RESEARCH PAPERS

Beyond Space Groups: the Arithmetic Symmetry of Deformable Multilattices

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Abstract

It is well known that the problem of classifying the symmetry of simple lattices leads to consideration of the conjugacy properties of the holohedral crystallographic point groups ('holohedries'). Classical results for the three-dimensional case then state that: (i) the *orthogonal* classification of the holohedries subdivides the simple lattices into the familiar *seven* crystal systems (this gives the 'geometric symmetry' of simple lattices); (ii) the stricter *arithmetic* classification of the holohedries subdivides the three-dimensional simple lattices into the well known *fourteen* Bravais lattice types (this gives the 'arithmetic symmetry' of simple lattices, which is more refined than the geometric one). There exists an analogous problem of studying the symmetry of the more complex periodic structures in three dimensions ('multilattices', that is, finite unions of translates of a given simple lattice), which describe in more detail the atomic lattices of the crystalline materials found in nature. In this case, the groups of affine isometries that leave a multilattice invariant, called the 'space groups', must be considered. Well known results subdivide the space groups into 219 affine conjugacy (or isomorphism) classes. This corresponds to classifying the 'geometric symmetry' of tridimensional multilattices. In crystallography, there does not exist a classical counterpart for multilattices of the above-mentioned arithmetic symmetry of simple lattices. In this paper, a natural framework is proposed in which to study the 'arithmetic symmetry of multilattices' and it is shown that the latter gives a finer classification than that based on the 219 classes of space groups, even if site symmetry is taken into account. This approach originates from the investigation of the changes of symmetry in deformable crystalline solids and proves useful for the modelling of phase transitions in crystals and related phenomena.

1. Introduction

1.1. *The symmetry of simple lattices*

A basic problem in crystallography is to describe and classify the symmetry of three-dimensional simple lattices. This question leads in a natural way to consider

the conjugacy classes, in the orthogonal group $O(3)$, of the 'crystallographic point groups', that is, of the finite subgroups of $O(3)$ leaving some simple lattice invariant.

Among the crystallographic point groups, the relevant ones for the description of the symmetry of simple lattices are the *maximal* subgroups of $O(3)$ leaving some simple lattice invariant, called the 'holohedries'. A classical result for the three-dimensional case states that there are *seven* orthogonal conjugacy classes of holohedries, called the *crystal systems*. Accordingly, the simple lattices are subdivided into seven crystal systems through the criterion that their holohedries be orthogonally conjugate. This point of view describes the 'geometric symmetry' of simple lattices.

As is well known, there is also a more refined (and equally natural) *arithmetic* classification of the holohedries, which leads to a description of the 'arithmetic symmetry' of simple lattices. The arithmetic criterion is based on the conjugacy properties of the symmetry groups within the group $GL(3, \mathbb{Z})$ of invertible 3×3 integral[1] matrices, rather than in $O(3)$. Thus, from the arithmetic point of view, two lattices are of the same type based on the fact that their symmetry groups be conjugate through an invertible *integral* matrix, that is, a matrix in $GL(3, \mathbb{Z})$ rather than one in $O(3)$.

It is a classical result that the arithmetic criterion is more stringent than the geometric one, giving rise to the *fourteen* familiar 'Bravais lattice types' within the seven crystal systems;[2] see for instance Bravais (1850), Miller (1972), Schwarzenberger (1972), Engel (1986), Sternberg (1994), Michel (1995) and Pitteri & Zanzotto (1996, 1998*a*).

In this context, it is natural to regard the space $\mathcal{B}$ of all the lattice bases, or the space $C^+(Q_3)$ of all the lattice metrics[3] as the natural *configuration spaces* of

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[1] As usual, here we denote by $\mathbb{Z}$ and $\mathbb{R}$ the sets of integral and real numbers, respectively.

[2] We recall that the different Bravais types within a given system correspond to possible different 'centerings' that exist for the primitive lattices in that system.

[3] Here $\mathcal{B}$ denotes the nine-dimensional space of all the triples of independent vectors of $\mathbb{R}^3$, and $C^+(Q_3)$ denotes the six-dimensional space (a convex cone) of all the 3×3 positive-definite symmetric real matrices.

(deformable) simple lattices – see §§2.2–2.3. Then one can see that $GL(3, \mathbb{Z})$ can be considered as the 'global symmetry group' of simple lattices, which encompasses all the crystallographic point groups, and induces a natural action on $\mathcal{B}$ or $C^+(\mathcal{Q}_3)$. In this context, the notion of arithmetic symmetry for simple lattices emerges readily by considering the action of the *finite* subgroups of $GL(3, \mathbb{Z})$ on the configuration spaces, and the lattice configurations that are invariant under such action. This makes arithmetic symmetry the natural instrument for describing and keeping track of the symmetry changes in simple lattices when their bases are deformed in the space $\mathcal{B}$. For this reason, the arithmetic symmetry proves to be very useful for the investigation of phase transitions in crystals and related phenomena.[4] For reviews of several aspects of the research in this field, see for instance Ericksen (1977, 1979, 1980, 1989, 1996), Ball & James (1987, 1992, 1998), Luskin (1996) and Pitteri & Zanzotto (1998a).

1.2. *The symmetry of multilattices*

In crystallography and physics, there is also the need to investigate the symmetry of (tridimensional) *multi-lattices*, *i.e.* of the finite unions of translates of a given simple lattice. These complex periodic structures describe in more detail the atomic lattices of the crystalline materials found in nature.[5] In the case of multilattices, one is first led to consider the groups of *affine* isometries that leave some multilattice invariant ('space groups'). Classical results subdivide such groups into 219 affine conjugacy classes (or, equivalently, isomorphism classes).[6] This corresponds to classifying the 'geometric symmetry' of multilattices.

There does not seem to exist in crystallography a counterpart for multilattices of the classical arithmetic symmetry of simple lattices mentioned in §1.1. Our aim here is to propose a framework for the investigation of the *arithmetic symmetry of (deformable) multilattices*. Analogously to the case of simple lattices, this gives a very useful tool for an accurate description of the symmetry changes and phase transitions in deformable complex crystals, as well as giving a classification of their symmetry which is *finer* than the one based on the 219 (or 230) classes of space groups (even if site-symmetry groups are taken into account).

Our approach closely follows the established treatment of arithmetic symmetry for simple lattices, which we briefly recalled in §1.1:

(*a*) First we indicate the natural 'configuration spaces' for multilattices.

(*b*) Secondly, we determine the 'global symmetry groups' of multilattices; these are suitable groups of integral matrices which generalize the global symmetry group $GL(3, \mathbb{Z})$ of simple lattices [see Pitteri (1985, 1996); see also the earlier works by Ericksen (1970) and Parry (1978) for the simplest special cases]. We then briefly describe the action of the global symmetry groups on the configuration spaces.

(*c*) Thirdly, the arithmetic symmetry of multilattices is described by means of the action of suitable *finite* subgroups of the global symmetry groups. As for simple lattices, the arithmetic symmetry proves to be a natural method for describing how a multilattice changes its symmetry while undergoing a (homogeneous) deformation.

We will see through an example that, in analogy to the case of simple lattices, also for multilattices the arithmetic symmetry is *finer* than the geometric (space-group) symmetry. The same example shows that the arithmetic symmetry is finer than the symmetry described when the 'site-symmetry groups' are also taken into account (a site-symmetry group is a subgroup of the space group whose operations stabilize a point of the multilattice).

The approach we propose originates from and proves useful in the investigation of solid-state phase transitions in crystalline materials (see for instance James, 1987; Bhattacharya *et al.*, 1993) and seems worth further study. We refer to Pitteri (1996) and Pitteri & Zanzotto (1998a,b) for further details on this and related subjects.

2. 'Geometric' and 'arithmetic' symmetries of simple lattices

This section gives some preliminary definitions and notions on the symmetry of simple lattices, a more comprehensive introduction to which can be found, for instance, in Engel (1986), Michel (1995), Pitteri & Zanzotto (1998a).

2.1. *The geometric symmetry of simple lattices and the seven crystal systems*

Let $\mathcal{L}(\mathbf{e}_a)$ be a three-dimensional simple lattice, defined by

$$\mathcal{L}(\mathbf{e}_a) = \{\mathbf{x} \in \mathbb{R}^3 : \mathbf{x} = M^a \mathbf{e}_a, \ a = 1, 2, 3, \ M^a \in \mathbb{Z}\}, \quad (1)$$

where[7] the three linearly independent vectors $\mathbf{e}_a$, $a = 1, 2, 3$, in the three-dimensional real Euclidean

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[4] That the Bravais types, and not only the crystal systems, are very significant in the phase changes of crystalline substances occurring in nature is a well known fact: for instance, one of the most important phase transformations in metallurgy, the so-called α–γ transformation in iron, is a transition of Bravais lattice type (from a body-centered cubic to a face-centered cubic structure) and not a transition of crystal system.

[5] For instance, the well known 'hexagonal close-packed' structure gives a very simple example of a multilattice that is *not* a simple lattice; also, typically, the metallic alloys have multilattice structures, as do various elements.

[6] There are 230 classes if conjugacy is sought through an orientation-preserving affine operation (*i.e.* with positive determinant).

[7] Here and in what follows, the summation convention over repeated indices will be understood.

space $\mathbb{R}^3$, are called the *lattice basis*; the positive-definite symmetric[8] matrix

$$g = g^t > 0, \quad \text{with} \quad g = (g_{ab}), \quad g_{ab} = \mathbf{e}_a \cdot \mathbf{e}_b, \quad (2)$$

is the *lattice metric*.

Given $\mathbf{e}_a$, it is classical to consider the *holohedry* $P(\mathbf{e}_a) \subset O(3)$, which is the group of orthogonal operations leaving the lattice $\mathcal{L}(\mathbf{e}_a)$ invariant:

$$P(\mathbf{e}_a) = \{\mathbf{Q} \in O(3) : \mathbf{Q}\mathcal{L}(\mathbf{e}_a) = \mathcal{L}(\mathbf{e}_a)\}. \quad (3)$$

As is well known, the holohedral subgroups of $O(3)$ are all finite groups, they all contain the central inversion, and all their elements have period 1, 2, 3, 4 or 6 ('crystallographic restriction').

Since by applying an orthogonal transformation to a simple lattice the holohedry changes by conjugacy in $O(3)$:

$$P(\mathbf{Q}\mathbf{e}_a) = \mathbf{Q}P(\mathbf{e}_a)\mathbf{Q}^t \quad \text{for} \quad \mathbf{Q} \in O(3), \quad (4)$$

the natural classification criterion for the holohedries is *orthogonal conjugacy*, which leads to the following classical result:

Theorem 1. There are *32* conjugacy classes of crystallographic point groups[9] in $O(3)$ (called *crystal classes*). Of these, the classes of holohedries, called the *crystal systems*, are *seven*.

As is well known, the crystal systems are denominated triclinic, monoclinic, orthorhombic, rhombohedral (or trigonal), tetragonal, hexagonal, and cubic.

