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The arithmetic symmetry of monoatomic 2-nets

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A recent paper [Pitteri & Zanzotto (1998). *Acta Cryst.* A**54**, 359–373] has proposed a framework for the study of the 'arithmetic symmetry' of multilattices (discrete triply periodic point sets in the affine space). The classical approach to multilattice symmetry considers the well known 'space groups', that is, the groups of affine isometries leaving a multilattice invariant. The ensuing classification counts 219 affine conjugacy (or isomorphism) classes of space groups in three dimensions, and 17 classes in two dimensions ('plane groups'). The arithmetic criterion gives a finer classification of multilattice symmetry than space (or plane) groups do. This paper is concerned with the systematic investigation of the arithmetic symmetry of multilattices in the simplest nontrivial case, that is, monoatomic 2-nets (planar lattices with two identical atoms in their unit cell). We show the latter to belong to *five* distinct arithmetic types. We also give the complete description of a fundamental domain for the action of the global symmetry group of 2-nets on the space of 2-net metrics.

1. Introduction

The detailed modelling of phase transitions in crystalline solids and the related phenomena of twinning and microstructure formation (see for instance Ericksen, 1980; Ball & James, 1992, 2000; Luskin, 1996; Müller, 1998; James, 1999; Pitteri & Zanzotto, 2000) has led workers to introduce a framework in which to study the 'arithmetic symmetry' of deformable simple lattices and multilattices. As a definition, multilattices are triply periodic discrete subsets of the affine space that are constituted by finite unions of translates of a given (simple) Bravais lattice; these structures describe the atomic arrangements found in crystalline materials in more detail than simple lattices do, in that they also account for the extra atoms that may be present in the unit cell of the crystal.

In this context, the notion of arithmetic symmetry arises as the natural tool for keeping track of the changes of symmetry that may occur in a crystal as it undergoes deformations and/or changes in the atomic positions while maintaining a periodic lattice structure, as is the case in many solid-state phase transitions. A recent paper, see Pitteri & Zanzotto (1998), for brevity hereafter referred to as I, gives an introduction to this subject. The approach in I is based on earlier work by Ericksen (1970), Parry (1978) and Pitteri (1985, 1998); see also Pitteri & Zanzotto (2000) for more details. The notions discussed in I allow for a natural extension to multilattices of the distinction, classically made for simple lattices, between their 'geometric' and their 'arithmetic' symmetry. For simple lattices, the geometric symmetry is described by the crystal systems, while the arithmetic symmetry is described by the Bravais lattice types.[1] As is well known, the notion of the crystal system is based on the conjugacy properties of the symmetry groups of simple lattices within the orthogonal group $O(3)$; the Bravais types, on the other hand, are distinguished by the conjugacy properties of the symmetry groups within the 'arithmetic' group $GL(3, \mathbb{Z})$ constituted by the invertible 3×3 matrices with integral entries.[2]

For the case of three-dimensional multilattices, the description of the geometric symmetry is based on the classification obtained through the well known 219 classes of space groups. Except for the literature recalled above, in crystallography there is no classical counterpart, for multilattices, of the notion of arithmetic symmetry. This paper follows the framework proposed in I for studying the latter, which in I has been shown to give a sharper classification

[1] For instance, the body-centred cubic (b.c.c.) and the face-centred cubic (f.c.c.) lattices are both 'cubic' simple lattices, *i.e.* they belong to the same 'cubic' crystal system; however, the sharper classification in Bravais lattice types evidences a difference in these structures that the mere crystal system cannot capture. We notice explicitly that such differences are very important in nature, as, for instance, the α–γ (b.c.c. to f.c.c.) transformation in iron is indeed a transition of Bravais type and not of crystal system.

[2] As usual, in this paper we denote by $\mathbb{Z}$ and $\mathbb{R}$ the sets of integral and real numbers, respectively. It is a classical result that the arithmetic criterion is in general more stringent than the geometric one, and that it gives rise, in three dimensions, to the 14 Bravais lattice types within the seven crystal systems. See, for instance, Schwarzenberger (1972), Engel (1986), Michel (1995) or Pitteri & Zanzotto (2000). Analogously with $GL(2, \mathbb{Z})$ and the planar simple lattices; see §3.2 for details.

Table 1
The Bravais types of two-dimensional simple lattices (1-nets), and the fixed sets intersecting the fundamental domain $\mathcal{D}'$ defined in (32) for the action (21), with the corresponding lattice groups.

See Fig. 2 for a geometric representation of $\mathcal{D}'$ and Fig. 3(*a*) for a picture of the lattice cells.

