'_{3m}\}$ generates G_m by the above remarks. Then from (4.10),

$$\begin{aligned} \boldsymbol{g}'^{A}_{im} = \boldsymbol{g}^A_{jm} P_{ji} &= \boldsymbol{g}^A_{jm} Q^{-1}_{ji} \\ &= \alpha_j Q^{-1}_{ji} = \delta_{i1}, \quad i = 1,2,3, \end{aligned} \tag{4.12}$$

where (δ_{ij}) is the Krönecker delta, and the result follows. □

To facilitate some of the following calculations, we introduce the notation

$$\boldsymbol{h}^{\boldsymbol{p}} = \boldsymbol{p}^{-1}\boldsymbol{h}\boldsymbol{p}, \quad \boldsymbol{h}, \boldsymbol{p} \in G, \tag{4.13}$$

for the conjugate of an element $\boldsymbol{h} \in G$. Then we have:

$$(\boldsymbol{x}^{\boldsymbol{y}})^{\boldsymbol{z}} = \boldsymbol{x}^{(\boldsymbol{y}\boldsymbol{z})},\ (\boldsymbol{x}\boldsymbol{y})^{\boldsymbol{z}} = \boldsymbol{x}^{\boldsymbol{z}}\boldsymbol{y}^{\boldsymbol{z}},\ (\boldsymbol{x}^{\boldsymbol{y}})^{-1} = \left(\boldsymbol{x}^{-1}\right)^{\boldsymbol{y}},\ \boldsymbol{x}^{\boldsymbol{x}^{-1}\boldsymbol{y}} = \boldsymbol{x}^{\boldsymbol{y}},\ (\boldsymbol{x}, \boldsymbol{y})^{\boldsymbol{z}} = (\boldsymbol{x}^{\boldsymbol{z}}, \boldsymbol{y}^{\boldsymbol{z}})\,, \tag{4.14}$$

for $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z} \in G$.

We define

$$\boldsymbol{x}^{n\boldsymbol{y}} \equiv (\boldsymbol{x}^n)^{\boldsymbol{y}} = (\boldsymbol{x}^{\boldsymbol{y}})^n,\ n \in \mathbb{Z}, \boldsymbol{x}, \boldsymbol{y} = G.$$

Also, for example,

$$\begin{aligned} (\boldsymbol{x}, \boldsymbol{z})^{\boldsymbol{y}\boldsymbol{x}} \left(\boldsymbol{y}^{-1}, \boldsymbol{x}\right)^{\boldsymbol{y}^{\boldsymbol{x}}} &= (\boldsymbol{x}, \boldsymbol{z}\boldsymbol{y})\,, \quad \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z} \in G; \\ (\boldsymbol{x}^m, \boldsymbol{y}) &= \prod_{j=1}^{m} (\boldsymbol{x}, \boldsymbol{y})^{\boldsymbol{x}^{m-j}}\,, \quad \boldsymbol{x}, \boldsymbol{y} \in G,\ m \in \mathbb{Z}_{>0}; \\ (\boldsymbol{x}, \boldsymbol{y}^m) &= \prod_{j=1}^{m} (\boldsymbol{x}, \boldsymbol{y})^{\boldsymbol{y}^{m-j}}\,, \quad \boldsymbol{x}, \boldsymbol{y} \in G,\ m \in \mathbb{Z}_{>0}; \end{aligned} \tag{4.15}$$

Now commutators commute in G, and since $(\boldsymbol{x}, \boldsymbol{y})^{\boldsymbol{z}} = (\boldsymbol{x}^{\boldsymbol{z}}, \boldsymbol{y}^{\boldsymbol{z}})$, terms of the form $(\boldsymbol{x}, \boldsymbol{y})^{\boldsymbol{z}}$ also commute in G, $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z} \in G$. Furthermore

(i) $\left(\boldsymbol{x}^{-1}, \boldsymbol{y}\right) = (\boldsymbol{x}, \boldsymbol{y})^{-\boldsymbol{x}^{-1}}\,,\ \left(\boldsymbol{x}, \boldsymbol{y}^{-1}\right) = (\boldsymbol{x}, \boldsymbol{y})^{-\boldsymbol{y}^{-1}}\,,\ \left(\boldsymbol{x}^{-1}, \boldsymbol{y}^{-1}\right) = (\boldsymbol{x}, \boldsymbol{y})^{\boldsymbol{x}^{-1}\boldsymbol{y}^{-1}}\,,\ \boldsymbol{x}, \boldsymbol{y}, \in G;$

(ii)
$$\begin{aligned} (\boldsymbol{x}, \boldsymbol{y})^{\boldsymbol{w}\boldsymbol{z}} &= (\boldsymbol{x}, \boldsymbol{y})^{(\boldsymbol{w}^{-1}, \boldsymbol{z}^{-1})\boldsymbol{z}\boldsymbol{w}} \\ &= (\boldsymbol{z}\boldsymbol{w})^{-1}(\boldsymbol{w}^{-1}, \boldsymbol{z}^{-1})^{-1}(\boldsymbol{x}, \boldsymbol{y})(\boldsymbol{w}^{-1}, \boldsymbol{z}^{-1})\boldsymbol{z}\boldsymbol{w} \\ &= (\boldsymbol{x}, \boldsymbol{y})^{\boldsymbol{z}\boldsymbol{w}}, \quad \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}, \boldsymbol{w} \in G, \end{aligned}$$

since $(\boldsymbol{w}^{-1}, \boldsymbol{z}^{-1})^{-1}$ is a commutator.