The result above allows one to classify also the simple lattices [and, indeed, also the bases in $\mathcal{B}$ and the metrics in $\mathcal{C}^+(\mathcal{Q}_3)$] into crystal systems, each of which collects all the simple lattices whose holohedries are orthogonally equivalent.

2.2. *The global symmetry of simple lattices*

The results recalled in the preceding subsection answer the following classical question of crystallography:

(*a*) To find all the orthogonal transformations $\mathbf{Q}$ of the vector space $\mathbb{R}^3$ mapping a simple lattice $\mathcal{L}(\mathbf{e}_a)$ onto itself: $\mathbf{Q}\mathcal{L}(\mathbf{e}_a) = \mathcal{L}(\mathbf{e}_a)$.

By (1) and the linearity of $\mathbf{Q}$, this clearly amounts to finding all the transformations $\mathbf{Q}$ such that

$$\mathcal{L}(\mathbf{Q}\mathbf{e}_a) = \mathcal{L}(\mathbf{e}_a), \quad (5)$$

that is, such that the *orthogonally* transformed vectors $\mathbf{Q}\mathbf{e}_a$ are again a basis for $\mathcal{L}(\mathbf{e}_a)$. This is a special case of the following more general question:

(*b*) To find all the *linearly* transformed vectors $\mathbf{H}\mathbf{e}_a$, with $\mathbf{H}$ an invertible linear transformation, that generate $\mathcal{L}(\mathbf{e}_a)$.

Problem (*b*) is connected to the observation that a simple lattice $\mathcal{L}$ does not uniquely determine its basis or its unit cell; the indeterminacy in the choice of the lattice basis is described precisely by the following Proposition (see Ericksen, 1979; Pitteri & Zanzotto, 1998*a*):

Proposition 1. A simple lattice $\mathcal{L}(\mathbf{e}_a)$ determines its basis up to transformations in $GL(3, \mathbb{Z})$:

$$\mathcal{L}(m_a^b \mathbf{e}_b) = \mathcal{L}(\mathbf{e}_a) \Leftrightarrow m \in GL(3, \mathbb{Z}). \quad (6)$$

As recalled in the *Introduction*, $GL(3, \mathbb{Z})$ denotes the infinite discrete group of invertible 3×3 matrices with integral entries (necessarily their determinant is unimodular).

Proposition 1 states that the vectors $\mathbf{e}_a'$ form a new basis for the lattice $\mathcal{L}(\mathbf{e}_a)$ if and only if

$$\mathcal{L}(\mathbf{e}_a') = \mathcal{L}(\mathbf{e}_a) \Leftrightarrow \mathbf{e}_a' = m_a^b \mathbf{e}_b, \quad \text{with} \quad m \in GL(3, \mathbb{Z}). \quad (7)$$

Thus the invariance of all simple lattices is abstractly the same, being given by the 'global symmetry group' $GL(3, \mathbb{Z})$.

We notice that under a transformation of lattice basis as in $(7)_2$ the lattice metric transforms, in obvious notation, as

$$g' = m^t g m, \quad m \in GL(3, \mathbb{Z}). \quad (8)$$

Formulas $(7)_2$ and (8) give natural *actions* of $GL(3, \mathbb{Z})$ on the spaces $\mathcal{B}$ and $\mathcal{C}^+(\mathcal{Q}_3)$. These spaces can be considered as natural 'configuration spaces' for deformable simple lattices. The actions $(7)_2$ or (8) of $GL(3, \mathbb{Z})$, and of its finite subgroups, on $\mathcal{B}$ and $\mathcal{C}^+(\mathcal{Q}_3)$ give a classical and very natural way of studying the (changes of) symmetry in simple lattices that undergo deformations, as is described hereafter.

2.3. *The arithmetic symmetry of simple lattices and the 14 Bravais lattice types*

In view of (3) and (6), the holohedry $P(\mathbf{e}_a)$ of a lattice $\mathcal{L}(\mathbf{e}_a)$ can be equivalently defined as

$$P(\mathbf{e}_a) = \{\mathbf{Q} \in O(3) : \mathbf{Q}\mathbf{e}_a = m_a^b \mathbf{e}_b, m \in GL(3, \mathbb{Z})\}. \quad (9)$$

Then the considerations in §2.2 regarding the 'global symmetry' of simple lattices are tied to the discussion in §2.1 by considering the *lattice groups*[10] of simple lattices.

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[8] Here the symbol t indicates the transpose of a matrix or tensor, while > 0 means positive-definiteness.

[9] By definition, a 'crystallographic point group' P is a subgroup of $O(3)$ whose elements leave some simple lattice invariant. If P has this property, it is a holohedry if and only if it is the maximal group leaving a simple lattice invariant, that is, $P = P(\mathbf{e}_a)$ for some $\mathbf{e}_a$, as in (3).

[10] Also the terms *integral* or *arithmetic holohedries* are used in the literature for our lattice groups. In fact, the name 'lattice group' is used by some authors [for instance Yale (1968) and Miller (1972)] to indicate the simple lattices themselves, regarded as groups of translations of the affine space $\mathbb{A}^3$. Following Ericksen (1979), we use the term 'lattice group' because, as we will see from Theorems 2 and 3 below, these groups of integral matrices determine the Bravais *lattice* types within each system.

By definition, the lattice group $L(\mathbf{e}_a)$ of a basis $\mathbf{e}_a$ is the finite group of integral matrices appearing in (9):

$$L(\mathbf{e}_a) = \{m \in GL(3, \mathbb{Z}) : m_a^b \mathbf{e}_b = \mathbf{Q}\mathbf{e}_a, \mathbf{Q} \in O(3)\}$$
$$\subset GL(3, \mathbb{Z}). \tag{10}$$

Since they are the integral representations of the holohedries of $O(3)$ in their own lattice bases, by definition the lattice groups are the maximal finite subgroups of $GL(3, \mathbb{Z})$ acting orthogonally on a simple lattice. Some main properties of these groups are investigated for instance by Janssen (1973), Ericksen (1979), Engel (1986), Opechowski (1986), Michel (1995), Pitteri & Zanzotto (1998a).

A change of lattice basis changes the lattice group to a conjugate in $GL(3, \mathbb{Z})$:

$$L(m_a^b \mathbf{e}_b) = m^{-1} L(\mathbf{e}_a) m \quad \text{if} \quad m \in GL(3, \mathbb{Z}), \tag{11}$$

while an orthogonal transformation does not change the lattice group:

$$L(\mathbf{Q}\mathbf{e}_a) = L(\mathbf{e}_a) \quad \text{if} \quad \mathbf{Q} \in O(3). \tag{12}$$

Owing to (12), $L(\mathbf{e}_a)$ can be equivalently defined as the stabilizer of the lattice metric g in (2), that is, as the maximal subgroup of $GL(3, \mathbb{Z})$ whose elements leave g invariant under the action (8):

$$L(g) = \{m \in GL(3, \mathbb{Z}) : m^t g m = g\} = L(\mathbf{e}_a). \tag{13}$$

Because of its definition, $L(\mathbf{e}_a)$ shares with $P(\mathbf{e}_a)$ a number of properties; thus, a subgroup of $GL(3, \mathbb{Z})$ is (a subgroup of) a lattice group if and only if it is finite; all lattice groups contain the inversion $-1 \in GL(3, \mathbb{Z})$; all the matrices in a lattice group satisfy the crystallographic restriction.

The transformation law (11) for lattice groups and Proposition 1 say that a lattice $\mathcal{L}(\mathbf{e}_a)$ determines an entire *conjugacy class* in $GL(3, \mathbb{Z})$ of lattice groups, also called an *arithmetic Bravais class*[11] (see Engel, 1986). Then the natural question is how many such Bravais classes exist. It is well known that conjugacy in $GL(3, \mathbb{Z})$ is a more stringent requirement than conjugacy in $O(3)$. This means that the number of Bravais classes is greater than the number of crystal systems (seven). Indeed, a classical result in mathematical crystallography states that (compare with Theorem 1):

Theorem 2. There are 73 arithmetic classes (conjugacy classes of finite subgroups) in $GL(3, \mathbb{Z})$, among which there are 14 arithmetic Bravais classes (conjugacy classes of *lattice groups*).

See for instance Niggli & Nowacki (1935), Burckhardt (1947), Sternberg (1994), Michel (1995).

By means of the Bravais classes in $GL(3, \mathbb{Z})$ and of Theorem 2, we obtain an arithmetic criterion giving a further classification of simple lattices, of their bases and their metrics; this classification is *finer* than the geometric one based on the crystal systems discussed in §2.2. Explicitly, since, as mentioned above, to any lattice $\mathcal{L}(\mathbf{e}_a)$ corresponds by (11) a Bravais class of equivalent lattice groups, one considers as arithmetically equivalent all the bases and lattices corresponding to the *same* Bravais class. Thus, two bases $\mathbf{e}_a$ and $\mathbf{e}_a'$ in $\mathcal{B}$ (and the lattices they generate) are arithmetically equivalent if their lattice groups are such that:

$$L(\mathbf{e}_a') = m^{-1} L(\mathbf{e}_a) m \quad \text{for some} \quad m \in GL(3, \mathbb{Z}). \tag{14}$$

Bases or lattices for which (14) holds are said to have the same *Bravais lattice type* and likewise for the metrics; we thus have the following classical corollary of Theorem 2:

Theorem 3. There are 14 distinct Bravais lattice types in three dimensions.

The construction of the 14 Bravais lattice types, which are subdivided among the seven crystal systems in the known way, can be found for instance in Bravais (1850), Seitz (1935), Miller (1972), Sternberg (1994).[12]

As is also well known, the geometric meaning of Theorem 3 is connected to the possible existence of distinct 'centerings' for the 'primitive' lattices within each crystal system; as a consequence, the Bravais classes and Bravais types have classical denominations such as 'body-centered cubic' (b.c.c.), 'face-centered cubic' (f.c.c.), 'body-centered tetragonal' *etc.*[13]

2.4. *Fixed sets in the configuration spaces of simple lattices*

The first step in the analysis of the changes of lattice symmetry that may be caused by the deformation of a lattice basis is establishing for which class of deformations the 'symmetry of a lattice remains the same'. By the definitions in §2.3, this leads to studying the structure of the sets of bases [or, equivalently, of metrics –

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[11] In general, the $GL(3, \mathbb{Z})$-conjugacy class of any finite subgroup of $GL(3, \mathbb{Z})$ is called an *arithmetic class*, and the groups in it are called *arithmetically equivalent.*

[12] Sometimes the classification of simple lattices in Bravais types is based on definitions that are different from (14). For instance, lattices can be equivalently partitioned in types based on the affine equivalence of their affine symmetry groups (see also footnote 24). Pitteri & Zanzotto (1996) show that the criterion originally used by Bravais (1850) and Cauchy for classifying simple lattices is not equivalent to the one based on condition (14) and actually leads to distinguishing only 11 types of lattices.