No.	Crystal system (International symbol)	Lattice type (International symbol)	Fixed set intersecting $\mathcal{D}'$	Lattice group
1	Oblique (2)	Oblique ($p2$)	$0 < K_{11} < K_{22}$ $0 < K_{12} < K_{11}/2$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}, \begin{pmatrix}-1&0\\0&-1\end{pmatrix}$
2	Rectangular ($2mm$)	Primitive rectangular ($p2mm$)	$0 < K_{11} < K_{22}$ $K_{12} = 0$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}, \begin{pmatrix}-1&0\\0&-1\end{pmatrix}, \begin{pmatrix}-1&0\\0&1\end{pmatrix}, \begin{pmatrix}1&0\\0&-1\end{pmatrix}$
3	Rectangular ($2mm$)	Rhombic or centred-rectangular ($c2mm$)	Fixed set I $0 < K_{11} = K_{22}$ $0 < K_{12} < K_{11}/2$ Fixed set II $0 < K_{11} < K_{22}$ $0 < K_{12} = K_{11}/2$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}, \begin{pmatrix}0&1\\1&0\end{pmatrix}, \begin{pmatrix}-1&0\\0&-1\end{pmatrix}, \begin{pmatrix}0&-1\\-1&0\end{pmatrix}$ $\begin{pmatrix}1&0\\0&1\end{pmatrix}, \begin{pmatrix}-1&0\\0&-1\end{pmatrix}, \begin{pmatrix}1&1\\0&-1\end{pmatrix}, \begin{pmatrix}-1&-1\\0&1\end{pmatrix}$
4	Square ($4mm$)	Square ($p4mm$)	$0 < K_{11}$ $K_{22}K_{12} = 0$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}, \begin{pmatrix}-1&0\\0&-1\end{pmatrix}, \begin{pmatrix}0&-1\\1&0\end{pmatrix}, \begin{pmatrix}0&1\\-1&0\end{pmatrix}$ $\begin{pmatrix}-1&0\\0&1\end{pmatrix}, \begin{pmatrix}1&0\\0&-1\end{pmatrix}, \begin{pmatrix}0&1\\1&0\end{pmatrix}, \begin{pmatrix}0&-1\\-1&0\end{pmatrix}$
5	Hexagonal ($6mm$)	Hexagonal ($p6mm$)	$0 < K_{11} = K_{22}$ $0 < K_{12} = K_{11}/2$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}, \begin{pmatrix}-1&0\\0&-1\end{pmatrix}, \begin{pmatrix}-1&-1\\1&0\end{pmatrix}, \begin{pmatrix}0&-1\\1&1\end{pmatrix}$ $\begin{pmatrix}0&1\\-1&-1\end{pmatrix}, \begin{pmatrix}1&1\\-1&0\end{pmatrix}, \begin{pmatrix}1&1\\0&-1\end{pmatrix}, \begin{pmatrix}-1&0\\1&1\end{pmatrix}$ $\begin{pmatrix}0&-1\\-1&0\end{pmatrix}, \begin{pmatrix}0&1\\1&0\end{pmatrix}, \begin{pmatrix}-1&-1\\0&1\end{pmatrix}, \begin{pmatrix}1&0\\-1&-1\end{pmatrix}$

of multilattice symmetry than the one produced by the space groups.[3]

The approach in I is based on the conjugacy properties of the symmetry groups of multilattices within suitable groups of integral matrices that describe the general indeterminacy in the choice of the 'multilattice descriptors'.[4] These groups suitably generalize the role played by the groups $GL(2, \mathbb{Z})$ and $GL(3, \mathbb{Z})$ for simple lattices, recalled above. See also Pitteri (1985).

Recent works have investigated some general properties of the arithmetic symmetry groups of multilattices; see for instance Ericksen (1999*a*) and Adeleke (1999). In the present paper, we make a *systematic* study of the arithmetic symmetry of multilattices in the simplest nontrivial case, *i.e.* the case of *monoatomic 2-nets* (planar lattices with two identical atoms in their unit cell). As is well known, *simple* nets (planar simple lattices or 1-nets) exhibit five distinct arithmetic (*i.e.* Bravais) types within four crystal systems, see Table 1. Correspondingly, we show that the monoatomic 2-nets have five distinct arithmetic types, which all have a distinct plane group. Table 2 summarizes these results; Fig. 3 also illustrates schematically the arithmetic types of monoatomic 2-nets and their symmetry hierarchies, and compares them with the classical Bravais types of simple nets.

The method we use for proving these results actually gives much more information than the sole classification of the arithmetic types of 2-nets. Indeed, we investigate in detail the structure of a fundamental domain for the action of the global symmetry group $\Gamma_{2,1}$, defined in (15)–(16) below, on the space of 2-net metrics, defined in (14). We determine, in the fundamental domain, the metrics that are stabilized by different (finite) subgroups of matrices of $\Gamma_{2,1}$ (called the 'lattice groups'). This allows one to give a complete local description of the configuration spaces of deformable 2-nets.

[3] The study of the arithmetic symmetry in the case of simple lattices can be interpreted as the investigation, for each holohedral point group (or crystal system), of how many 'distinct' simple lattices can be constructed sharing that point group (see Bravais, 1850; Pitteri & Zanzotto, 1996). For instance, as was recalled in footnote **1**, the b.c.c. and the f.c.c. structures give distinct arrangements of points in space (as simple lattices) that share the same (cubic) point group. Analogously, for multilattices with a *given* number of atoms per unit cell, the investigation of the arithmetic symmetry can be thought of as the problem of finding in how many distinct ways such atoms can be arranged, for each given space group.

[4] In the classical case of simple lattices, the descriptors are given by the vectors forming the lattice basis; for multilattices, one also needs to take into account the 'shift' vectors giving the positions of the further simple lattices constituting the multilattice.

From this analysis, we also obtain a finite number of lattice groups in $\Gamma_{2,1}$, whose conjugacy properties we investigate completely, thereby determining all the distinct arithmetic types of monoatomic 2-nets. This procedure is analogous to the classical one used for studying the fundamental domains and the Bravais types of simple lattices (see for instance the literature quoted in footnote **2**).

2. 2-nets

In this paper, we shall make constant use of the notions introduced in Pitteri & Zanzotto (1998), hereafter referred to as I. For instance, §I2.2 refers to §2.2 in I.