So one can define $(\boldsymbol{x}, \boldsymbol{y})^P$, where P is a polynomial with integer coefficients in the generators of $G = gp(\boldsymbol{g}_1, \boldsymbol{g}_2, \boldsymbol{g}_3)$, and their inverses, as follows. Let P be written (uniquely) in the form $P = \sum_{\boldsymbol{\alpha}} \varepsilon_{\boldsymbol{\alpha}} p_{\boldsymbol{\alpha}}$, where $\varepsilon_{\boldsymbol{\alpha}}$ is nonzero only for a finite number of choices of multi-index $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$, $\varepsilon_{\boldsymbol{\alpha}} \in \mathbb{Z}, \alpha_1, \alpha_2, \alpha_3 \in \mathbb{Z}$, where $p_{\boldsymbol{\alpha}} \equiv \boldsymbol{g}_1^{\alpha_1} \boldsymbol{g}_2^{\alpha_2} \boldsymbol{g}_3^{\alpha_3}$, and let $P' = \sum_{\boldsymbol{\alpha}} \varepsilon'_{\boldsymbol{\alpha}} p'_{\boldsymbol{\alpha}}$ be similarly defined. Then put

$$(\boldsymbol{x}, \boldsymbol{y})^P = \prod_{\boldsymbol{\alpha}} (\boldsymbol{x}, \boldsymbol{y})^{\varepsilon_{\boldsymbol{\alpha}} p_{\boldsymbol{\alpha}}}, \tag{4.16}$$

and also put

$$\{(\boldsymbol{x}, \boldsymbol{y})^P\}^{P'} = \prod_{\boldsymbol{\alpha}'} \left\{(\boldsymbol{x}, \boldsymbol{y})^P\right\}^{\varepsilon'_{\boldsymbol{\alpha}} p'_{\boldsymbol{\alpha}}}. \tag{4.17}$$

It is straightforward to show that, with these definitions,

$$\begin{aligned} &(\boldsymbol{x}, \boldsymbol{y})^{nP} = \{(\boldsymbol{x}, \boldsymbol{y})^n\}^P = \{(\boldsymbol{x}, \boldsymbol{y})^P\}^n, \\ &(\boldsymbol{x}, \boldsymbol{y})^P (\boldsymbol{x}, \boldsymbol{y})^{P'} = (\boldsymbol{x}, \boldsymbol{y})^{P+P'}, \\ &\{(\boldsymbol{x}, \boldsymbol{y})^P\}^{P'} = \{(\boldsymbol{x}, \boldsymbol{y})^{P'}\}^P = (\boldsymbol{x}, \boldsymbol{y})^{PP'}. \end{aligned} \tag{4.18}$$

Lemma 2. *Let $\boldsymbol{g}$ be arbitrary element of $G = gp(\boldsymbol{g}_1, \boldsymbol{g}_2, \boldsymbol{g}_3)$. Then $\boldsymbol{g}$ can be written in the form*

$$\boldsymbol{g}_1^{\alpha} \boldsymbol{g}_2^{\beta} \boldsymbol{g}_3^{\gamma} (\boldsymbol{g}_1, \boldsymbol{g}_2)^{P_3} (\boldsymbol{g}_2, \boldsymbol{g}_3)^{P_1} (\boldsymbol{g}_3, \boldsymbol{g}_1)^{P_2}, \tag{4.19}$$

where P_1, P_2, P_3 are polynomials in $\boldsymbol{g}_1, \boldsymbol{g}_2, \boldsymbol{g}_3$ and their inverses.

Proof

Any non trivial $\boldsymbol{g} \in G$ can be written in the form

$$\boldsymbol{g} = \boldsymbol{g}_1^{\varepsilon_1} \boldsymbol{g}_2^{\nu_1} \boldsymbol{g}_3^{\mu_1} \cdots \boldsymbol{g}_1^{\varepsilon_r} \boldsymbol{g}_2^{\nu_r} \boldsymbol{g}_3^{\mu_r} \tag{4.20}$$

for $\varepsilon_i, \nu_i, \mu_i \in \{0, -1, 1\},\ i = 1 \ldots r$, r a positive integer. We proceed by induction on r. Note that the lemma holds in the case $r = 1$, and suppose that it also holds for $r \leq k-1$. Then

$$\boldsymbol{g} = \boldsymbol{g}_1^{\varepsilon_1} \boldsymbol{g}_2^{\nu_1} \boldsymbol{g}_3^{\mu_1} \cdots \boldsymbol{g}_1^{\varepsilon_k} \boldsymbol{g}_2^{\nu_k} \boldsymbol{g}_3^{\mu_k} = \boldsymbol{g}_1^{\varepsilon_1} \boldsymbol{g}_2^{\nu_1} \boldsymbol{g}_3^{\mu_1} \left(\boldsymbol{g}_1^{\alpha'} \boldsymbol{g}_2^{\beta'} \boldsymbol{g}_3^{\gamma'} (\boldsymbol{g}_1, \boldsymbol{g}_2)^{P'_3} (\boldsymbol{g}_2, \boldsymbol{g}_3)^{P'_1} (\boldsymbol{g}_3, \boldsymbol{g}_1)^{P'_2} \right) \tag{4.21}$$

where $\alpha' = \varepsilon_2 + \cdots + \varepsilon_k$, etc. Noting that terms of the form $(\boldsymbol{x}, \boldsymbol{y})^{\boldsymbol{z}}$, and therefore terms of the form $(\boldsymbol{x}, \boldsymbol{y})^P$, commute and also that $(\boldsymbol{x}, \boldsymbol{y})\, \boldsymbol{z} = \boldsymbol{z}\, (\boldsymbol{x}, \boldsymbol{y})^{\boldsymbol{z}}$ this can be rearranged as follows:

$$\begin{aligned} \boldsymbol{g} &= \boldsymbol{g}_1^{\varepsilon_1} \boldsymbol{g}_2^{\nu_1} \boldsymbol{g}_3^{\mu_1} \left(\boldsymbol{g}_1^{\alpha'} \boldsymbol{g}_2^{\beta'} \boldsymbol{g}_3^{\gamma'} (\boldsymbol{g}_1, \boldsymbol{g}_2)^{P'_3} (\boldsymbol{g}_2, \boldsymbol{g}_3)^{P'_1} (\boldsymbol{g}_3, \boldsymbol{g}_1)^{P'_2} \right) \\ &= \boldsymbol{g}_1^{\varepsilon_1} \boldsymbol{g}_2^{\nu_1} \boldsymbol{g}_1^{\alpha'} \boldsymbol{g}_3^{\mu_1} (\boldsymbol{g}_3^{\mu_1}, \boldsymbol{g}_1^{\alpha'}) \boldsymbol{g}_2^{\beta'} \boldsymbol{g}_3^{\gamma'} (\boldsymbol{g}_1, \boldsymbol{g}_2)^{P'_3} (\boldsymbol{g}_2, \boldsymbol{g}_3)^{P'_1} (\boldsymbol{g}_3, \boldsymbol{g}_1)^{P'_2} \\ &= \boldsymbol{g}_1^{\varepsilon_1} \boldsymbol{g}_2^{\nu_1} \boldsymbol{g}_1^{\alpha'} \boldsymbol{g}_3^{\mu_1} \boldsymbol{g}_2^{\beta'} \boldsymbol{g}_3^{\gamma'} (\boldsymbol{g}_1, \boldsymbol{g}_2)^{P'_3} (\boldsymbol{g}_2, \boldsymbol{g}_3)^{P'_1} (\boldsymbol{g}_3, \boldsymbol{g}_1)^{P'_2} (\boldsymbol{g}_3^{\mu_1}, \boldsymbol{g}_1^{\alpha'})^{\boldsymbol{g}_2^{\beta'} \boldsymbol{g}_3^{\gamma'}} \\ &= \boldsymbol{g}_1^{\varepsilon_1 + \alpha'} \boldsymbol{g}_2^{\nu_1 + \beta'} \boldsymbol{g}_3^{\mu_1 + \gamma'} (\boldsymbol{g}_1, \boldsymbol{g}_2)^{P'_3} (\boldsymbol{g}_2^{\nu_1}, \boldsymbol{g}_1^{\alpha'})^{\boldsymbol{g}_2^{\beta'} \boldsymbol{g}_3^{\mu_1 + \gamma'}} (\boldsymbol{g}_2, \boldsymbol{g}_3)^{P'_1} (\boldsymbol{g}_3^{\mu_1}, \boldsymbol{g}_2^{\beta'})^{\boldsymbol{g}_3^{\gamma'}} (\boldsymbol{g}_3, \boldsymbol{g}_1)^{P'_2} (\boldsymbol{g}_3^{\mu_1}, \boldsymbol{g}_1^{\alpha'})^{\boldsymbol{g}_2^{\beta'} \boldsymbol{g}_3^{\gamma'}} \end{aligned}$$

Next, observe that the commutator $(\boldsymbol{g}_2^{\nu_1},\boldsymbol{g}_1^{\alpha'})^{\boldsymbol{g}_2^{\beta'}\boldsymbol{g}_3^{\mu_1+\gamma'}}$ is the identity if $\nu_1=0$, and if $\nu_1=\pm 1$ then using point (ii) above and (4.15) it can be rewritten as

$$(\boldsymbol{g}_2^{\nu_1},\boldsymbol{g}_1^{\alpha'})^{\boldsymbol{g}_2^{\beta'}\boldsymbol{g}_3^{\mu_1+\gamma'}} = \begin{cases} (\boldsymbol{g}_2,\boldsymbol{g}_1^{\alpha'})^{\boldsymbol{g}_2^{\beta'}\boldsymbol{g}_3^{\mu_1+\gamma'}} = \prod_{j=1}^{\alpha'}(\boldsymbol{g}_2,\boldsymbol{g}_1)^{\boldsymbol{g}_1^{\alpha'-j}\boldsymbol{g}_2^{\beta'}\boldsymbol{g}_3^{\mu_1+\gamma'}} & \text{when } \nu_1=1,\ \alpha'>0,\\ (\boldsymbol{g}_1^{-\alpha'},\boldsymbol{g}_2)^{\boldsymbol{g}_1^{\alpha'}\boldsymbol{g}_2^{\beta'}\boldsymbol{g}_3^{\mu_1+\gamma'}} = \prod_{j=1}^{-\alpha'}(\boldsymbol{g}_1,\boldsymbol{g}_2)^{\boldsymbol{g}_1^{-j}\boldsymbol{g}_2^{\beta'}\boldsymbol{g}_3^{\mu_1+\gamma'}} & \text{when } \nu_1=1,\ \alpha'<0,\\ (\boldsymbol{g}_1^{\alpha'},\boldsymbol{g}_2)^{\boldsymbol{g}_2^{\beta'-1}\boldsymbol{g}_3^{\mu_1+\gamma'}} = \prod_{j=1}^{\alpha'}(\boldsymbol{g}_1,\boldsymbol{g}_2)^{\boldsymbol{g}_1^{\alpha'-j}\boldsymbol{g}_2^{\beta'-1}\boldsymbol{g}_3^{\mu_1+\gamma'}} & \text{when } \nu_1=-1,\ \alpha'>0,\\ (\boldsymbol{g}_2,\boldsymbol{g}_1^{-\alpha'})^{\boldsymbol{g}_1^{\alpha'}\boldsymbol{g}_2^{\beta'-1}\boldsymbol{g}_3^{\mu_1+\gamma'}} = \prod_{j=1}^{-\alpha'}(\boldsymbol{g}_2,\boldsymbol{g}_1)^{\boldsymbol{g}_1^{-j}\boldsymbol{g}_2^{\beta'-1}\boldsymbol{g}_3^{\mu_1+\gamma'}} & \text{when } \nu_1=-1,\ \alpha'<0. \end{cases}$$

Hence $(\boldsymbol{g}_2^{\nu_1},\boldsymbol{g}_1^{\alpha'})^{\boldsymbol{g}_2^{\beta'}\boldsymbol{g}_3^{\mu_1+\gamma'}} = (\boldsymbol{g}_1,\boldsymbol{g}_2)^{Q_3}$ where Q_3 is the polynomial given by

$$Q_3 = \begin{cases} \sum_{j=1}^{\alpha'} -\boldsymbol{g}_1^{\alpha'-j}\boldsymbol{g}_2^{\beta'}\boldsymbol{g}_3^{\mu_1+\gamma'} & \text{when } \nu_1=1,\ \alpha'>0,\\ \sum_{j=1}^{-\alpha'} \boldsymbol{g}_1^{-j}\boldsymbol{g}_2^{\beta'}\boldsymbol{g}_3^{\mu_1+\gamma'} & \text{when } \nu_1=1,\ \alpha'<0,\\ \sum_{j=1}^{\alpha'} \boldsymbol{g}_1^{\alpha'-j}\boldsymbol{g}_2^{\beta'-1}\boldsymbol{g}_3^{\mu_1+\gamma'} & \text{when } \nu_1=-1,\ \alpha'>0,\\ \sum_{j=1}^{-\alpha'} -\boldsymbol{g}_1^{-j}\boldsymbol{g}_2^{\beta'-1}\boldsymbol{g}_3^{\mu_1+\gamma'} & \text{when } \nu_1=-1,\ \alpha'<0. \end{cases}$$