[13] We already mentioned that the 'arithmetic symmetry' described by the lattice groups has great physical relevance. For instance, the phase transformation in iron mentioned in footnote 4 changes the crystalline structure from b.c.c. to f.c.c: in this case, the crystal system of both phases is cubic, so that the symmetry change cannot be described in terms of the holohedries, which are (orthogonally) equivalent; it can only be captured by the change in the phases' *inequivalent* lattice groups. Further classifications of simple lattices that are *finer* than the arithmetic one are discussed in detail by Gruber (1997).

see (13)] sharing the same lattice group. These subsets of the spaces $\mathcal{B}$ or $\mathcal{C}^+(\mathcal{Q}_3)$ are very important in the study of phase transitions in crystals and in this section we briefly mention some of their main properties.

Any subgroup $L \subset GL(3, \mathbb{Z})$ determines a connected set $I(L)$ in the space $\mathcal{C}^+(\mathcal{Q}_3)$, called its *fixed set*, consisting of all the metrics stabilized by the elements of L (see Ericksen, 1979; Michel, 1995; Pitteri & Zanzotto, 1998a):

$$I(L) = \{g \in \mathcal{C}^+(\mathcal{Q}_3) : m^t g m = g \quad \text{for all } m \in L\};$$
(15)

in the space $\mathcal{Q}_3$ of all symmetric 3×3 real matrices, formula (15) defines a suitable vector subspace that depends on the group L; in the space $\mathcal{C}^+(\mathcal{Q}_3)$ of positive-definite matrices formula (15) only defines a linear convex cone. In the same way, L determines an $O(3)$-invariant set in the space $\mathcal{B}$ of lattice bases, again called the fixed set of L, consisting of all the bases on which the elements of L act orthogonally:

$$E(L) = \{\mathbf{e}_a \in \mathcal{B} : (\mathbf{e}_a \cdot \mathbf{e}_b) \in I(L)\}.$$
(16)

The basic observation here is that the metrics or bases admitting a given lattice group, which belong to the *same fixed set*, all correspond by definition to lattices of the *same* Bravais symmetry type, while the metrics or bases of lattices of different type never belong to the same fixed set. Thus by analyzing the arrangement of the fixed sets we can see how a lattice changes its symmetry when undergoing a (homogeneous) deformation, that is, when a 'path' is given in the configuration space $\mathcal{B}$ [or in $\mathcal{C}^+(\mathcal{Q}_3)$] .[14]

We briefly recall here some of the main properties of the fixed sets of any subgroup of $GL(3, \mathbb{Z})$ (see Ericksen, 1979; Michel, 1995); these give useful information regarding the symmetry changes that are possible for deformable simple lattices. See also Pitteri & Zanzotto (1998a) for more details.

Proposition 2.
(i) The fixed set of a subgroup of $GL(3, \mathbb{Z})$ is nonempty if and only if the subgroup is included in a lattice group.
(ii) The fixed set of any finite subgroup of $GL(3, \mathbb{Z})$ is a linear subspace of the space $\mathcal{Q}_3$ of all symmetric 3×3

real matrices and a convex cone in the space $\mathcal{C}^+(\mathcal{Q}_3)$ of the positive-definite elements of $\mathcal{Q}_3$.

(iii) The fixed sets $I(L_1), I(L_2)$ of two finite subgroups L_1 and L_2 of $GL(3, \mathbb{Z})$ have a nonempty intersection if and only if L_1 and L_2 together generate a finite subgroup of $GL(3, \mathbb{Z})$, whose fixed set is $I(L_1) \cap I(L_2)$.

(iv) The fixed set $I(L)$ of a lattice group L contains, as a submanifold of strictly smaller dimension, the fixed set of any lattice group L' larger than L:

$$I(L') \subset I(L) \Leftrightarrow L \subset L'.$$
(17)

(v) For any lattice group $L(C)$ and any $m \in GL(3, \mathbb{Z})$, the lattice group and its fixed set transform as follows [see also (11)]:

$$L(m^t g m) = m^{-1} L(g) m$$
$$\text{and} \quad I(m^{-1} L(g) m) = m^t I(L(g)) m.$$
(18)

Analogous properties hold for the fixed sets in the space $\mathcal{B}$.

3. Multilattices and their 'geometric symmetry': space groups

3.1. *Deformable multilattices, their descriptors and their configuration spaces*

Throughout this section and the following one, we will adopt the usual Grassmann notation for the points and translation vectors in the three-dimensional real affine space $\mathbb{A}^3$; the group of all the affine transformations of $\mathbb{A}^3$ is denoted by Aff(3), and the subgroups of all the affine isometries of $\mathbb{A}^3$ and of the translational isometries are denoted by $E(3)$ and $T(3)$, respectively [$T(3)$ is of course isomorphic to $\mathbb{R}^3$].

An ideal crystal is an infinite and discrete subset $\mathcal{M}$ of points in $\mathbb{A}^3$ which admits a simple lattice of translations, say $\mathcal{L}(\mathbf{e}_a)$, mapping $\mathcal{M}$ to itself. This expresses the fact that $\mathcal{M}$ has three-dimensional 'periodicity', and implies (see Engel, 1986; Pitteri, 1990) that $\mathcal{M}$ is the *finite union* of translates of a suitable affine simple lattice $\mathcal{L}(P, \mathbf{e}_a)$, the latter being defined as

$$\mathcal{L}(P, \mathbf{e}_a) = P + \mathcal{L}(\mathbf{e}_a) \subset \mathbb{A}^3, \quad \text{with} \quad P \in \mathbb{A}^3. \quad (19)$$

Our starting point is thus the following:

Definition 1. A (monatomic) *multilattice* $\mathcal{M}$ in the affine space $\mathbb{A}^3$ is a subset of $\mathbb{A}^3$ such that

$$\mathcal{M} = \bigcup_{i=0}^{\nu} \mathcal{L}(P_i, \mathbf{e}_a) = \bigcup_{i=0}^{\nu} \{P_i + \mathcal{L}(\mathbf{e}_a)\}, \quad (20)$$

where $\mathcal{L}(\mathbf{e}_a)$ denotes a simple lattice in the translation space $\mathbb{R}^3$ of $\mathbb{A}^3$ as in (1). In (20), ν is a suitable integer and the points $P_i \in \mathcal{M}$ are all distinct and do not differ by any vector in $\mathcal{L}(\mathbf{e}_a)$.

The name '($\nu + 1$)-lattice' will be used when it is necessary to specify the number of simple lattices

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[14] It is useful to consider the six independent entries g_{ab}, $a \le b$, of a typical lattice metric $g \in \mathcal{C}^+(\mathcal{Q}_3)$ to be coordinates in the space of all symmetric 3×3 matrices and, by definition (15), describe the fixed sets of lattice groups by means of linear equations in the variables g_{ab}. For example, the fixed set of a primitive cubic basis given by three mutually orthogonal unit vectors is constituted by all the positive-definite diagonal matrices diag(g_{11}, g_{11}, g_{11}), $g_{11} > 0$, as is geometrically intuitive. In this case, the linear equations are $g_{11} = g_{22} = g_{33} > 0$, $g_{ab} = 0$ for $a < b$. Then one can study the metrics that have primitive tetragonal symmetry, such as diag(g_{11}, g_{11}, g_{22}), with $g_{11} \ne g_{22}$, and so on, with the other symmetries.

composing $\mathcal{M}$; in particular, 1-lattices are affine simple lattices.

Remark. For simplicity, in this paper, we will only consider multilattices that are monatomic as in the above definition, that is, whose points are all of the same atomic species. It is possible to extend the considerations presented here to the polyatomic case if all the constituent simple lattices carrying different atomic species have the same periodicity.

A convenient set of *descriptors* for $(v + 1)$-lattices can be defined if we choose a 'base point' in $\mathcal{M}$, for instance P_0, and introduce the v *shift vectors* or *shifts*

$$\mathbf{p}_i = P_0 P_i \quad \text{for} \quad i = 1, \ldots, v; \qquad (21)$$

the $(v + 1)$-lattice $\mathcal{M}$ is then uniquely determined by P_0 and the $v + 3$ vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{p}_1, \ldots, \mathbf{p}_v$:

$$\mathcal{M} = \mathcal{M}(P_0, \mathbf{e}_a, \mathbf{p}_1, \ldots, \mathbf{p}_v) = \bigcup_{i=0}^{v} \{P_0 + \mathbf{p}_i + \mathcal{L}(\mathbf{e}_a)\}. \qquad (22)$$

The basis and shifts satisfy the conditions

$$\mathbf{e}_1 \cdot \mathbf{e}_2 \times \mathbf{e}_3 \neq 0, \quad \mathbf{p}_i \neq l_i^a \mathbf{e}_a \quad \text{and} \quad \mathbf{p}_i \neq \mathbf{p}_j + l_{ij}^a \mathbf{e}_a, \qquad (23)$$

for $i, j = 1, \ldots, v$, $i \neq j$, and l_i^a, l_{ij}^a any integers; this guarantees that the simple lattices $\mathcal{L}(P_i, \mathbf{e}_a)$ included in $\mathcal{M}$ are three-dimensional and mutually disjoint. We will denote the above vectors by ε_σ, for $\sigma = 1, \ldots, v + 3$:

$$\varepsilon_a = \mathbf{e}_a, \quad a = 1, 2, 3 \quad \text{and} \quad \varepsilon_{3+i} = \mathbf{p}_i, \quad i = 1, \ldots, v; \qquad (24)$$

accordingly, we denote the multilattice $\mathcal{M}$ in (22) by

$$\mathcal{M}(P_0, \varepsilon_\sigma). \qquad (25)$$

The set of all $(v + 3)$-tuples of vectors of $\mathbb{R}^3$ satisfying the conditions in (23) ('multilattice descriptors') is denoted by $\mathcal{D}_{v+3}^m$, and is called the *configuration space* for deformable $(v + 1)$-lattices.[15]

The simple lattice $\mathcal{L}(\mathbf{e}_a) \subset \mathbb{R}^3$ appearing in (20) is called the *skeletal* lattice of $\mathcal{M}(P_0, \varepsilon_\sigma)$ in the given description, and its unit cell and basis are also called the *cell* and *basis* of $\mathcal{M}$ in that description. $\mathcal{L}(\mathbf{e}_a)$ can be interpreted as a group of translational isometries that map $\mathcal{M}$ onto itself. Notice that we can think of $\mathcal{M}(P_0, \varepsilon_\sigma)$ as a triply periodic distribution of congruent clusters of 'atoms', of which a representative atom is placed at each point of the base lattice $\mathcal{L}(P_0, \mathbf{e}_a)$. Such clusters create the microstructural *motif* which contributes in an essential way to the characterization of the symmetry of $\mathcal{M}$. The shifts $\mathbf{p}_i$ can be thought of as

giving the position of the atoms of the motif of $\mathcal{M}$ with respect to the representative atom. An equivalent interpretation is that the $\mathbf{p}_i$ give the displacement from the base lattice $\mathcal{L}(P_0, \mathbf{e}_a)$ of the remaining simple lattices constituting $\mathcal{M}$. For this reason, the shift vectors $\mathbf{p}_i$ are quite natural 'internal' variables in the kinematics and energetics of deformable multilattices (see Ericksen, 1970; James, 1987; Bhattacharya *et al.*, 1993; Pitteri & Zanzotto, 1998*a*).