2.1. Descriptors and configuration spaces of 2-nets

We adopt the usual Grassmann notation for the points and translation vectors in the two-dimensional real affine space $\mathbb{A}^2$, whose origin is denoted by O.

A 2-net is an infinite and discrete subset $\mathcal{M}$ of points in $\mathbb{A}^2$, coinciding with the union of two 'affine simple nets' (also called 1-nets):

$$\mathcal{M} = \mathcal{M}(\mathbf{e}_a, \mathbf{p}) = \{O + \mathcal{L}(\mathbf{e}_a)\} \bigcup \{O + \mathbf{p} + \mathcal{L}(\mathbf{e}_a)\}. \qquad (1)$$

Here, $\mathcal{L}(\mathbf{e}_a)$ denotes a (linear) simple net in the translation space $\mathbb{R}^2$ of $\mathbb{A}^2$, generated by the basis $\mathbf{e}_a$ ($a = 1, 2$):

$$\mathcal{L}(\mathbf{e}_a) = \{ v \in \mathbb{R}^2 \, : \, v = v^a \mathbf{e}_a, \; v^a \in \mathbb{Z} \}. \qquad (2)$$

In (2) and hereafter, the summation convention over repeated indices will be understood.

Given a 2-net $\mathcal{M}$ in $\mathbb{A}^2$, for definiteness in this paper the origin O will always be chosen on a point of $\mathcal{M}$, as is implicit in (1). The simple net $\mathcal{L}(\mathbf{e}_a)$ appearing in (2) is called the *skeletal* net of $\mathcal{M}$; its basis $\mathbf{e}_a$ and its unit cell are also called the skeletal basis and unit cell of $\mathcal{M}$. The skeleton $\mathcal{L}(\mathbf{e}_a)$ can be interpreted, as usual, as a group of translational isometries that map $\mathcal{M}$ onto itself, giving the (two-dimensional) periodicity of the 2-net $\mathcal{M}$. The vector

$$\mathbf{p} = p^1 \mathbf{e}_1 + p^2 \mathbf{e}_2 \qquad (3)$$

in (1) is called the 'shift vector' or simply the 'shift' of $\mathcal{M}$: it gives the separation of the two simple nets constituting $\mathcal{M}$. The vectors ($\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{p}$) are called the *descriptors* of $\mathcal{M}$.

The basis and shift satisfy the conditions:

$$\mathbf{e}_1 \times \mathbf{e}_2 \neq 0 \quad \text{and} \quad \mathbf{p} \neq l^a \mathbf{e}_a, \quad \text{for } l^a \in \mathbb{Z}, \; a = 1, 2; \qquad (4)$$

these guarantee that the simple nets included in $\mathcal{M}$ are two-dimensional and not coincident. We often denote the above vectors by $\boldsymbol{\varepsilon}_\sigma$, $\sigma = 1, 2, 3$, where

$$\boldsymbol{\varepsilon}_a = \mathbf{e}_a, \quad a = 1, 2, \quad \text{and} \quad \boldsymbol{\varepsilon}_3 = \mathbf{p}; \qquad (5)$$

accordingly, we denote the multilattice $\mathcal{M}$ in (1) by $\mathcal{M}(\boldsymbol{\varepsilon}_\sigma)$.

The set of all triples of vectors of $\mathbb{R}^2$ satisfying the conditions in (4) is denoted by $\mathcal{D}_{2,1}$ and is called the space of descriptors or the *configuration space* of 2-nets.

Let $\mathcal{Q}_3$ denote the six-dimensional vector space of all symmetric 3×3 real matrices; it is useful to extend to multilattices the usual notion of lattice metric (or 'Gram matrix') and define the space $\mathcal{Q}_{2,1} \subset \mathcal{Q}_3$ of the *2-net metrics K* such that

$$K = (K_{\sigma\tau}), \quad K_{\tau\sigma} = K_{\sigma\tau} = \boldsymbol{\varepsilon}_\sigma \cdot \boldsymbol{\varepsilon}_\tau \quad \text{for} \quad \boldsymbol{\varepsilon}_\sigma \in \mathcal{D}_{2,1} \qquad (6)$$

($\sigma, \tau = 1, 2, 3$), where the $\boldsymbol{\varepsilon}_\sigma$ satisfy conditions (3)–(5). An element $K \in \mathcal{Q}_{2,1}$ is a 3×3 symmetric matrix which is only positive semi-definite because the vectors $\boldsymbol{\varepsilon}_\sigma$ are not linearly independent in $\mathbb{R}^2$. However, not all the symmetric positive semi-definite matrices belong to $\mathcal{Q}_{2,1}$ because, by definition, the $\boldsymbol{\varepsilon}_\sigma$ in (6) must also satisfy conditions (3)–(5). If we define the usual dual basis

$$\mathbf{e}^a = K^{ab} \mathbf{e}_b \qquad (K^{ab} K_{bc} = \delta^a_c) \qquad (7)$$

of $\mathbf{e}_a$ and express the shift $\mathbf{p}$ as [see (3)]

$$p = p_a \mathbf{e}^a = p^a \mathbf{e}_a, \qquad (8)$$

we see that the explicit form of a 2-net metric $K \in \mathcal{Q}_{2,1}$ defined in (6) is the following (only the entries with $\sigma \geq \tau$ are shown):

$$(K_{\sigma\tau}) = (K_{\tau\sigma}) = \left(\begin{array}{cc|c} K_{11} & K_{12} & K_{13} = p_1 = K_{1a} p^a \\ & K_{22} & K_{23} = p_2 = K_{2a} p^a \\ \hline & & K_{33} = K_{ab} p^a p^b = p_a p^a \end{array} \right), \qquad (9)$$

where p^1 and p^2 are not both in $\mathbb{Z}$. Clearly, $K_{ab} = \mathbf{e}_a \cdot \mathbf{e}_b$ ($a, b = 1, 2$) is but the metric of the skeletal net $\mathcal{L}(\mathbf{e}_a)$. Also, notice that, by (3), (7), (8), $K_{33} = \|\mathbf{p}\|^2$ in (9) is a rational function of the five other independent entries of K; thus the space $\mathcal{Q}_{2,1}$ is a five-dimensional nonlinear submanifold of the six-dimensional vector space $\mathcal{Q}_3$.