Similarly, one can rewrite the commutators $(\boldsymbol{g}_3^{\mu_1},\boldsymbol{g}_2^{\beta'})^{\boldsymbol{g}_3^{\gamma'}}$ and $(\boldsymbol{g}_3^{\mu_1},\boldsymbol{g}_1^{\alpha'})^{\boldsymbol{g}_2^{\beta'}\boldsymbol{g}_3^{\gamma'}}$ as terms of the form $(\boldsymbol{g}_2,\boldsymbol{g}_3)^{Q_1}$ and $(\boldsymbol{g}_3,\boldsymbol{g}_1)^{Q_2}$ respectively where Q_1,Q_2 are polynomials in $\boldsymbol{g}_1,\boldsymbol{g}_2,\boldsymbol{g}_3$ and their inverses, computed in the same way as Q_3 above. So from (4.20) we have

$$\begin{aligned} \boldsymbol{g} &= \boldsymbol{g}_1^{\varepsilon_1+\alpha'}\boldsymbol{g}_2^{\nu_1+\beta'}\boldsymbol{g}_3^{\mu_1+\gamma'}(\boldsymbol{g}_1,\boldsymbol{g}_2)^{P_3'}(\boldsymbol{g}_1,\boldsymbol{g}_2)^{Q_3}(\boldsymbol{g}_2,\boldsymbol{g}_3)^{P_1'}(\boldsymbol{g}_2,\boldsymbol{g}_3)^{Q_1}(\boldsymbol{g}_3,\boldsymbol{g}_1)^{P_2'}(\boldsymbol{g}_3,\boldsymbol{g}_1)^{Q_2}\\ &= \boldsymbol{g}_1^{\varepsilon_1+\alpha'}\boldsymbol{g}_2^{\nu_1+\beta'}\boldsymbol{g}_3^{\mu_1+\gamma'}(\boldsymbol{g}_1,\boldsymbol{g}_2)^{P_3'+Q_3}(\boldsymbol{g}_2,\boldsymbol{g}_3)^{P_1'+Q_1}(\boldsymbol{g}_3,\boldsymbol{g}_1)^{P_2'+Q_2} \end{aligned}$$

which is in the form (4.19), where $\alpha=\varepsilon_1+\alpha'=\varepsilon_1+\varepsilon_2+\ldots\varepsilon_k$, $P_3=P_3'+Q_3$ etc. This proves the lemma. $\square$

Corrollary 3. *Let $\boldsymbol{g}'\in G'\equiv(G,G)$. Then $\boldsymbol{g}'$ can be written in the form*

$$(g_1,g_2)^{P_3}(g_2,g_3)^{P_1}(g_3,g_1)^{P_2}, \tag{4.22}$$

which is a product of terms of the form

$$(\boldsymbol{g}_i,\boldsymbol{g}_j)^{\boldsymbol{g}_1^{\alpha}\boldsymbol{g}_2^{\beta}\boldsymbol{g}_3^{\gamma}},\quad \alpha,\beta,\gamma\in\mathbb{Z},\quad i,j=1,2,3. \tag{4.23}$$

Proof

That $\boldsymbol{g}'$ can be written in the form (4.22) follows immediately from the proof of the lemma since $\alpha=\beta=\gamma=0$, when $\boldsymbol{g}'$ is a commutator. That $\boldsymbol{g}'$ can be written in the form (4.23) follows from the definition (4.16) and $(\boldsymbol{g}_i,\boldsymbol{g}_j)^{-1}=(\boldsymbol{g}_j,\boldsymbol{g}_i)$. $\square$

5 Generators of G'

Let $\boldsymbol{g}_i \in D,\ i = 1,2,3,$, let $\boldsymbol{g}_{im} \equiv r_m(\boldsymbol{g}_i),\ i = 1,2,3$, and suppose that (4.2) holds. Then

$$\begin{aligned} \boldsymbol{g}_i = r_m^{-1}(\boldsymbol{g}_{im}) &= r_m^{-1}\left(A^{\alpha_i} B^{\beta_i} C^{\gamma_i}\right) \\ &= r_m^{-1}\left(\begin{array}{cc|cc} \multicolumn{2}{c|}{\phi(\alpha_i)} & \begin{matrix} 0 \\ 0 \end{matrix} & \phi(\alpha_i)\begin{pmatrix} \beta_i \\ \gamma_i \end{pmatrix} \\ \hline 0 & 0 & 1 & \alpha_i \\ 0 & 0 & 0 & 1 \end{array}\right), \end{aligned} \tag{5.1}$$

according to (3.9) with no summation over i. So

$$\boldsymbol{g}_i = \begin{pmatrix} \theta^{\alpha_i}\begin{pmatrix} \beta_i \\ \gamma_i \end{pmatrix} \\ \alpha_i \end{pmatrix}, \tag{5.2}$$

since $\phi(\alpha_i) = (\phi(1))^{\alpha_1} \equiv \theta^{\alpha_i},\ \alpha_i \in \mathbb{Z}$.

So from (2.22)

$$\boldsymbol{\psi}(\boldsymbol{g}_i, \boldsymbol{g}_j) \equiv \begin{pmatrix} \theta^{(\alpha_i+\alpha_j)}\left(\theta^{-\alpha_j}\begin{pmatrix} \beta_i \\ \gamma_i \end{pmatrix} + \begin{pmatrix} \beta_j \\ \gamma_j \end{pmatrix}\right) \\ \alpha_i + \alpha_j \end{pmatrix}. \tag{5.3}$$