Let $\mathcal{Q}_{v+3}$ denote the space of all symmetric $(v + 3) \times (v + 3)$ real matrices; it is useful to extend to multilattices the notion of lattice metric introduced in (2) and define the space $\mathcal{Q}_{v+3}^m \subset \mathcal{Q}_{v+3}$ of the *multilattice metrics* K:

$$K = (K_{\sigma\tau}), \quad K_{\tau\sigma} = K_{\sigma\tau} = \varepsilon_\sigma \cdot \varepsilon_\tau, \\ \sigma, \tau = 1, \ldots, v + 3, \qquad (26)$$

where the ε_σ satisfy conditions (23) and (24). An element $K \in \mathcal{Q}_{v+3}^m$ is a $(v + 3) \times (v + 3)$ symmetric matrix which is only positive semi-definite because the vectors ε_σ are not linearly independent; but not all the symmetric positive semi-definite matrices belong to $\mathcal{Q}_{v+3}^m$ because, by definition, the ε_σ in (26) must also satisfy conditions (23) and (24).

It is not difficult to see that, for any two sets of descriptors ε_σ and ε_σ' as in (23)$_1$ and (24), we have

$$K' = K \Leftrightarrow \varepsilon_\sigma' = \mathbf{Q}\varepsilon_\sigma \quad \text{for some} \quad \mathbf{Q} \in O(3). \qquad (27)$$

Owing to (27), also the space of metrics $\mathcal{Q}_{v+3}^m$ will be referred to as the configuration space of $(v + 1)$-lattices, as was the case for the space $\mathcal{C}^+(\mathcal{Q}_3)$ of simple lattice metrics, to which $\mathcal{Q}_{v+3}^m$ reduces for $v = 0$.

3.2. *Essential descriptors of multilattices*

A basic remark about the descriptive parameters $(P_0, \varepsilon_\sigma)$ of a multilattice $\mathcal{M}$ is that in (20) or (22) the number v is *not* determined by $\mathcal{M}$. This ambiguity arises because in general the skeletal lattice $\mathcal{L}(\mathbf{e}_a)$ in (20) may not describe the full translational invariance (periodicity) of $\mathcal{M}$, which is independent of the descriptors. Clearly, Definition 1 implies that there is a *maximal* lattice, that is, a maximal subgroup of translations, $\mathcal{R}$ say,[16] mapping $\mathcal{M}$ onto itself. The lattice $\mathcal{R}$ is generated by suitable maximal bases for $\mathcal{M}$, and when the latter are used in (20) or (22) the description of $\mathcal{M}$ is called *essential*. In this case, the number v of shifts as well as the volume of the elementary cells of $\mathcal{M}$ are *minimal* and no longer arbitrary, and the descriptors $\varepsilon_\sigma \in \mathcal{D}_{v+3}$ are themselves called essential for $\mathcal{M}$.

It is not difficult to see that any description with the same number of shifts as an essential description is also essential. In a non-essential description of $\mathcal{M}$, the basis only generates a sublattice of $\mathcal{R}$, and the number of

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[15] For simple lattices (1-lattices), $v = 0$ and, as mentioned at the end of §2.1, their configuration space is given by the space $\mathcal{D}_3^m = \mathcal{B}$ of all bases of $\mathbb{R}^3$.

[16] From the French word 'réseau' utilized for the maximal skeletal lattice of a multilattice.

shifts must be suitably increased to take all the lattice points of $\mathcal{M}$ into account. As an example, one can consider the (essential) lattice vectors $\mathbf{e}_a$ in Fig. 1(a), which generate a body-centered cubic 1-lattice $\mathcal{L}$. The same $\mathcal{L}$ can be described by three primitive cubic lattice vectors, $\tilde{\mathbf{e}}_a$, say, together with the shift

$$\tilde{\mathbf{p}} = \tfrac{1}{2}(\tilde{\mathbf{e}}_1 + \tilde{\mathbf{e}}_2 + \tilde{\mathbf{e}}_3) \qquad (28)$$

(see Fig. 1b). The skeletal lattice $\mathcal{L}(\tilde{\mathbf{e}}_a)$ in this case is obviously not maximal for $\mathcal{L}$ (its unit cell is twice the unit cell given by $\mathbf{e}_a$) and the descriptors $(\tilde{\mathbf{e}}_a, \mathbf{p})$ are not essential.

Non-essential descriptors must sometimes be used to model certain phase changes in crystals (for instance, they must be used in a model if it is to describe phase transitions from the body-centered cubic to the hexagonal close-packed lattice configurations, such as observed in Li, Ti, Zn or Hf (see Nishiyama, 1978, pp. 68 and 344). However, there are various problems associated with non-essential descriptors, as we analyze in Pitteri & Zanzotto (1998a); see also Ericksen (1998). Thus:

Remark. For simplicity, in this paper we will always suppose that the descriptors used for a multilattice are essential. Also, we will drop P_0 from the notation (25) whenever this does not create confusion.

3.3. Symmetry operations of multilattices

As is well known, once an origin O is chosen in the affine space $\mathbb{A}^3$, any isometry $e \in E(3)$ can be represented by a pair[17] $(\mathbf{t}, \mathbf{Q})$, where $\mathbf{t}$ is the vector from O to $e(O)$ and $\mathbf{Q} \in O(3)$. Given a multilattice $\mathcal{M}(\varepsilon_\sigma)$ in its essential description, for convenience we identify O with one of its points, say P_0.

An isometry $e \in E(3)$ mapping $\mathcal{M}$ onto itself: $e(\mathcal{M}) = \mathcal{M}$, is called a *symmetry operation* of $\mathcal{M}$. By definition, any symmetry operation $e = (\mathbf{t}, \mathbf{Q})$ of $\mathcal{M}$ produces new essential descriptors ($\bar{P}_0$ and) $\bar{\varepsilon}_\sigma$ for $\mathcal{M}$ given by

$$\bar{P}_0 = e(P_0) = P_0 + \mathbf{t}, \quad \text{and} \quad \bar{\varepsilon}_\sigma = \mathbf{Q}\varepsilon_\sigma, \qquad (29)$$

for which

$$\mathcal{M}(P_0, \varepsilon_\sigma) = \mathcal{M}(\bar{P}_0, \bar{\varepsilon}_\sigma). \qquad (30)$$

Some characteristic features of the symmetry operations of multilattices are not encountered in simple lattices. For instance, it is well known that a multilattice can admit non-trivial *screw rotations* or *glide reflections* as symmetry operations, unlike simple lattices, which only admit trivial ones whose translational component is a lattice vector. Furthermore, unlike simple lattices, multilattices may lack central symmetry.

3.4. Space groups

The *space group* of a monoatomic multilattice $\mathcal{M}$, denoted by $S(\mathcal{M})$, collects all the affine isometries mapping $\mathcal{M}$ onto itself:

$$S(\mathcal{M}) = \{e \in E(3) : e(\mathcal{M}) = \mathcal{M}\}. \qquad (31)$$

In analogy to (4), if an affine symmetry e is applied to $\mathcal{M}$, its space group $S(\mathcal{M})$ changes to a conjugate in $E(3)$:

$$S(e\mathcal{M}) = eS(\mathcal{M})e^{-1}. \qquad (32)$$

Also, the following groups are considered in connection with $\mathcal{M}$: the group

$$T(\mathcal{M}) = S(\mathcal{M}) \cap T(3) \qquad (33)$$

and the group $P(\mathcal{M})$ collecting all the the orthogonal transformations $\mathbf{Q}$ preserving $\mathcal{M}$ when coupled with a suitable translation.

Clearly, the groups $S(\mathcal{M})$, $T(\mathcal{M})$, $P(\mathcal{M})$ only depend on the lattice $\mathcal{M}$ and not on any choice of its descriptors. When essential descriptors $\varepsilon_\sigma = (\mathbf{e}_a, \mathbf{p}_i)$ of $\mathcal{M} = \mathcal{M}(\varepsilon_\sigma)$ are considered, several properties of these groups can be easily seen. For instance, since $T(\mathcal{M})$ is the abelian normal subgroup of $S(\mathcal{M})$ consisting of all the translations mapping $\mathcal{M}$ onto itself, $T(\mathcal{M})$ is isomorphic to the maximal skeletal lattice $\mathcal{R}(\mathbf{e}_a)$ of $\mathcal{M}$.

Also, owing to (47) below, one can check that the group $P(\mathcal{M})$ is in general a *non-holohedral* crystallographic point group contained in the holohedry $P(\mathbf{e}_a)$ of $\mathcal{R}(\mathbf{e}_a)$:

$$P(\mathcal{M}(\mathbf{e}_a, \mathbf{p}_i)) \subseteq P(\mathbf{e}_a). \qquad (34)$$

The group $P(\mathcal{M})$ is indeed called the *point group* of $\mathcal{M}$ and determines an orthogonal conjugacy class called the *crystal class* of the multilattice $\mathcal{M}$; since $P(\mathcal{M})$ may be non-holohedral, the class of $\mathcal{M}$ may be any one of the 32 classes[18] mentioned in Theorem 1.

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[18] Recall that simple lattices can only realise the seven holohedral crystal classes (crystal systems). Multilattices, on the other hand, do realise, in theory and in nature, all the 32 crystal classes that exist in three dimensions.
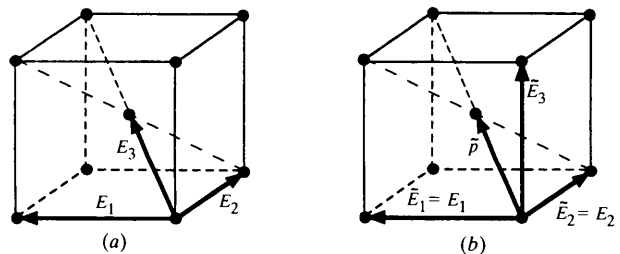

Fig. 1. (a) The basis $\mathbf{e}_a$ (essential descriptors) for the body-centered cubic simple lattice $\mathcal{L}$. (b) Non-essential descriptors $(\tilde{\mathbf{e}}_a, \tilde{\mathbf{p}})$ for the same simple lattice $\mathcal{L}$ viewed as a 2-lattice.

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[17] We follow the notational convention proposed in the Appendix to Michel (1996).

The classification criterion adopted for space groups is the natural one given by conjugacy within the affine group Aff(3) (see, for instance, Farkas, 1981; Miller, 1972; Sternberg, 1994). By a known theorem of Bieberbach (1912) stating that any two isomorphic discrete subgroups of $E(3)$ are affinely conjugate, this classification actually coincides with the classification of space groups based on group isomorphism.

The following classical result, which is an analog for multilattices of Theorem 1, was obtained at the end of the last century:

Theorem 4. There are 219 conjugacy classes of space groups within Aff(3). The number increases to 230 if conjugacy is considered only through orientation-preserving affine transformations.

Numerous descriptions of the space groups can be found in the literature: see for instance Burckhardt (1947), Janssen (1973), Sternberg (1994) or *International Tables for X-ray Crystallography* (1952); see also Miller (1972) or Senechal (1990).