It is not difficult to see that, for any two sets of descriptors $\boldsymbol{\varepsilon}_\sigma$ and $\boldsymbol{\varepsilon}'_\sigma$ as in (4)–(6), we have

$$K' = K \;\Leftrightarrow\; \boldsymbol{\varepsilon}'_\sigma = \mathbf{Q} \boldsymbol{\varepsilon}_\sigma \quad \text{for some} \quad \mathbf{Q} \in O(2). \qquad (10)$$

Since we are often interested in properties that are independent of the orientation of a multilattice in $\mathbb{A}^2$, owing to (10) also the space of metrics $\mathcal{Q}_{2,1}$ will be referred to as the 'configuration space' of 2-nets.

Remark. The 2-nets considered so far are, implicitly, *monoatomic*, in that all their points are considered to be physically indistinguishable. However, it is possible to extend the considerations presented here to the *diatomic* case, in which the two simple nets constituting the 2-net in (1) are made of atoms belonging to different species. The only change necessary in what follows is that, in the diatomic case, the variable α defined in formula (16) below can only have the value 1, rather than ± 1 as in the monoatomic case. See point (iii) in §8 for further details.

2.2. Essential descriptors of monoatomic 2-nets

As remarked in §I3.2, certain descriptors $\boldsymbol{\varepsilon}_\sigma$ of monoatomic 2-nets actually give a 1-net in $\mathbb{A}^2$ (see for instance Fig. 1 in I). Such $\boldsymbol{\varepsilon}_\sigma$ are called *nonessential* descriptors of 1-nets, and will be avoided hereafter, as they give rise to various problems [see Ericksen (1998) and Pitteri & Zanzotto (2000) for some details]. This will not hurt our systematic investigation of the arithmetic types of monoatomic 2-nets, for no actual (monoatomic) 2-net is missed if only essential descriptors are considered [for diatomic 2-nets, see point (iii) in §8]. Explicitly, in the configuration space $\mathcal{D}_{2,1}$, the nonessential descriptors are the following:

$$(\mathbf{e}_1,\ \mathbf{e}_2,\ \mathbf{p}) \in \mathcal{D}_{2,1} \text{ is nonessential } \Leftrightarrow\ \mathbf{p} = \tfrac{1}{2}\beta^a \mathbf{e}_a + \mathbf{t}, \quad (11)$$

where $\mathbf{t} \in \mathcal{L}(\mathbf{e}_a)$ and the numbers β^a are

$$\text{either } (1,\ 1) \text{ or a permutation of } (1,\ 0) \quad (12)$$

[also recall the conditions $(4)_2$ on the shift $\mathbf{p}$].

In the rest of the paper, we shall confine ourselves to the portions of the configuration spaces of 2-nets that only contain essential descriptors not satisfying (11)–(12), thus generating monoatomic 2-nets that are *not* 1-nets. Explicitly, we shall consider

$$\mathcal{D}^{\text{ess}}_{2,1} = \left\{(\mathbf{e}_a,\ \mathbf{p}) \in \mathcal{D}_{2,1}\ :\ \mathbf{p} \neq \tfrac{1}{2}\beta^a \mathbf{e}_a + \mathbf{t},\ \beta^a \text{ as in (12)}\right\} \subset \mathcal{D}_{2,1} \quad (13)$$

and

$$\mathcal{Q}^{\text{ess}}_{2,1} = \left\{K \in \mathcal{Q}_{2,1}\ :\ K_{\sigma\tau} = \boldsymbol{\varepsilon}_\sigma \cdot \boldsymbol{\varepsilon}_\tau,\ \boldsymbol{\varepsilon}_\sigma \in \mathcal{D}^{\text{ess}}_{2,1}\right\} \subset \mathcal{Q}_{2,1}. \quad (14)$$

Accordingly, we shall call any $\mathcal{M}(\boldsymbol{\varepsilon}_\sigma)$ as in (1), with $\boldsymbol{\varepsilon}_\sigma \in \mathcal{D}^{\text{ess}}_{2,1}$, an 'essential' monoatomic 2-net. For brevity, also the spaces $\mathcal{D}^{\text{ess}}_{2,1}$ and $\mathcal{Q}^{\text{ess}}_{2,1}$ are referred to as the 'configuration spaces' of (essential) 2-nets.

3. The global symmetry group of monoatomic 2-nets

From now on, we consider only monoatomic essential 2-nets unless otherwise stated.