One calculates that $\boldsymbol{g}_i^{-1} = -\boldsymbol{g}_i$, and also that

$$\begin{aligned} \boldsymbol{g}_j^{-1}\boldsymbol{g}_i\boldsymbol{g}_j &= \begin{pmatrix} (\theta^{\alpha_i} - \mathbb{I}_2)\begin{pmatrix} \beta_j \\ \gamma_j \end{pmatrix} + \theta^{\alpha_i-\alpha_j}\begin{pmatrix} \beta_i \\ \gamma_i \end{pmatrix} \\ \alpha_i \end{pmatrix}, \\ (\boldsymbol{g}_i, \boldsymbol{g}_j) &= \begin{pmatrix} (\theta^{-\alpha_j} - \mathbb{I}_2)\begin{pmatrix} \beta_i \\ \gamma_i \end{pmatrix} - (\theta^{-\alpha_i} - \mathbb{I}_2)\begin{pmatrix} \beta_j \\ \gamma_j \end{pmatrix} \\ 0 \end{pmatrix}, \\ \boldsymbol{g}_j^{-1}\boldsymbol{g}_i\boldsymbol{g}_j &= \boldsymbol{g}_i + \theta^{\alpha_i}\left(\boldsymbol{g}_i, \boldsymbol{g}_j\right). \end{aligned} \tag{5.4}$$

Now it follows from Corollary 3 that G' is generated by $(\boldsymbol{g}_i, \boldsymbol{g}_j)^{\boldsymbol{h}}$, for all $\boldsymbol{h}$ of the form $\boldsymbol{g}_1^{\alpha}\boldsymbol{g}_2^{\beta}\boldsymbol{g}_3^{\gamma}$, $\alpha, \beta, \gamma \in \mathbb{Z}$. Also from $(5.4)_3$,

$$\begin{aligned} \left(\boldsymbol{g}_i, \boldsymbol{g}_j\right)^{\boldsymbol{h}} &= \boldsymbol{h}^{-1}(\boldsymbol{g}_i, \boldsymbol{g}_j)\boldsymbol{h} \\ &= (\boldsymbol{g}_i, \boldsymbol{g}_j) + \left((\boldsymbol{g}_i, \boldsymbol{g}_j), \boldsymbol{h}\right), \end{aligned} \tag{5.5}$$

noting that $r_m\left((\boldsymbol{g}_i, \boldsymbol{g}_j)\right) = B^{\beta}C^{\gamma}$, for some $\beta, \gamma \in \mathbb{Z}$.

So from $(5.4)_2$,

$$\begin{aligned}(\boldsymbol{g}_i, \boldsymbol{g}_j)^{\boldsymbol{h}} &= (\boldsymbol{g}_i, \boldsymbol{g}_j) + \left(\theta^{-h_3} - \mathbb{I}_2\right)(\boldsymbol{g}_i, \boldsymbol{g}_j) \\ &= \theta^{-h_3}(\boldsymbol{g}_i, \boldsymbol{g}_j),\end{aligned} \tag{5.6}$$

where h_3 is found as the exponent of A in the expression for $r_m(\boldsymbol{h})$:

$$\boldsymbol{g}_{1m}^{\alpha}\boldsymbol{g}_{2m}^{\beta}\boldsymbol{g}_{3m}^{\gamma} = \left(A^{\alpha_1}B^{\beta_1}C^{\gamma_1}\right)^{\alpha}\left(A^{\alpha_2}B^{\beta_2}C^{\gamma_2}\right)^{\beta}\left(A^{\alpha_3}B^{\beta_3}C^{\gamma_3}\right)^{\gamma}. \tag{5.7}$$

Hence

$$h_3 = \alpha\alpha_1 + \beta\alpha_2 + \gamma\alpha_3. \tag{5.8}$$

Since $\alpha_1, \alpha_2, \alpha_3$ are relatively prime, h_3 assumes all integer values as α, β, γ range over $\mathbb{Z}$.

Lemma 4.

$$G' = \left\langle(\boldsymbol{g}_i, \boldsymbol{g}_j), \theta(\boldsymbol{g}_i, \boldsymbol{g}_j);\ i<j,\ i,j = 1,2,3\right\rangle \tag{5.9}$$

Proof

First $\boldsymbol{\psi}(\boldsymbol{a}, \boldsymbol{b}) = \boldsymbol{a} + \boldsymbol{b},\ \boldsymbol{a}, \boldsymbol{b} \in G'$. By the preceding remarks, G' consists of all integer linear combinations of $\theta^h(\boldsymbol{g}_i, \boldsymbol{g}_j)$, $i, j, \in 1,2,3, h \in \mathbb{Z}$. From (3.6)

$$\theta^h = U_h\theta - U_{h-1}\mathbb{I}_2, \quad h \in \mathbb{Z}, \tag{5.10}$$

and $U_h \in \mathbb{Z}$ for all $h \in \mathbb{Z}$. Since $(\boldsymbol{g}_i, \boldsymbol{g}_j)^{-1} = (\boldsymbol{g}_j, \boldsymbol{g}_i) = -(\boldsymbol{g}_i, \boldsymbol{g}_j)$, the result follows. □

Recall that, according to Lemma 1, $G = gp(\boldsymbol{g}_1, \boldsymbol{g}_2, \boldsymbol{g}_3)$ has a set of generators $\{\boldsymbol{g}_1', \boldsymbol{g}_2', \boldsymbol{g}_3'\}$ such that $\boldsymbol{g}_{im}' \equiv r_m(\boldsymbol{g}_i')$, $i = 1,2,3$ have the form (4.6). We deal with sets of generators of G of this form henceforward, and write (dropping the primes),

$$\boldsymbol{g}_{1m} = AB^{\beta_1}C^{\gamma_1}, \boldsymbol{g}_{2m} = B^{\beta_2}C^{\gamma_2},\ \boldsymbol{g}_{3m} = B^{\beta_3}C^{\gamma_3}. \tag{5.11}$$

Then from (5.4):

$$(\boldsymbol{g}_1, \boldsymbol{g}_k) = -\begin{pmatrix} (\theta^{-1} - \mathbb{I}_2)\begin{pmatrix}\beta_k \\ \gamma_k\end{pmatrix} \\ 0 \end{pmatrix}, \quad k = 2,3; \quad (\boldsymbol{g}_2, \boldsymbol{g}_3) = \boldsymbol{0}. \tag{5.12}$$

So from Lemma 4, with generators of G_m chosen in the form (4.6),

$$G' = \langle \boldsymbol{a}, \boldsymbol{b}, \theta\boldsymbol{a}, \theta\boldsymbol{b}\rangle, \tag{5.13}$$

where $\boldsymbol{a} \equiv (\boldsymbol{g}_1, \boldsymbol{g}_2)$, $\boldsymbol{b} \equiv (\boldsymbol{g}_1, \boldsymbol{g}_3)$.