As with the geometric symmetry of simple lattices in §2.1, based on the classification in crystal systems within $\mathcal{B}$ or $\mathcal{C}^+(\mathcal{Q}_3)$, it is possible to introduce an analogous subdivision into crystal classes (and systems) also for the configuration spaces $\mathcal{D}^m_{v+3}$ or $\mathcal{Q}^m_{v+3}$ of $(v+1)$ lattices.

4. The arithmetic symmetry of multilattices

In the previous section, we have briefly recalled the main facts regarding the geometric symmetry of multilattices, which is based on their classification through the affine (or isomorphism) classes of the space groups. In this section, we discuss the notion of the *arithmetic symmetry* of multilattices; this is not a classical subject of crystallography and, as mentioned in the *Introduction*, so far it has only been partially investigated.

We will follow rather closely the structure of §§2.2–2.4, where we briefly introduced the classical arithmetic symmetry of simple lattices. Thus we will seek to generalize to the case of multilattices the action of a 'global symmetry group' on a suitable 'configuration space' [in §§2.2–2.4 these were given respectively by $GL(3, \mathbb{Z})$ and $\mathcal{B}$ or $\mathcal{C}^+(\mathcal{Q}_3)$ – see $(7)_2$ and (8)].

Recall that in §3.1 we have already identified the natural configuration spaces for the deformable $(v+1)$-lattices, that is, the spaces $\mathcal{D}^m_{v+3}$ or $\mathcal{Q}^m_{v+3}$. We now indicate a natural counterpart, for $(v+1)$-lattices, of the global symmetry group $GL(3, \mathbb{Z})$ of simple lattices.

4.1. *Indeterminacy of the multilattice descriptors ε_σ and global symmetry groups of multilattices*

To the end of finding the global symmetry groups of multilattices, we give a result, see Proposition 3 below, analogous to Proposition 1 for simple lattices.

Let us first introduce the (sub)group

$$\Gamma_{v+3} \subset GL(v+3, \mathbb{Z}) \tag{35}$$

constituted by the unimodular integral $(v+3) \times (v+3)$ matrices, which, by definition, have the following structure: for $a, b = 1, 2, 3$ and $i, j = 1, \ldots, v$,

$$\mu \in \Gamma_{v+3} \Leftrightarrow (\mu^\tau_\sigma) = \left(\begin{array}{ccc|c} & m^b_a & & l^b_1 \ldots l^b_v \\ \hline 0 & 0 & 0 & \\ & \vdots & & \alpha^j_i \\ 0 & 0 & 0 & \end{array} \right), \tag{36}$$

where (m^b_a) is any matrix in $GL(3, \mathbb{Z})$, l^b_i are arbitrary integers and $\alpha = (\alpha^j_i)$ is a $v \times v$ matrix belonging to the finite non-commutative group of matrices generated by the *permutation matrices*[19] of the set $\{1, \ldots, v\}$ and by the matrices of the form

$$\left(\begin{array}{ccccc} 1 & 0 & \ldots & 0 & 0 \\ 0 & 1 & \ldots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ -1 & -1 & \ldots & -1 & -1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \ldots & 1 & 0 \\ 0 & 0 & \ldots & 0 & 1 \end{array} \right), \tag{37}$$

which are obtained from the identity by replacing one of its rows by a row of -1s. The set Γ_{v+3} introduced in (36)–(37) is indeed a subgroup of $GL(v+3, \mathbb{Z})$, as can be checked by means of a direct computation. Notice that the submatrix α of a $\mu \in \Gamma_{v+3}$ either is a permutation matrix or is a permutation matrix one of whose rows is substituted by a row of -1s.[20]

As examples, we give the explicit forms of the elements of the groups Γ_4 ($v = 1$: 2-lattices) and Γ_5 ($v = 2$: 3-lattices):

$$\Gamma_4 = \left\{ \mu = \left(\begin{array}{ccc|c} & m^a_b & & l^1 \\ & & & l^2 \\ & & & l^3 \\ \hline 0 & 0 & 0 & \alpha \end{array} \right) : m \in GL(3, \mathbb{Z}), \right.$$

$$\left. l^b \in \mathbb{Z}, \alpha = \pm 1 \right\}, \tag{38}$$

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[19] The $v \times v$ permutation matrix α of a permutation f of $\{1, \ldots, v\}$ is defined as usual by $\alpha^j_i v_j = v_{f(i)}$ for any numbers $v_1, \ldots, v_v$; so the entries of the matrix α are all 0s, except for 1s in the $f(i)$th row of the ith column.

[20] For $v = 0$ (1-lattices or affine simple lattices), the definitions (36)–(37) give back the group $\Gamma_3 = GL(3, \mathbb{Z})$ of Proposition 1.

and

$$\Gamma_5 = \left\{ \mu = \begin{pmatrix} & & & l_1^1 & l_2^1 \\ & m_a^b & & l_1^2 & l_2^2 \\ & & & l_1^3 & l_2^3 \\ \hline 0 & 0 & 0 & & \\ 0 & 0 & 0 & & \alpha_i^j \end{pmatrix} : m \in GL(3, \mathbb{Z}), \right.$$

$$\left. l_i^b \in \mathbb{Z}, (\alpha_i^j) \in A \right\}, \qquad (39)$$

where A denotes the following group of matrices:

$$\left\{ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & -1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} -1 & -1 \\ 0 & 1 \end{pmatrix} \right.$$

$$\left. \begin{pmatrix} 1 & 0 \\ -1 & -1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ -1 & -1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right\}. \qquad (40)$$

The structure of the matrices $\mu \in \Gamma_{\nu+3}$ is justified by the following result, showing that the essential descriptors ε_σ of a multilattice transform by means of a matrix in $\Gamma_{\nu+3}$ and that the changes of essential descriptors are in a one-to-one correspondence with such matrices (compare with Proposition 1 for simple lattices).

Proposition 3. Let $\mathcal{M}(\varepsilon_\sigma)$ be a monoatomic $(\nu + 1)$-lattice in an *essential description*.[21] Then $\bar\varepsilon_\sigma$ are new essential descriptors for $\mathcal{M}$ up to a translation [that is, $\mathcal{M}(\bar\varepsilon_\sigma) = \mathcal{M}(\varepsilon_\sigma) + \mathbf{t}$] if and only if there exists a matrix $\mu \in \Gamma_{\nu+3}$ such that

$$\bar\varepsilon_\sigma = \mu_\sigma^\tau \varepsilon_\tau \quad \text{for} \quad \mu \in \Gamma_{\nu+3}. \qquad (41)$$

The matrix $\mu \in \Gamma_{\nu+3}$ determines uniquely the new descriptors $\bar\varepsilon_\sigma$ and *vice versa*.[22]

The proof of this result is given in Appendix $A1$. We notice explicitly that, by (36) and (41), the new lattice vectors and shifts are given by

$$\bar{\mathbf{e}}_a = m_a^b \mathbf{e}_b, \quad \bar{\mathbf{p}}_i = \alpha_i^j \mathbf{p}_j + l_i^a \mathbf{e}_a, \qquad (42)$$

where $(m_a^b) \in GL(3, \mathbb{Z})$, $l_i^a \in \mathbb{Z}$, and (α_i^j) is a permutation or a matrix (37) times a permutation, with $a = 1, 2, 3$, $i, j = 1, \ldots, \nu$. Note that the skeletal basis transforms to an equivalent triple as in (7).

As anticipated above, this result shows that the global symmetry of any monoatomic $(\nu + 1)$-lattice in its essential description is given abstractly by the arithmetic group $\Gamma_{\nu+3}$, and evidences the central role played

by the integral matrices μ defined in (36)–(37) in the account of multilattice symmetry.

A change of descriptors as in (41) induces, in obvious notation, the following transformation of the multilattice metric K in (26):

$$\bar{K} = \mu^t K \mu, \qquad (43)$$

where, in general, $\bar{K} \neq K$. Formulas (41) and (43) give natural actions of the group $\Gamma_{\nu+3}$ on the configuration spaces $\mathcal{D}_{\nu+3}^m$ and $\mathcal{Q}_{\nu+3}^m$, which generalize the actions $(7)_2$ and (8) obtained in the case of simple lattices: this is one of the central notions of this section. By (27), for any choice of ε_σ with multilattice metric K, the following holds:

$$\mu^t K \mu = K \Leftrightarrow \mu_\sigma^\tau \varepsilon_\tau = \mathbf{Q}\varepsilon_\sigma \quad \text{for some } \mathbf{Q} \in O(3), \quad (44)$$

that is, two multilattices have the same metric if and only if their descriptions are orthogonally related.

4.2. Lattice groups of multilattices

As for simple lattices in §2.3, also the arithmetic symmetry of multilattices is based on the analysis of the finite subgroups of $\Gamma_{\nu+3}$ that act *isometrically* on some multilattice or, equivalently, that stabilize some multilattice metric under the action (43). Indeed, we will see in Corollary 1 that, as a particular case of the changes of essential descriptors considered in Proposition 3, the affine symmetry operations $e = (\mathbf{t}, \mathbf{Q})$ belonging to the space group $S(\mathcal{M})$ of a $(\nu + 1)$-lattice $\mathcal{M}$ are in a one-to-one correspondence with the pairs (n_0^a, μ) where n_0^a is a triple of integers and μ is a matrix in a suitable *finite* subgroup of $\Gamma_{\nu+3}$.

For the purposes of this Corollary, it is necessary to revert to the notation $\mathcal{M}(P_0, \varepsilon_\sigma)$ for multilattices, in which also the base point P_0 is explicitly indicated, as in (25). See Pitteri & Zanzotto (1998a) for more details, also for the case of non-essential descriptors.

Corollary 1. Let $\mathcal{M}(P_0, \varepsilon_\sigma)$ be a monoatomic $(\nu + 1)$-lattice in an essential description and let $K \in \mathcal{Q}_{\nu+3}^m$ be the corresponding multilattice metric. Then an isometry $e = (\mathbf{t}, \mathbf{Q}) \in E(3)$ is a symmetry operation for $\mathcal{M}$, that is, $e \in S(\mathcal{M})$ if and only if there exist a set of integers n_0^a and a matrix $\mu \in \Gamma_{\nu+3}$ that are (mutually independent and) such that

$$\mathbf{t} = P_0 e(P_0) = \mathbf{p}_{i(\mu)} + n_0^a \mathbf{e}_a \quad \text{and} \quad \mathbf{Q}\varepsilon_\sigma = \mu_\sigma^\tau \varepsilon_\tau, \quad (45)$$

that is, μ preserves the metric K:

$$\mu^t K \mu = K. \qquad (46)$$

The integers n_0^a and the matrix $\mu \in \Gamma_{\nu+3}$ uniquely determine the affine symmetry $e \in E(3)$ and *vice versa*. The index $i(\mu)$ in (45) is determined by the submatrix α of μ in (36) as follows: if α is a permutation matrix, $i(\mu) = 0$; if the rth row of α is a row of -1s, $i(\mu) = r$.