3.1. The global symmetry group and its action on the configuration spaces

As discussed in I and in Pitteri & Zanzotto (2000), the group of operations describing the general indeterminacy in the choice of multilattice descriptors is the basis for the study of their arithmetic classification; this generalizes the classical procedure used for simple lattices. Here we apply the approach of I to 2-nets: the indeterminacy in the choice of their essential descriptors leads to considering the following discrete group of 'global symmetry' (see Pitteri, 1985):

$$\Gamma_{2,1} < GL(3, \mathbb{Z}), \quad (15)$$

constituted by the unimodular integral 3 × 3 matrices, which, by definition, have the following structure: for $a, b = 1, 2$,

$$\mu \in \Gamma_{2,1}\ \Leftrightarrow\ \mu^\tau_\sigma = \left(\begin{array}{cc|c} \multicolumn{2}{c|}{\multirow{2}{*}{m^b_a}} & l^1 \\ & & l^2 \\ \hline 0 & 0 & \alpha \end{array}\right), \quad (16)$$

where[5] (m^b_a) is any matrix in $GL(2, \mathbb{Z})$, $l^b \in \mathbb{Z}$ and $\alpha = \pm 1$ (recall the *Remark* at the end of §2.1).

[5] $GL(2, \mathbb{Z})$ denotes the group of (invertible) 2 × 2 matrices with integral entries and determinant ±1.

The structure of the matrices $\mu \in \Gamma_{2,1}$ is justified by Proposition 3 in I, which for clarity we recall here for the case of 2-nets:

Proposition 1. Let $\mathcal{M}(\boldsymbol{\varepsilon}_\sigma)$ be an essential monoatomic 2-net. Then, $\bar{\boldsymbol{\varepsilon}}_\sigma$ are new essential descriptors for $\mathcal{M}$ up to a translation [that is, $\mathcal{M}(\bar{\boldsymbol{\varepsilon}}_\sigma) = \mathcal{M}(\boldsymbol{\varepsilon}_\sigma) + \mathbf{t}$, $\mathbf{t} \in \mathbb{R}^2$] if and only if there exists a matrix μ such that

$$\bar{\boldsymbol{\varepsilon}}_\sigma = \mu^\tau_\sigma \boldsymbol{\varepsilon}_\tau, \quad \mu \in \Gamma_{2,1}. \quad (17)$$

The matrix $\mu \in \Gamma_{2,1}$ in (17) determines uniquely the new essential descriptors $\bar{\boldsymbol{\varepsilon}}_\sigma$ and *vice versa*.[6]

Owing to (16) and (17), the new net basis and shift are given explicitly by

$$\bar{\mathbf{e}}_a = m^b_a \mathbf{e}_b, \quad \bar{\mathbf{p}} = \alpha\mathbf{p} + l^a \mathbf{e}_a, \quad (18)$$

where $(m^b_a) \in GL(2, \mathbb{Z})$, $l^a \in \mathbb{Z}$ and $\alpha = \pm 1$.

Proposition 1 shows that the essential descriptors $\boldsymbol{\varepsilon}_\sigma \in \mathcal{D}^{\text{ess}}_{2,1}$ of a 2-net transform by means of a matrix in $\Gamma_{2,1}$ and that the changes of essential descriptors are in a one-to-one correspondence with such matrices. For this reason, we refer to $\Gamma_{2,1}$ as the global symmetry group of monoatomic 2-nets.

A change of descriptors as in (17) induces, in obvious notation, the following transformation of the multilattice metric K in (6):

$$\bar{K} = \mu^T K \mu, \quad (19)$$

where, in general, $\bar{K} \neq K$.[7] Formulae (17) and (19) give natural actions of the group $\Gamma_{2,1}$ on the configuration spaces $\mathcal{D}^{\text{ess}}_{2,1}$ and $\mathcal{Q}^{\text{ess}}_{2,1}$; for instance, the orbit of a given $K \in \mathcal{Q}^{\text{ess}}_{2,1}$ under $\Gamma_{2,1}$ is the set

$$\left\{\mu^T K \mu,\ \mu \in \Gamma_{2,1}\right\} \subset\ \mathcal{Q}^{\text{ess}}_{2,1}. \quad (20)$$

Based on these actions, the arithmetic symmetry of 2-nets will be studied; as we shall need it later on, we explicitly recall that the action (19) of $\Gamma_{2,1}$ on $\mathcal{Q}^{\text{ess}}_{2,1}$ generalizes to 2-nets the usual action

$$C \mapsto m^T C m, \quad C \in \mathcal{C}^+(\mathcal{Q}_2), \quad m \in GL(2, \mathbb{Z}), \quad (21)$$

considered in crystallography for classifying the arithmetic symmetry of *simple* nets (1-nets). In (21), the symbol $\mathcal{C}^+(\mathcal{Q}_2)$ indicates the set of 2 × 2 positive definite symmetric matrices (1-net metrics).

3.2. Lattice groups, point groups, and arithmetic types of 2-nets

Analogously to the case of 1-nets, the arithmetic classification of 2-net symmetry is based on the analysis of the subgroups of $\Gamma_{2,1}$ that act *isometrically* on some 2-net [or, equivalently, that stabilize some 2-net metric under the action (19)], and that are maximal for this property. Therefore, one main focus in what follows will be establishing the (conjugacy

[6] Of course, since the vectors $\boldsymbol{\varepsilon}_i$, $i = 1, 2, 3$, are not linearly independent in $\mathbb{R}^2$, there are infinitely many 3 × 3 matrices relating them to the vectors $\bar{\boldsymbol{\varepsilon}}_\sigma$. This Proposition states that when $\boldsymbol{\varepsilon}_\sigma$ and $\bar{\boldsymbol{\varepsilon}}_\sigma$ are essential, there always is one and only one such matrix in the group $\Gamma_{2,1}$.