6 Necessary and sufficient conditions that $G = D$

6.1 Conditions that $G' = D'$

From §3.3, $D' = \langle (\theta^{-1} - \mathbb{I}_2)\, \boldsymbol{e}_1, (\theta^{-1} - \mathbb{I}_2)\boldsymbol{e}_2 \rangle$, and from §5,

$$G' = \left\langle (\theta^{-1} - \mathbb{I}_2) \begin{pmatrix} \beta_2 \\ \gamma_2 \end{pmatrix},\ (\theta^{-1} - \mathbb{I}_2) \begin{pmatrix} \beta_3 \\ \gamma_3 \end{pmatrix},\ \theta(\theta^{-1} - \mathbb{I}_2) \begin{pmatrix} \beta_2 \\ \gamma_2 \end{pmatrix},\ \theta(\theta^{-1} - \mathbb{I}_2) \begin{pmatrix} \beta_3 \\ \gamma_3 \end{pmatrix} \right\rangle. \tag{6.1}$$

Define $\boldsymbol{\tau}_1, \boldsymbol{\tau}_2, \boldsymbol{\tau}_3, \boldsymbol{\tau}_4 \in \mathbb{Z}^2$ by

$$\boldsymbol{\tau}_1 = \begin{pmatrix} \beta_2 \\ \gamma_2 \end{pmatrix}, \boldsymbol{\tau}_2 = \begin{pmatrix} \beta_3 \\ \gamma_3 \end{pmatrix}, \boldsymbol{\tau}_3 = \theta \begin{pmatrix} \beta_2 \\ \gamma_2 \end{pmatrix}, \boldsymbol{\tau}_4 = \theta \begin{pmatrix} \beta_3 \\ \gamma_3 \end{pmatrix}. \tag{6.2}$$

Then since $(\theta^{-1} - \mathbb{I}_2)$ is non singular, it follows that $D' = G'$ if and only if

$$\langle \boldsymbol{\tau}_1, \boldsymbol{\tau}_2, \boldsymbol{\tau}_3, \boldsymbol{\tau}_4 \rangle = \langle \boldsymbol{e}_1, \boldsymbol{e}_2 \rangle. \tag{6.3}$$

To determine conditions necessary and sufficient in order that (6.3) hold, it is convenient to introduce a matrix B such that

$$\begin{pmatrix} \beta_2 & \beta_3 \\ \gamma_2 & \gamma_3 \end{pmatrix} B = \theta \begin{pmatrix} \beta_2 & \beta_3 \\ \gamma_2 & \gamma_3 \end{pmatrix}, \tag{6.4}$$

so that

$$\begin{aligned} B &= \left(\operatorname{adj} \begin{pmatrix} \beta_2 & \beta_3 \\ \gamma_2 & \gamma_3 \end{pmatrix} \right) \theta \begin{pmatrix} \beta_2 & \beta_3 \\ \gamma_2 & \gamma_3 \end{pmatrix} / \Delta \\ &\equiv \begin{pmatrix} b_1 & c_1 \\ b_2 & c_2 \end{pmatrix} / \Delta, \end{aligned} \tag{6.5}$$

where $\Delta \equiv \beta_2\gamma_3 - \beta_3\gamma_2 \in \mathbb{Z}$, where $\operatorname{adj} \begin{pmatrix} \beta_2 & \beta_3 \\ \gamma_2 & \gamma_3 \end{pmatrix} \equiv \begin{pmatrix} \gamma_3 & -\beta_3 \\ -\gamma_2 & \beta_2 \end{pmatrix}$, and the elements of $\begin{pmatrix} b_1 & c_1 \\ b_2 & c_2 \end{pmatrix}$ are integers.

From (6.3), there are integers $\lambda_i, \mu_i,\ i = 1, 2, 3, 4$ such that

$$\lambda_1\boldsymbol{\tau}_1 + \lambda_2\boldsymbol{\tau}_2 + \lambda_3\boldsymbol{\tau}_3 + \lambda_4\boldsymbol{\tau}_4 = \boldsymbol{e}_1,\ \mu_1\boldsymbol{\tau}_1 + \mu_2\boldsymbol{\tau}_2 + \mu_3\boldsymbol{\tau}_3 + \mu_4\boldsymbol{\tau}_4 = \boldsymbol{e}_2, \tag{6.6}$$

and it follows, in particular, that if we write that the components of $\boldsymbol{\tau}_i,\ i = 1, 2, 3, 4$, are $\begin{pmatrix} \tau_{1i} \\ \tau_{2i} \end{pmatrix}$ then,

$$hcf\,(\tau_{11}, \tau_{12}, \tau_{13}, \tau_{14}) = hcf\,(\tau_{21}, \tau_{22}, \tau_{23}, \tau_{24}) = 1. \tag{6.7}$$

Also from (6.3), with $\begin{pmatrix} p \\ q \end{pmatrix} \wedge \begin{pmatrix} r \\ s \end{pmatrix} \equiv ps - rq$, one sees that some integer linear combination of the quantities $\boldsymbol{\tau}_i \wedge \boldsymbol{\tau}_j,\ i < j$, equals $\boldsymbol{e}_1 \wedge \boldsymbol{e}_2 = 1$, and it follows that

$$hcf\left(\{\boldsymbol{\tau}_i \wedge \boldsymbol{\tau}_j; i < j, i, j = 1, 2, 3, 4\}\right) = 1. \tag{6.8}$$

Note that $\boldsymbol{\tau}_1 \wedge \boldsymbol{\tau}_2 = \boldsymbol{\tau}_3 \wedge \boldsymbol{\tau}_4$, since $\det \theta = 1$, and that one can re-express (6.8) as

$$hcf(b_1, b_2, c_1, c_2, \Delta) = 1, \tag{6.9}$$

after a short calculation.