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[21] See §4.2.3 of Pitteri & Zanzotto (1998a) for more details regarding the case of non-essential descriptors.

[22] Of course, since the vectors $\varepsilon_1, \ldots, \varepsilon_{\nu+3}$ are not linearly independent, there are infinitely many $(\nu + 3) \times (\nu + 3)$ matrices relating them to the vectors $\bar\varepsilon_\sigma$. This Proposition states that when the ε_σ and the $\bar\varepsilon_\sigma$ are essential there always is one and only one such matrix in the group $\Gamma_{\nu+3}$.

The proof of Corollary 1 is given in Appendix $A2$. Notice that, by (36) or (42), $(45)_3$ can be written explicitly as

$$\mathbf{Q}\mathbf{e}_a = m_a^b \mathbf{e}_b, \quad \mathbf{Q}\mathbf{p}_i = \alpha_i^j \mathbf{p}_j + l_i^a \mathbf{e}_a. \quad (47)$$

Formula (47) says that $e = (\mathbf{t}, \mathbf{Q}) \in E(3)$ is a symmetry operation for the essential multilattice $\mathcal{M}(\mathbf{e}_a, \mathbf{p}_i)$ only if the orthogonal tensor $\mathbf{Q}$ transforms the maximal skeletal lattice basis to an equivalent one according to $(47)_1$ [that is, $\mathbf{Q} \in P(\mathbf{e}_a)$] *and* satisfies the further conditions $(47)_2$. This proves the group–subgroup relation (34) between the point group $P(\mathcal{M})$ of $\mathcal{M}$ and its maximal skeletal holohedry $P(\mathbf{e}_a)$. In what follows, for brevity we use the notation $P(\varepsilon_\sigma) = P(\mathcal{M}(\varepsilon_\sigma))$ for the point group of the multilattice described by ε_σ.

If $\mathcal{M}(\varepsilon_\sigma)$ is a $(\nu + 1)$-lattice with metric K, based on Corollary 1 and by analogy with the definitions (10)–(13) for simple lattices, we define the *lattice group* $\Lambda(\varepsilon_\sigma)$ of $\mathcal{M}$:

$$\Lambda(\varepsilon_\sigma) \subset \Gamma_{\nu+3} \subset GL(\nu + 3, \mathbb{Z}), \quad (48)$$

as the subgroup of all the integral matrices $\mu \in \Gamma_{\nu+3}$ acting isometrically on $\mathcal{M}$, that is, for which there is $\mathbf{Q} \in O(3)$ such that $(45)_3$ holds:

$$\Lambda(\varepsilon_\sigma) = \{\mu \in \Gamma_{\nu+3} : \mu_\sigma^\tau \varepsilon_\tau = \mathbf{Q}\varepsilon_\sigma, \mathbf{Q} \in O(3)\}$$
$$= \{\mu \in \Gamma_{\nu+3} : \mu^t K \mu = K\}. \quad (49)$$

Analogously to the case of simple lattices, due to (46), $\Lambda(\varepsilon_\sigma)$ can be equivalently defined as the group of matrices μ preserving the multilattice metric K, as stated by $(49)_2$ [compare with (10) and (13)]. The analogs for multilattices of the transformation rules (11) for lattice groups are

$$\Lambda(\mu_\sigma^\tau \varepsilon_\tau) = \mu^{-1} \Lambda(\varepsilon_\sigma)\mu \quad \text{and} \quad \Lambda(\mathbf{R}\varepsilon_\sigma) = \Lambda(\varepsilon_\sigma), \quad (50)$$

for any $\mu \in \Gamma_{\nu+3}$ and any $\mathbf{R} \in O(3)$.

By Corollary 1, when the description is essential, each matrix $\mu \in \Lambda(\varepsilon_\sigma)$ uniquely determines an element $\mathbf{Q} \in P(\varepsilon_\sigma)$ and *vice versa*; the groups $\Lambda(\varepsilon_\sigma)$ and $P(\varepsilon_\sigma)$ are indeed isomorphic and $\Lambda(\varepsilon_\sigma)$ is necessarily finite. However, $\Lambda(\varepsilon_\sigma)$ carries more information than $P(\varepsilon_\sigma)$: indeed, unlike with the point group $P(\varepsilon_\sigma)$, given the group of matrices $\Lambda(\varepsilon_\sigma)$ it is possible to reconstruct uniquely the (isomorphism class of the) space group $S(\mathcal{M}(\varepsilon_\sigma))$ – see Proposition 5 in §5.

The natural (arithmetic) equivalence relation for the lattice groups and for the metrics of $(\nu + 1)$-lattices is conjugacy within $\Gamma_{\nu+3}$, as it was conjugacy in $GL(3, \mathbb{Z})$ in the case of simple lattices. Moreover, similarly to the latter, a $(\nu + 1)$-lattice determines by $(50)_1$ and (43) an entire $\Gamma_{\nu+3}$-conjugacy class of lattice groups. Then one can study the conjugacy properties of the lattice groups

and their arithmetic classes in $\Gamma_{\nu+3}$ in order to get information on the arithmetic symmetry of multilattices. For instance, in this context, it is natural to ask how many distinct conjugacy classes of lattice groups there are in $\Gamma_{\nu+3}$, with the aim of obtaining a result similar to Theorem 2. This would classify the 'arithmetic symmetry types' of $(\nu + 1)$-lattices, giving an analog of the subdivision in Bravais symmetry types for simple lattices.

4.3. Fixed sets in the configuration spaces of multilattices

The considerations in §2.4 on simple lattices, to a large extent, can be generalized in order to investigate the (changes of) symmetry of deformable $(\nu + 1)$-lattices.

In analogy to (15), we define the fixed set $I(\Lambda) \subset \mathcal{Q}_{\nu+3}^m$ of any subgroup Λ of $\Gamma_{\nu+3}$:

$$I(\Lambda) = \{K \in \mathcal{Q}_{\nu+3}^m : \mu^t K \mu = K \quad \text{for all} \quad \mu \in \Lambda\}. \quad (51)$$

We may also define the corresponding $O(3)$-invariant fixed sets in the configuration space $\mathcal{D}_{\nu+3}^m$; in this way, we get the analog to the definitions (15) and (16) for simple lattices. Similarly to §§2.3–2.4, one can then investigate the structure of the fixed sets in the configuration spaces $\mathcal{Q}_{\nu+3}^m$ or $\mathcal{D}_{\nu+3}^m$ to see how symmetry changes along any 'phase transition' paths in these spaces.[23]

In the rest of this paper, we only report some very basic results giving partial counterparts for multilattices to some of the remarks in Proposition 2 (see also Pitteri & Zanzotto, 1998a,b).

Proposition 4.

(i) Any element μ in the lattice group $\Lambda(\varepsilon_\sigma)$ of essential ε_σ, has period 1, 2, 3, 4, or 6.

(ii) A subgroup $\Lambda \subset \Gamma_{\nu+3}$ is a subgroup of a lattice group if and only if $I(\Lambda)$ contains a multilattice metric $K \in \mathcal{Q}_{\nu+3}^m$, that is, a symmetric $(\nu + 3) \times (\nu + 3)$ matrix satisfying (23) and (26).

(iii) $\Lambda \subset \Gamma_{\nu+3}$ is a subgroup of a lattice group if and only if it is finite and it satisfies the additional conditions originating from (58) below.

See Appendix $A3$ below for a proof of these statements. Notice that according to statement (iii), unlike for simple lattices, it is not enough that $I(\Lambda)$ be non-empty to guarantee that Λ be (included in) the lattice group of a multilattice, but it must be $I(\Lambda) \cap \mathcal{Q}_{\nu+3}^m \neq \emptyset$. It is also possible to obtain the analogs to statements (ii)–(iv) in Proposition 2. However, a complete analysis of the structure of the fixed sets in $\mathcal{D}_{\nu+3}^m$ or $\mathcal{Q}_{\nu+3}^m$ is not yet available [see the references above and Ericksen (1998) for some related results].

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[23] Remark that, given an element $K \in \mathcal{Q}_{\nu+3}^m$ with a known lattice group $\Lambda(K)$, the problem of finding all the $K' \in I(\Lambda(K))$ that belong to the same fixed set as K is linear.

5. Inequivalence of the geometric and arithmetic symmetry of multilattices

In this section, we give one main property of the fixed sets in the configuration space $\mathcal{Q}_{\nu+3}^m$ of multilattices: we show that also for multilattices the arithmetic symmetry is more refined than the geometric (space-group) symmetry. This derives from the following proposition, which gives a counterpart, for multilattices, of some of the properties of the fixed sets of simple lattices stated in §2.4, and indicates the relation between the classical affine (or isomorphism) classes of space groups of Theorem 4 and the arithmetic classes of lattice groups in the group $\Gamma_{\nu+3}$.

Proposition 5. The space-group symmetry of multi-lattices is strictly *coarser* than their arithmetic symmetry; that is:

(i) Two $(\nu + 1)$-lattices in their essential description, whose lattice groups coincide, have isomorphic space groups. More, in general, if their lattice groups are conjugate in $\Gamma_{\nu+3}$, their space groups are isomorphic.

(ii) For $\nu > 0$, the converse of (i) in general does not hold:[24] there are $(\nu + 1)$-lattices whose space groups are isomorphic but whose essential descriptors give lattice groups that are not conjugate in $\Gamma_{\nu+3}$.

A proof is given in Appendix $A4$ below (see also Fig. 2). Statements (i)–(ii) above show that multilattices with equivalent lattice groups always have isomorphic space groups but not *vice versa*. Thus, in principle, certain phase transitions with a change of symmetry in multilattices can only be detected through the analysis of the lattice groups and not by means of the space groups (even if complemented by the site-symmetry groups, as we remark below). Fig. 2 shows a theoretical example of this, which is analogous to the transitions changing the Bravais type but not the crystal system of a simple lattice, mentioned in footnotes 4 and 13.

Remark. To describe in more detail the symmetry of multilattices, the notion of 'site symmetry' is also used. The 'site-symmetry group' of a point of a multilattice is the subgroup of operations of the space group that stabilize that point [the site-symmetry groups of points belonging to the same space-group orbit are all conjugate, see for instance Senechal (1990)]. By considering both the space group and the site-symmetry group(s), one describes the symmetry of multilattices in a finer way than by using only the space groups (see *International Tables for X-ray Crystallography*, 1952). The example in Fig. 2 shows that the arithmetic symmetry

gives a classification of multilattices that is even finer than the one obtained by means of the space groups together with the site-symmetry groups (see at the end of Appendix $A4$).

6. Conclusions

In this paper, we have proposed a framework for the investigation of the kinematics and arithmetic symmetry of deformable multilattices, by generalizing the approach to this subject that is classical for simple lattices. For $(\nu + 1)$-lattices, we consider the action of a 'global symmetry group' $\Gamma_{\nu+3} \subset GL(\nu + 3, \mathbb{Z})$ in (36), and of its finite lattice (sub)groups on the configuration spaces $\mathcal{D}_{\nu+3}^m$ or $\mathcal{Q}_{\nu+3}^m$ defined by (23)–(26); by investigating the structure and arrangement of the fixed sets of such an action, one can describe in detail the symmetry changes in a multilattice that undergoes a deformation.