[7] As usual, μ^T denotes the transpose of any matrix μ.

properties of the) subgroups of matrices $\mu \in \Gamma_{2,1}$ such that the equation

$$\mu^T K \mu = K \tag{22}$$

holds for some $K \in \mathcal{Q}_{2,1}^{\rm ess}$ – as we shall see, such groups are necessarily finite.

To be precise, let $\boldsymbol{\varepsilon}_\sigma \in \mathcal{D}_{2,1}^{\rm ess}$ with metric $K \in \mathcal{Q}_{2,1}^{\rm ess}$ be given; we define the *lattice group* $\Lambda(\boldsymbol{\varepsilon}_\sigma)$ of the 2-net $\mathcal{M}(\boldsymbol{\varepsilon}_\sigma)$:

$$\Lambda(\boldsymbol{\varepsilon}_\sigma) < \Gamma_{2,1} < GL(3, \mathbb{Z}), \tag{23}$$

as the subgroup of all the integral matrices $\mu \in \Gamma_{2,1}$ such that

$$\begin{aligned}\Lambda(\boldsymbol{\varepsilon}_\sigma) &= \{\mu \in \Gamma_{2,1} \,:\, \mu_\sigma^\tau \boldsymbol{\varepsilon}_\tau = \mathbf{Q}\boldsymbol{\varepsilon}_\sigma,\ \mathbf{Q} \in O(2)\} \\ &= \{\mu \in \Gamma_{2,1} \,:\, \mu^T K \mu = K\} \\ &= \Lambda(K).\end{aligned} \tag{24}$$

By (10), for $\boldsymbol{\varepsilon}_\sigma \in \mathcal{D}_{2,1}^{\rm ess}$ with metric K, the following holds:

$$\mu^T K \mu = K \;\Leftrightarrow\; \mu_\sigma^\tau \boldsymbol{\varepsilon}_\tau = \mathbf{Q}\boldsymbol{\varepsilon}_\sigma \quad \text{for some } \mathbf{Q} \in O(2). \tag{25}$$

For this reason, $(24)_2$ above is true and the lattice group $\Lambda(\boldsymbol{\varepsilon}_\sigma)$ is also denoted $\Lambda(K)$ as in $(24)_3$, for it depends only on the metric K of the descriptors $\boldsymbol{\varepsilon}_\sigma$. This means that, given any $\boldsymbol{\varepsilon}_\sigma \in \mathcal{D}_{2,1}^{\rm ess}$,

$$\Lambda(\mathbf{Q}\boldsymbol{\varepsilon}_\sigma) = \Lambda(\boldsymbol{\varepsilon}_\sigma) \quad \text{for all } \mathbf{Q} \in O(2), \tag{26}$$

so that the lattice group is independent of the orientation of the 2-net in $\mathbb{A}^2$. Furthermore, under a change of descriptors $\bar{\boldsymbol{\varepsilon}}_\sigma = \mu_\sigma^\tau \boldsymbol{\varepsilon}_\tau$ for the 2-net $\mathcal{M}(\boldsymbol{\varepsilon}_\sigma)$ [see (17)], the lattice group transforms as follows, as can be checked directly through (24):

$$\Lambda(\mu_\sigma^\tau \boldsymbol{\varepsilon}_\tau) = \mu^{-1}\Lambda(\boldsymbol{\varepsilon}_\sigma)\mu \quad \text{for all} \quad \mu \in \Gamma_{2,1}. \tag{27}$$

By Proposition 1, this means that any given 2-net $\mathcal{M}(\boldsymbol{\varepsilon}_\sigma)$ determines an entire *conjugacy class* of lattice groups in $\Gamma_{2,1}$. In analogy to the case of 1-lattices, we define two 2-nets $\mathcal{M}$ and $\mathcal{M}'$ to be of the same *arithmetic type* when their lattice groups are $\Gamma_{2,1}$ conjugate. We also say that two metrics K and K' (or two sets of descriptors $\boldsymbol{\varepsilon}_\sigma$ and $\boldsymbol{\varepsilon}'_\sigma$) are of the same arithmetic type when their lattice groups are conjugate in $\Gamma_{2,1}$. This generates a subdivision of $\mathcal{Q}_{2,1}^{\rm ess}$ into equivalence classes [the 'strata' of the action (19)], which are called the arithmetic types within $\mathcal{Q}_{2,1}^{\rm ess}$ (analogously for $\mathcal{D}_{2,1}^{\rm ess}$). We shall thus determine and study the properties of all the conjugacy classes of lattice groups in $\Gamma_{2,1}$ in order to obtain a complete description of the 'arithmetic symmetry types' of 2-nets. In this way, we shall produce an analogue of the subdivision into Bravais types that is classical for simple nets.[8]

To find the lattice groups in $\Gamma_{2,1}$, it will be more convenient to analyse, rather than equation (22), the equations[9]

$$\mathbf{Q}\mathbf{e}_a = m_a^b \mathbf{e}_b, \quad \mathbf{Q}\mathbf{p} = \alpha\mathbf{p} + l^a \mathbf{e}_a \tag{28}$$

for $(\mathbf{e}_a, \mathbf{p}) \in \mathcal{D}_{2,1}^{\rm ess}$ K, $\mathbf{Q} \in O(2)$, $\alpha = \pm 1$, $l^a \in \mathbb{Z}$. By (5), (6), (16), (18) and (25), conditions (28) are equivalent to (22).