Lemma 5. *Condition* (6.7) *and* (6.9) *are necessary and sufficient that* (6.3) *should hold.*

Proof

The above remarks show the necessity of (6.7) and (6.9). To prove sufficiency, note that (6.7) and (6.9) imply that the invariant factors (see Gantmacher [21]) of the two matrices

$$T \equiv \begin{pmatrix} \tau_{11} & \tau_{12} & \tau_{13} & \tau_{14} \\ \tau_{21} & \tau_{22} & \tau_{23} & \tau_{24} \end{pmatrix} \quad \text{and} \quad E \equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \tag{6.10}$$

coincide. So there exist unimodular matrices $P, Q\,(P \in SL_2(\mathbb{Z}), Q \in SL_4(\mathbb{Z}))$ such that

$$PTQ = E. \tag{6.11}$$

Hence

$$TQ = P^{-1}E. \tag{6.12}$$

Let the first two columns of Q be $(\lambda_1', \lambda_2', \lambda_3', \lambda_4')^T, (\mu_1', \mu_2', \mu_3', \mu_4')^T$. Then (6.12) gives that $\lambda_1'\boldsymbol{\tau}_1 + \lambda_2'\boldsymbol{\tau}_2 + \lambda_3'\boldsymbol{\tau}_3 + \lambda_4'\boldsymbol{\tau}_4 = \boldsymbol{p}_1^{-1}$, $\mu_1'\boldsymbol{\tau}_1 + \mu_2'\boldsymbol{\tau}_2 + \mu_3'\boldsymbol{\tau}_3 + \mu_4'\boldsymbol{\tau}_4 = \boldsymbol{p}_2^{-1}$, where $\boldsymbol{p}_1^{-1}, \boldsymbol{p}_2^{-1}$ are the first and second columns of $P^{-1} \in SL_2(\mathbb{Z})$. Since $\{\boldsymbol{p}_1^{-1}, \boldsymbol{p}_2^{-1}\}$ is a basis of $\mathbb{Z}^2$, it follows that each of $\boldsymbol{e}_1, \boldsymbol{e}_2$ is expressible as an integer linear combination of $\boldsymbol{\tau}_1, \boldsymbol{\tau}_2, \boldsymbol{\tau}_3, \boldsymbol{\tau}_4$ and this is enough to prove that (6.3) holds. $\square$

6.2 Conditions that $D \cap N = G \cap N$

In §3.4 we showed that $D \cap N = \{\mathbb{Z}^2, +\}$. From Lemma 2, if $\boldsymbol{g} \in G$, then $\boldsymbol{g}$ can be written in the form $\boldsymbol{g}_1^\alpha \boldsymbol{g}_2^\beta \boldsymbol{g}_3^\gamma (\boldsymbol{g}_1, \boldsymbol{g}_2)^{P_3} (\boldsymbol{g}_2, \boldsymbol{g}_3)^{P_1} (\boldsymbol{g}_3, \boldsymbol{g}_1)^{P_2}$. Recall that we are now dealing with generators $\boldsymbol{g}_1, \boldsymbol{g}_2, \boldsymbol{g}_3$ such that (4.6) holds, so if $\boldsymbol{g} \in G \cap N$, then $\alpha = 0$. It follows that $G \cap N$ is generated by $\boldsymbol{g}_2, \boldsymbol{g}_3$ and the generators of $G' = G' \cap N$. So, using the results of the previous section,

$$G \cap N = \left\langle \boldsymbol{\tau}_1, \boldsymbol{\tau}_2, (\theta^{-1} - \mathbb{I}_2)\boldsymbol{\tau}_1, (\theta^{-1} - \mathbb{I}_2)\boldsymbol{\tau}_2, \theta(\theta^{-1} - \mathbb{I}_2)\boldsymbol{\tau}_1, \theta(\theta^{-1} - \mathbb{I}_2)\boldsymbol{\tau}_2 \right\rangle. \tag{6.13}$$

Now since $\det\theta = 1, \theta^2 = (a+d)\theta - \mathbb{I}_2$, so $\theta = (a+d)\mathbb{I}_2 - \theta^{-1}$, and

$$\theta(\theta^{-1} - \mathbb{I}_2)\boldsymbol{\tau}_1 = \boldsymbol{\tau}_1 - \theta\boldsymbol{\tau}_1 = (\theta^{-1} - \mathbb{I}_2)\boldsymbol{\tau}_1 - (a+d-2)\boldsymbol{\tau}_1, \tag{6.14}$$

which is an integer linear combination of $\boldsymbol{\tau}_1, (\theta^{-1} - \mathbb{I}_2)\boldsymbol{\tau}_1$. It follows quickly that

$$G \cap N = \langle \boldsymbol{\tau}_1, \boldsymbol{\tau}_2, \boldsymbol{\tau}_3, \boldsymbol{\tau}_4 \rangle, \tag{6.15}$$

recalling that $\boldsymbol{\tau}_3 \equiv \theta\boldsymbol{\tau}_1$, etc.. So conditions (6.7) and (6.9), which are necessary and sufficient that $G' = D'$, are also necessary and sufficient that $G \cap N = D \cap N$.

6.3 Conditions that $G = D$

It is necessary, in order that $G = D$, that conditions (6.7) and (6.9) hold. These conditions are also sufficient for this purpose, for if they hold, then any $\boldsymbol{n} = \begin{pmatrix} r \\ s \\ 0 \end{pmatrix} \in D$ lies in $D \cap N = G \cap N$ and so is a product of elements $\boldsymbol{g}_1, \boldsymbol{g}_2, \boldsymbol{g}_3$ of the form (4.6). Note that $\boldsymbol{g}_1^\alpha = \begin{pmatrix} r' \\ s' \\ \alpha \end{pmatrix}$ for some integers r, s. Therefore $\boldsymbol{\psi}(\boldsymbol{n}, \boldsymbol{g}_1^\alpha) = \boldsymbol{n} + \boldsymbol{g}_1^\alpha$, from (2.22), is a product of elements $\boldsymbol{g}_1, \boldsymbol{g}_2, \boldsymbol{g}_3$ (and their inverses), and can be set equal to any element of $(\mathbb{Z}^3, \boldsymbol{\psi})$ by choice of the integers r, s, α, which concludes the argument.