The arithmetic symmetry of simple lattices distinguishes different centerings in each crystal system and has great relevance in the phase transitions of real materials. In the same way, although geometrically not as transparent, the arithmetic symmetry of multilattices is expected to be relevant in the description of phase changes in complex crystals (see Fig. 2), and is well worth investigating further. Although our example is theoretical and not taken from nature, it is apparent that if two lattice structures as in Fig. 2 were to be observed in a crystalline material, it would be natural to call them two different 'phases' of that solid. These two arithmetically inequivalent multilattices have the same space group and the same site symmetry, yet exhibit markedly different geometries: their atomic configurations, for instance their nearest-neighbor relations, are clearly distinct. It would be impossible to describe such a 'phase transition' by means of the space group and site symmetries of the crystal because these do not change in the two phases. Only through their inequivalent lattice groups is it possible to take their symmetry change into account (this is analogous, for multilattices, to the phase transformations in simple lattices mentioned in footnotes 4 and 13). Further study

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[24] Statement (i) in Proposition 5 *can* indeed be reversed if $\nu = 0$, that is, for simple lattices: two simple lattices $\mathcal{L}$ and $\mathcal{L}'$ have arithmetically equivalent lattice groups, that is, have the same Bravais lattice type [see (14)], if and only if their space groups are isomorphic. This well known result (see for instance Janssen, 1973, p. 120) can be used to *define* the Bravais lattice types as the affine conjugacy classes of the space groups of 1-lattices (see, for instance, Schwarzenberger, 1972).
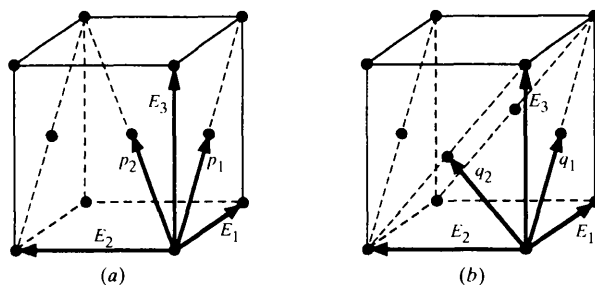

Fig. 2. Two 3-lattices whose space groups and site-symmetry groups are the same but whose lattice groups are not arithmetically equivalent [see Appendix $A4$, formulas (64)–(67) for an explicit description].

of the arithmetic symmetry of multilattices, and a more detailed knowledge of the spaces $\mathcal{D}_{v+3}^m$ and $\mathcal{Q}_{v+3}^m$ will thus improve our understanding of phase transitions in complex crystalline structures.

It is worthwhile to remark that the systematic analysis, mentioned at the end of §4.2, of the arithmetic symmetry of $(v+1)$-lattices for any v is a difficult problem. The reason is that in order to have a complete knowledge it is necessary to investigate all the conjugacy classes of the lattice (sub)groups of $\Gamma_{v+3} \subset GL(v+3, \mathbb{Z})$, which is far from trivial [recall from Proposition 4 that the lattice groups are special finite subgroups of $GL(v+3, \mathbb{Z})$ – see also Appendix A3]. A special case of this was the systematic analysis of the arithmetic symmetry of simple lattices, carried out at the beginning of this century, which required finding the conjugacy classes of all the finite subgroups of $GL(3, \mathbb{Z})$ and resulted in Theorem 2 of §2.3. The arithmetic symmetry of multilattices is therefore a problem similar but not equivalent to that of the arithmetic symmetry of *higher-dimensional* simple lattices, which is based on the investigation of the conjugacy properties of the finite subgroups of the groups $GL(n, \mathbb{Z})$. The latter are known for low n (see Engel, 1986): this would help in the systematic study of the arithmetic symmetry of the simplest multilattices, such as the two- and three-dimensional 2- and 3-lattices. At this stage, however, it is likely that the analysis of interesting special cases encountered in crystallography, mechanics, physics, chemistry or materials science, may prove more illuminating. See Ericksen (1998) and Pitteri & Zanzotto (1998a,b) for some related results.

APPENDIX A
Some proofs

A1. Proof of Proposition 3

For the 'only if' part: the maximal skeletal lattice of $\mathcal{M}$ is independent of the essential descriptors used, that is, $\mathcal{R}(\bar{\mathbf{e}}_a) = \mathcal{R}(\mathbf{e}_a)$; thus, Proposition 1 implies that $(42)_1$ necessarily holds for some element m of $GL(3, \mathbb{Z})$. To prove that $\bar{v} = v$, let us assume $\bar{v} \geq v$ for definiteness. Since $\mathcal{M}(\bar{P}_0, \bar{\varepsilon}_\alpha) = \mathcal{M}(P_0, \varepsilon_\alpha) + \mathbf{t}$, $\bar{P}_i$ is a point of $\mathcal{M} + \mathbf{t}$ for any $i = 0, \ldots, \bar{v}$, see (20); hence, there exist a map $f : \{0, \ldots, \bar{v}\} \to \{0, \ldots, v\}$ and integers n_i^a such that

$$\bar{P}_i = P_{f(i)} + n_i^a \mathbf{e}_a + \mathbf{t}. \qquad (52)$$

We show that f is injective, hence $(\bar{v} = v$ and) f is a permutation of $\{0, \ldots, v\}$: by contradiction, assume that $f(i) = f(j)$ for some choice of i and $j \neq i$; then $(42)_1$ and (52), together with the analog of (21) for $\bar{\mathbf{p}}_i$ with the definition $\bar{\mathbf{p}}_0 = \mathbf{0}$, imply

$$\bar{\mathbf{p}}_i - \bar{\mathbf{p}}_j = (n_i^a - n_j^a)\mathbf{e}_a = (n_i^a - n_j^a)(m^{-1})_a^b \bar{\mathbf{e}}_b, \qquad (53)$$

which contradicts (23) for $\bar{\mathbf{e}}_a$ and $\bar{\mathbf{p}}_i$.

We now write (52) – the right-hand side first for convenience – in the form

$$P_0 + \mathbf{t} + \mathbf{p}_{f(i)} + n_i^a \mathbf{e}_a = \bar{P}_0 + \bar{\mathbf{p}}_i$$
$$= P_0 + \mathbf{t} + \mathbf{p}_{f(0)} + n_0^a \mathbf{e}_a + \bar{\mathbf{p}}_i, \qquad (54)$$

whence, for $i = 1, \ldots, v$ and $a = 1, 2, 3$,

$$\bar{\mathbf{p}}_i = \mathbf{p}_{f(i)} - \mathbf{p}_{f(0)} + l_i^a \mathbf{e}_a, \quad l_i^a = n_i^a - n_0^a. \qquad (55)$$

If $f(0) = 0$, equation (55) has the form $(42)_2$ in which α is the permutation matrix of the restriction of f to $\{1, \ldots, v\}$; if $f(0) \neq 0$, (55) coincides with $(42)_2$, where α is the matrix of the form (37) in which the row of -1s is the $f(0)$th, multiplied by the matrix of the permutation $\{1, \ldots, f(0) - 1, 0, f(0) + 1, \ldots, v\} \mapsto \{f(1), \ldots, f(v)\}$.

The relationship established above between the maximal skeletal bases $\bar{\mathbf{e}}_a$ and $\mathbf{e}_a$ and relation (55) show that the two sets of essential descriptors $\bar{\varepsilon}_\sigma$ and ε_σ are indeed related by a matrix $\mu \in \Gamma_{v+3}$ as in (41) – compare with (36), (37).

The permutation $f : \{0, \ldots, v\} \to \{0, \ldots, v\}$ defined above is uniquely determined by the matrix $\mu \in \Gamma_{v+3}$ through its submatrix α; f is called the permutation associated with μ.

For the 'if' part: when (41) holds, so does $(55)_1$ and the definitions of $\bar{P}_0$ through (52) for $i = 0$, with arbitrary n_0^a and $\mathbf{t}$, and of n_i^a through $(55)_2$, imply (54), hence (52) also for $i \neq 0$. Thus,

$$\mathcal{M}(\bar{P}_0, \ldots \bar{P}_v, \bar{\mathbf{e}}_a) = \bigcup_{i=0}^{v} \mathcal{R}(\bar{P}_i, \bar{\mathbf{e}}_a) = \bigcup_{i=0}^{v} \mathcal{R}(P_{f(i)}, \mathbf{e}_a) + \mathbf{t},$$
$$(56)$$

whence the conclusion.

A2. Proof of Corollary 1

This corollary is a consequence of (44), (30) and Proposition 3, complemented by formula (52) for $i = 0$ and $\mathbf{t} = \mathbf{0}$.

Referring to (52), we notice that the index $i(\mu)$ mentioned in this corollary coincides with the value $f(0)$, f being the permutation associated with the matrix $\mu \in \Gamma_{v+3}$, defined in §A1.

A3. Proof of Proposition 4

Statement (i) derives from (36), (37), $(45)_3$ and the crystallographic restrictions for $\mathbf{Q} \in P(\varepsilon_\sigma)$.[25]

Statement (ii) is an easy consequence of the definitions of lattice group and of fixed set, and of (27).

For statement (iii), the finiteness of Λ is a consequence of $(45)_3$, (49) and of the finiteness of the point

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[25] If the ε_σ are not essential, the period of the elements $\mu \in \Lambda(\varepsilon_\sigma)$ is a *multiple* of a crystallographic period 1, 2, 3, 4, 6.

group $P(\varepsilon_\sigma)$. Moreover, with the definitions

$$b_i^a = |\Lambda|^{-1} \sum_{r=1}^{|\Lambda|} (m_r^{-1})_b^a (l_r)_i^b,$$

$$B_{i\,b}^{aj} = |\Lambda|^{-1} \sum_{r=1}^{|\Lambda|} (\alpha_r)_i^j (m_r^{-1})_b^a - \delta_b^a \delta_i^j, \tag{57}$$

$|\Lambda|$ being the number of elements in Λ, the technical condition mentioned in statement (iii) is that the system of equations

$$B_{i\,b}^{aj} k_j^b + b_i^a = 0 \tag{58}$$

in the unknown vectors $(k_1^1, k_1^2, k_1^3), \ldots, (k_v^1, k_v^2, k_v^3)$ have at least one solution such that no vector and no difference of any two vectors be a triple of integers. This holds if $I(\Lambda)$ contains a matrix K satisfying (23) and (26), as requested by (ii), and is not otherwise a very suggestive condition.

For the converse, we can use the finiteness of the group of submatrices $m(\mu) \in GL(3, \mathbb{Z})$ of $\mu \in \Lambda$ to select a lattice metric C such that $m(\mu)^t C m(\mu) = C$ for any $\mu \in \Lambda$: for any $\bar{C} \in C^+(\mathcal{Q}_3)$, the 'average'

$$C = |\Lambda|^{-1} \sum_{r=1}^{|\Lambda|} m(\mu_r)^t \bar{C} m(\mu_r) \tag{59}$$

has this property. Then, choose any basis $\mathbf{e}_a$ whose metric is C, any vectors $(k_1^1, k_1^2, k_1^3), \ldots, (k_v^1, k_v^2, k_v^3)$ satisfying the conditions mentioned below (58), and define $\mathbf{p}_i = k_i^a \mathbf{e}_a$. Then the matrix of the scalar products of the descriptors $(\mathbf{e}_a, \mathbf{p}_i)$ is a multilattice metric in $I(\Lambda)$, as required by (ii).