[8] The five Bravais types in two dimensions, recalled in the *Introduction*, are obtained in fact by considering the conjugacy classes of lattice groups for 1-nets in $GL(2, \mathbb{Z})$ – see below equation (28). See for instance Theorem 7.8 in Engel (1986), page 141, and §6 below.

[9] Indeed, as in Ericksen (1999*a*), rather than $(28)_2$, we shall study the equivalent equation $m_a^b p^a = \alpha p^b + l^b$.

Given a 2-net $\mathcal{M}(\boldsymbol{\varepsilon}_\sigma)$ with $\boldsymbol{\varepsilon}_\sigma = (\mathbf{e}_a, \mathbf{p})$, the operations $\mathbf{Q} \in O(2)$ that solve $(28)_1$ for some $\mathbf{e}_a$ and $m \in GL(2, \mathbb{Z})$ belong, by definition, to the (holohedral) point group $P(\mathbf{e}_a)$ of the skeletal lattice $\mathcal{L}(\mathbf{e}_a)$; the skeletal lattice group $L(\mathbf{e}_a)$ collects the corresponding matrices $m \in GL(2, \mathbb{Z})$ – see I. The operations $\mathbf{Q} \in O(2)$ satisfying *both* the equations in (28) belong by definition to the point group $P(\boldsymbol{\varepsilon}_\sigma)$ of the 2-net $\mathcal{M}(\boldsymbol{\varepsilon}_\sigma)$. In general, the skeletal point group $P(\mathbf{e}_a)$ is thus larger than the multilattice point group $P(\boldsymbol{\varepsilon}_\sigma)$, as is well known, and is easily seen since the operations in $P(\boldsymbol{\varepsilon}_\sigma)$ must also solve equation $(28)_2$.

We recall (see I) that the lattice group $\Lambda(\boldsymbol{\varepsilon}_\sigma)$ is isomorphic to the point group $P(\boldsymbol{\varepsilon}_\sigma)$ of $\mathcal{M}(\boldsymbol{\varepsilon}_\sigma)$ and is thus necessarily finite. However, $\Lambda(\boldsymbol{\varepsilon}_\sigma)$ carries more information than $P(\boldsymbol{\varepsilon}_\sigma)$: indeed, unlike with the point group, given the group of matrices $\Lambda(\boldsymbol{\varepsilon}_\sigma)$, it is possible to reconstruct uniquely the (isomorphism class of the) space group of $\mathcal{M}(\boldsymbol{\varepsilon}_\sigma)$ – see Proposition 5 in I. This, together with the example in Appendix *A* in I, shows that the arithmetic symmetry of multilattices gives in general a finer classification than their space-group symmetry.

3.3. Fixed sets in the configuration spaces of 2-nets

One main way of obtaining information about the action of $\Gamma_{2,1}$ on the configuration space $\mathcal{Q}_{2,1}^{\rm ess}$ is studying the sets of metrics that share the same lattice group. Thus, given any subgroup Λ of $\Gamma_{2,1}$, we define the *fixed set* $I(\Lambda) \subset \mathcal{Q}_{2,1}^{\rm ess}$ of Λ as follows:

$$I(\Lambda) = \{K \in \mathcal{Q}_{2,1}^{\rm ess} \,:\, \mu^T K \mu = K \text{ for all } \mu \in \Lambda\} \tag{29}$$

[we shall always consider Λ to be a lattice group as in (24), unless otherwise stated]. It can be seen that, by its very definition, if considered in $\mathcal{Q}_3$ rather than in $\mathcal{Q}_{2,1}^{\rm ess}$, the fixed set $I(\Lambda)$ is a linear subspace of $\mathcal{Q}_3$ which contains as subspaces of strictly smaller dimension the fixed sets of any larger lattice group:

$$I(\Lambda') \subset I(\Lambda) \;\Leftrightarrow\; \Lambda < \Lambda'. \tag{30}$$

For a precise description of the symmetry properties of multilattice metrics, it is often useful to consider the *proper fixed set* $I^*(\Lambda)$ of a lattice group Λ, which is defined as the set of metrics K such that their invariance group is exactly Λ and not merely containing Λ as in (29); thus, in general, $I^*(\Lambda) \subseteq I(\Lambda)$ and $I^*(\Lambda)$ is obtained by not considering fixed sets contained in $I(\Lambda)$, that is, any fixed sets of lattice groups $\Lambda' > \Lambda$.

It is not difficult to check that the lattice groups in the same $\Gamma_{2,1}$ conjugacy class as in (27) have fixed sets that are related through the action (19):

$$I(\mu^{-1}\Lambda\mu) = \mu^T I(\Lambda)\mu, \quad \mu \in \Gamma_{2,1}. \tag{31}$$

This means that an arithmetic type in $\mathcal{Q}_{2,1}^{\rm ess}$ is given by an 'orbit' of fixed sets as in (31).

Remark. All the notions introduced here in connection with 2-nets and the related action (19), such as lattice groups, point groups, (proper) fixed sets *etc.*, can be given in a completely analogous way for simple nets and the related action (21). We shall need and use these notions later, and refer to Pitteri & Zanzotto (1998, 2000) for details. Some such definitions were briefly recalled at the end of §3.2.