7 Conclusion

The purpose of the calculations given in the body of the paper is to determine the symmetries that should be imposed on a continuum strain energy density per unit volume that has the constitutive form $w = w(\{\boldsymbol{\ell}_1, \boldsymbol{\ell}_2, \boldsymbol{\ell}_3\}, \mathcal{S})$. We take the point of view that the kinematical quantities $\boldsymbol{\ell}_1, \boldsymbol{\ell}_2, \boldsymbol{\ell}_3, \mathcal{S}$ that are the arguments of the strain energy determine a discrete structure whose symmetries are to transfer to the continuum strain energy (just as the symmetries of a lattice $L = \{\boldsymbol{x} : \boldsymbol{x} = n_a\boldsymbol{\ell}_a, n_a \in \mathbb{Z}, a = 1,2,3\}$ transfer to the continuum strain energy $w = w(\{\boldsymbol{\ell}_1, \boldsymbol{\ell}_2, \boldsymbol{\ell}_3\}, 0)$ of a perfect crystal). The discrete structure is a discrete subgroup of the Lie group whose structure constants $C \equiv (C_{ijk})$ are related to the dislocation density tensor $\mathcal{S}$ via (1.17), with $\boldsymbol{\ell}_r(\mathbf{0})$, $r = 1,2,3$, determined by the values of $\boldsymbol{\ell}_r$, $r = 1,2,3$. (It is a matter of choice, whether or not one interprets the given values $\boldsymbol{\ell}_1, \boldsymbol{\ell}_2, \boldsymbol{\ell}_3$ as elements in the Lie algebra $\mathfrak{g}$, so that $\boldsymbol{\ell}_r(\mathbf{0}) = \boldsymbol{\ell}_r$, $r = 1,2,3$, or interprets $\boldsymbol{\ell}_1, \boldsymbol{\ell}_2, \boldsymbol{\ell}_3$ as group generators, in which case $e^{(\boldsymbol{\ell}_r(\mathbf{0}))} = \boldsymbol{\ell}_r, r = 1,2,3$. In either case, there is a one to one correspondence between $\boldsymbol{\ell}_r(\mathbf{0})$ and

$\boldsymbol{\ell}_r$, here. We choose the latter interpretation, below, for ease of presentation). Bearing (1.17) in mind, we can rewrite the strain energy as

$$w(\{\boldsymbol{\ell}_1, \boldsymbol{\ell}_2, \boldsymbol{\ell}_3\}, \mathcal{S}) \equiv \tilde{w}(\{\boldsymbol{\ell}_1, \boldsymbol{\ell}_2, \boldsymbol{\ell}_3\}, C). \tag{7.1}$$

Thus the strain energy relates to a particular subgroup, with generators $\boldsymbol{\ell}_1, \boldsymbol{\ell}_2, \boldsymbol{\ell}_3$, of a Lie group with structure constants C. The elements of that subgroup correspond to a discrete set of points in $\mathbb{R}^3$, and it is only the relative disposition of those points in $\mathbb{R}^3$ that determines the energy (i.e. the description of the set of points in terms of Lie groups and generators does not does not affect the energy). So if kinematical quantities $\boldsymbol{\ell}'_1, \boldsymbol{\ell}'_2, \boldsymbol{\ell}'_3, C'$ lead to the same set of points, then

$$\tilde{w}(\{\boldsymbol{\ell}_1, \boldsymbol{\ell}_2, \boldsymbol{\ell}_3\}, C = \tilde{w}(\{\boldsymbol{\ell}'_1, \boldsymbol{\ell}'_2, \boldsymbol{\ell}'_3\}, C'). \tag{7.2}$$

In this paper we have dealt with a single solvable Lie group of a particular class, and implicitly decomposed tensor quantities with respect to a single basis, so in (7.2) we have $C = C'$. We have considered what different sets of generators lead to a given discrete subgroup and so shown that

$$\tilde{w}(\{\boldsymbol{\ell}_1, \boldsymbol{\ell}_2, \boldsymbol{\ell}_3\}, C) = \tilde{w}(\{\boldsymbol{\ell}'_1, \boldsymbol{\ell}'_2, \boldsymbol{\ell}'_3\}, C). \tag{7.3}$$

provided that, given generators $\{\boldsymbol{\ell}_1, \boldsymbol{\ell}_2, \boldsymbol{\ell}_3\} \equiv \{\boldsymbol{g}_1, \boldsymbol{g}_2, \boldsymbol{g}_3\}$, different generators $\{\boldsymbol{\ell}'_1, \boldsymbol{\ell}'_2, \boldsymbol{\ell}'_3\} \equiv \{\boldsymbol{g}'_1, \boldsymbol{g}'_2, \boldsymbol{g}'_3\}$ are constructed as follows:

(i) One recalls (6.2) and chooses $\begin{pmatrix} \beta_2 \\ \gamma_2 \end{pmatrix}, \begin{pmatrix} \beta_3 \\ \gamma_3 \end{pmatrix}$ such that (6.7) and (6.9) (or(6.8)) hold. This gives that $\tilde{g}_{1m} \equiv AB^{\beta_1}C^{\gamma_1}$, $\tilde{g}_{2m} \equiv B^{\beta_2}C^{\gamma_2}$, $\tilde{g}_{3m} \equiv B^{\beta_3}C^{\gamma_3}$ generate the matrix representation of the same discrete subgroup, for arbitrary β_1, γ_1;

(ii) Let $P \in SL_3(\mathbb{Z})$ be arbitrary and define $\{g'_{1m}, g'_{2m}, g'_{3m}\} \equiv \{\tilde{g}_{1m}, \tilde{g}_{2m}, \tilde{g}_{3m}\}P$, recalling (4.8). Then if $\boldsymbol{g}'_i$, $i = 1, 2, 3$, is such that $g'_{im} = r_m(\boldsymbol{g}'_i)$, $i = 1, 2, 3$, it follows that $\{\boldsymbol{g}'_1, \boldsymbol{g}'_2, \boldsymbol{g}'_3\}$ is a set of generators of the same subgroup. Moreover, all sets of generators are obtained in this way.

Finally, we have remarked in the introduction that the symmetries, (7.3) above, which guarantee that the elements of D (as points of $\mathbb{R}^3$) are preserved, may be classified according as to whether or not they are (restrictions of) elastic deformations of the continuum (or, automorphisms of the Lie group). We intend to provide the explicit classification, into elastic and inelastic symmetries, in future work.

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