A4. Proof of Proposition 5

A proof of statement (i) can be given as follows.

Given two essential $(v + 1)$-lattices with arithmetically equivalent lattice groups in Γ_{v+3}, by (50) we can always choose their descriptors so that they have the same lattice group, say Λ. So, P_0 being an arbitrary point[26] in $\mathbb{A}^3$, suppose that two essential $(v + 1)$-lattices $\mathcal{M}' = \mathcal{M}(P_0, \varepsilon_\sigma')$ and $\mathcal{M}'' = \mathcal{M}(P_0, \varepsilon_\sigma'')$ have the same lattice group Λ, and let $S' = S(\mathcal{M}')$, $S'' = S(\mathcal{M}'')$ be the corresponding space groups.

For an element $e' = (\mathbf{t}', \mathbf{Q}') \in \mathcal{M}'$, write equations $(47)_2$ and $(45)_1$ in the equivalent form (set $\mathbf{p}_0' = \mathbf{0}$):

$$\mathbf{Q}' \mathbf{p}_i' + \mathbf{t}' = \mathbf{p}_{f(i)}' + n_i^a \mathbf{e}_a', \quad i = 0, \ldots, v, \quad a = 1, 2, 3; \tag{60}$$

then consider the map $\Phi' : S' \to \mathbb{Z}^{3(v+1)} \times \Lambda$, where $\Phi' : (\mathbf{t}', \mathbf{Q}') \mapsto (\{n_i^a\}, \mu)$; here, $\{n_i^a\}$ are the integers in (60) and μ is the unique element of Λ that corresponds to $\mathbf{Q}'$ through equation $(45)_2$. Also, define the product $*$

of pairs $(\{n_i^a\}, \mu)$ by the rule:[27]

$$\left(\{(n_1)_i^a\}, \mu_1 \right) * \left(\{(n_2)_i^a\}, \mu_2 \right)$$
$$= \left(\{(n_1)_{f_2(i)}^a + (n_2)_i^a (m_1)_b^a\}, \mu_1 \mu_2 \right), \tag{61}$$

where f_r is the permutation associated with $\mu_r, r = 1, 2$ (see §A1), and m_r is the m-component of μ_r [see (36)]. Then the standard composition rules for affine maps:

$$a = (\tau, \mathbf{A}), \bar{a} = (\bar{\tau}, \bar{\mathbf{A}}) \Rightarrow a\bar{a} = (\tau + \mathbf{A}\bar{\tau}, \mathbf{A}\bar{\mathbf{A}}) \quad \text{and}$$
$$a^{-1} = (-\mathbf{A}^{-1}\tau, \mathbf{A}^{-1}), \tag{62}$$

together with (60) and the uniqueness assertion in Corollary 1, imply (that the permutation associated with $\mu_1 \mu_2$ is $f_1 \circ f_2$ and) that

$$\Phi'(e_1 e_2) = \Phi'(e_1) * \Phi'(e_2)$$
$$\text{and} \quad \Phi'(e_1) = \Phi'(e_2) \Leftrightarrow e_1 = e_2 \tag{63}$$

for any e_1 and e_2 in S''; hence, Φ' is a group isomorphism. In the same way, we can construct a group isomorphism $\Phi'' : S'' \to \mathbb{Z}^{3(v+1)} \times \Lambda$, so that $\Phi'(\Phi'')^{-1} : S' \to S''$ is a group isomorphism too.

For statement (ii), we give an example. Take three mutually orthogonal vectors $\mathbf{e}_a$, not of equal length, and consider the two sets $\hat{\varepsilon}_\sigma$ and $\bar{\varepsilon}_\sigma$ of 3-lattice descriptors ($v = 2$) given by:

$$\hat{\varepsilon}_\sigma = (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{p}_1, \mathbf{p}_2), \quad \bar{\varepsilon}_\sigma = (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{q}_1, \mathbf{q}_2), \tag{64}$$

where

$$\mathbf{p}_1 = \tfrac{1}{2}(\mathbf{e}_1 + \mathbf{e}_3), \qquad \mathbf{p}_2 = \tfrac{1}{2}(\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3),$$
$$\mathbf{q}_1 = \tfrac{1}{2}(\mathbf{e}_1 + \mathbf{e}_3) = \mathbf{p}_1, \qquad \mathbf{q}_2 = \tfrac{1}{2}(\mathbf{e}_2 + \mathbf{e}_3). \tag{65}$$

These two sets of descriptors give two distinct essential 3-lattices whose primitive orthorhombic skeletal cells contain two extra points (see Fig. 2). It is not difficult to see that the (symmorphic) space groups of the multilattices $\mathcal{M} = \mathcal{M}(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{p}_1, \mathbf{p}_2)$ and $\bar{\mathcal{M}} = \mathcal{M}(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{q}_1, \mathbf{q}_2)$ coincide, and belong to the isomorphism class denoted by $Pmmm$ in the standard notation of International Tables for X-ray Crystallography (1952) or Janssen (1973). Indeed:

$$S(\hat{\mathcal{M}}) = \{(\mathbf{t}, \mathbf{Q}) : \mathbf{t} \in \mathcal{L}(\mathbf{e}_a),$$
$$\mathbf{Q} \in \pm \mathbf{1}, \pm \mathbf{R}_{\mathbf{e}_1}^\pi, \pm \mathbf{R}_{\mathbf{e}_2}^\pi, \pm \mathbf{R}_{\mathbf{e}_3}^\pi\} = S(\bar{\mathcal{M}}) \tag{66}$$

(here the symbol $\mathbf{R}_\mathbf{v}^\pi$ denotes the rotation of π about the axis $\mathbf{v}$). This means that the common point group $P(\hat{\mathcal{M}}) = P(\bar{\mathcal{M}}) = \{\pm \mathbf{1}, \pm \mathbf{R}_{\mathbf{e}_1}^\pi, \pm \mathbf{R}_{\mathbf{e}_2}^\pi, \pm \mathbf{R}_{\mathbf{e}_3}^\pi\}$ of the two multilattices coincides with the full orthorhombic holohedry mmm.

Furthermore, one can check that the lattice groups obtained from equations (64) and $(45)_2$ are as follows:

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[26] Choosing the same base point for the two multilattices does not change the conclusion because translating a multilattice changes its space group by conjugacy with the translation.

[27] The transformation of $\mathbb{Z}^{3(v+1)}$ defined by (61) is an example of a 'Frobenius congruence' – see Senechal (1980) or Jarić & Senechal (1984).

$\Lambda(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{p}_1, \mathbf{p}_2) = \{1, \hat{\mu}_{-1}, \hat{\mu}^\pi_{\mathbf{e}_a}, \hat{\mu}_{-1}\hat{\mu}^\pi_{\mathbf{e}_a}, a = 1, 2, 3\},$

$\Lambda(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{q}_1, \mathbf{q}_2) = \{1, \bar{\mu}_{-1}, \bar{\mu}^\pi_{\mathbf{e}_a}, \bar{\mu}_{-1}\bar{\mu}^\pi_{\mathbf{e}_a}, a = 1, 2, 3\},$

$$(67)$$

where the matrices $\hat{\mu}_{-1}$, $\bar{\mu}_{-1}$, $\hat{\mu}^\pi_{\mathbf{e}_a}$, and $\bar{\mu}^\pi_{\mathbf{e}_a}$ all belong to Γ_5 in (39), and are given explicitly by:

$$\hat{\mu}_{-1} = \left(\begin{array}{ccc|cc} -1 & 0 & 0 & -1 & -1 \\ 0 & -1 & 0 & 0 & -1 \\ 0 & 0 & -1 & -1 & -1 \\ \hline 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{array}\right),$$

$$\bar{\mu}_{-1} = \left(\begin{array}{ccc|cc} -1 & 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 & -1 \\ 0 & 0 & -1 & -1 & -1 \\ \hline 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{array}\right),$$

$$\hat{\mu}^\pi_{\mathbf{e}_1} = \left(\begin{array}{ccc|cc} 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & -1 \\ 0 & 0 & -1 & -1 & -1 \\ \hline 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{array}\right) = \bar{\mu}^\pi_{\mathbf{e}_1},$$

$$\hat{\mu}^\pi_{\mathbf{e}_2} = \left(\begin{array}{ccc|cc} -1 & 0 & 0 & -1 & -1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & -1 & -1 \\ \hline 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{array}\right),$$

$$\bar{\mu}^\pi_{\mathbf{e}_2} = \left(\begin{array}{ccc|cc} -1 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & -1 & -1 \\ \hline 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{array}\right),$$

$$\hat{\mu}^\pi_{\mathbf{e}_3} = \left(\begin{array}{ccc|cc} -1 & 0 & 0 & -1 & -1 \\ 0 & -1 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{array}\right),$$

$$\bar{\mu}^\pi_{\mathbf{e}_3} = \left(\begin{array}{ccc|cc} -1 & 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{array}\right).$$

Notice that for each index $a = 1, 2, 3$ the couples of integral matrices $(\hat{\mu}^\pi_{\mathbf{e}_a}, \bar{\mu}^\pi_{\mathbf{e}_a})$ and $(\hat{\mu}_{-1}, \bar{\mu}_{-1})$ represent, respectively, through equations (64) and (45)$_2$, the same orthogonal operations $\mathbf{R}^\pi_{\mathbf{e}_a}$ and -1, which belong to the point group of the multilattices.

It can be verified that the two (finite) lattice groups $\Lambda(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{p}_1, \mathbf{p}_2)$ and $\Lambda(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{q}_1, \mathbf{q}_2)$ defined in (67) are *not* conjugate in Γ_5. This can be concluded by analyzing the matrices in Γ_5 that: (*a*) conjugate $\hat{\mu}_{-1}$ to $\bar{\mu}_{-1}$, and (*b*) conjugate the subset of generators $\{\hat{\mu}^\pi_{\mathbf{e}_1}, \hat{\mu}^\pi_{\mathbf{e}_2}\}$ for $\Lambda(\hat{\boldsymbol{\varepsilon}}_\sigma)$ to any subset of matrices in $\Lambda(\bar{\boldsymbol{\varepsilon}}_\sigma)$. It can be verified that no integral matrices in Γ_5 do the job because these conjugacy requirements lead to a contradiction.

It should be remarked that the two multilattices $\hat{\mathcal{M}}$ and $\mathcal{M}$ share not only their space group but also the site-symmetry group of all their points; in both cases, the latter coincides with the entire point group. Consequently, this example shows that the arithmetic classification is also finer than the one based on the space-group and site-group symmetries.

We thank a referee for his interesting comments and suggestions, which led to the Remark at the end of §5.

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