4. Fundamental domains

As was mentioned in §3.2, the investigation of the conjugacy classes of lattice groups in $\Gamma_{2,1}$ and of the arithmetic types in $\mathcal{Q}_{2,1}^{\rm ess}$ (and $\mathcal{D}_{2,1}^{\rm ess}$) rests on the study of the solutions of equation (22) for $K \in \mathcal{Q}_{2,1}^{\rm ess}$. A main step for this is the determination of a *fundamental domain*, say $\mathcal{D} \subset \mathcal{Q}_{2,1}^{\rm ess}$ for the action (19). This is because one can generate all the solutions to (22) for $K \in \mathcal{Q}_{2,1}^{\rm ess}$ from the knowledge of the solutions to (22) for $K \in \mathcal{D}$, owing to the properties of a fundamental domain $\mathcal{D}$ – see below. Examining the solutions of (22) for $K \in \mathcal{D}$ is a manageable task because, for the action of a discrete group like $\Gamma_{2,1}$, such solutions are constituted by a *finite* number of lattice groups with their fixed sets. Studying these will be our goal in the rest of this paper.

4.1. Fundamental domain for the action of the group $\Gamma_{2,1}$ on $\mathcal{Q}_{2,1}^{\rm ess}$

A fundamental domain $\mathcal{D} \subset \mathcal{Q}_{2,1}^{\rm ess}$ is a (simply connected) region such that each $\Gamma_{2,1}$ orbit in $\mathcal{Q}_{2,1}^{\rm ess}$ has *one and only one* element in $\mathcal{D}$. The elements $K \in \mathcal{Q}_{2,1}^{\rm ess}$ satisfying conditions (32)–(33) below ('reduced forms' in $\mathcal{Q}_{2,1}^{\rm ess}$) define a fundamental domain $\mathcal{D} \subset \mathcal{Q}_{2,1}^{\rm ess}$ for the action (19):

$$0 < K_{11} \le K_{22}, \quad 0 \le K_{12} \le K_{11}/2, \tag{32}$$

$$\begin{aligned} -K_{11}/2 &< K_{13} \equiv p_1 \le K_{11}/2, \\ -K_{22}/2 &< K_{23} \equiv p_2 \le K_{22}/2, \\ -(K_{11} - 2K_{12} + K_{22})/2 &< K_{23} - K_{13} \le (K_{11} - 2K_{12} + K_{22})/2 \end{aligned} \tag{33}$$

[recall the exclusions for $\mathbf{p}$ indicated in (13)]. There is an explicit geometrical interpretation of formulae (32)–(33), indicated by Parry (1978),[10] who implicitly proves that $\mathcal{D}$ is indeed a fundamental domain. Given a 2-net $\mathcal{M} = \mathcal{M}(\tilde{\boldsymbol{\varepsilon}}_\sigma)$, whose descriptors $\tilde{\boldsymbol{\varepsilon}}_\sigma = (\tilde{\mathbf{e}}_a, \tilde{\mathbf{p}}) \in \mathcal{D}_{2,1}^{\rm ess}$ have metric $\tilde{K}$, the reduced form K of $\tilde{K}$, *i.e.* the element of the $\Gamma_{2,1}$ orbit of $\tilde{K}$ that satisfies (32)–(33), is the metric K of the unique set of descriptors $\boldsymbol{\varepsilon}_\sigma = (\mathbf{e}_a, \mathbf{p})$ of $\mathcal{M}$ obtained through the following procedure:

(i) Select as basis of the skeletal net $\mathcal{L}(\mathbf{e}_a)$ of $\mathcal{M}(\boldsymbol{\varepsilon}_\sigma)$ two noncollinear vectors $\mathbf{e}_1$, $\mathbf{e}_2$ in such a way that

$$\|\mathbf{e}_1\| \le \|\mathbf{e}_2\| \quad \text{and} \quad (\mathbf{e}_1 \cdot \mathbf{e}_2) \le \mathbf{e}_1^2/2. \tag{34}$$

This skeletal basis always exists and is unique; it involves the two shortest elementary translation vectors in $\mathcal{L}(\mathbf{e}_a)$, suitably ordered and forming an acute (or right) angle. From (34), we get the reduction conditions (32); see §4.2 below for further details.

(ii) Construct the *Wigner–Seitz elementary cell* $\mathcal{W}(\mathbf{e}_a)$[11] of $\mathcal{L}(\mathbf{e}_a)$, defined by (see Fig. 1)

$$\mathcal{W}(\mathbf{e}_a) = \Big\{\mathbf{v} = v_a \mathbf{e}^a \in \mathbb{R}^2 \,:\, -\mathbf{e}_a^2/2 < v_a \le \mathbf{e}_a^2/2, \\ -(\mathbf{e}_1 \pm \mathbf{e}_2)^2/2 < v_2 \pm v_1 \le (\mathbf{e}_1 \pm \mathbf{e}_2)^2/2\Big\}, \tag{35}$$

and take the unique shift vector $\mathbf{p}$ of $\mathcal{M}(\boldsymbol{\varepsilon}_\sigma)$, such that $\mathbf{p} \in \mathcal{W}(\mathbf{e}_a)$. Parry (1978) has shown that under (34) such $\mathbf{p}$ always exists and is the shortest shift vector for $\mathcal{M}$:

$$\|\mathbf{p}\| \le \|\mathbf{p} + m^a \mathbf{e}_a\| \tag{36}$$

for all $m^a \in \mathbb{Z}$. A vector $\mathbf{p} \in \mathcal{W}(\mathbf{e}_a)$ satisfies the conditions (recall that p_1 and p_2 are not both zero):

$$\begin{aligned} -K_{11}/2 &< p_1 \equiv K_{13} \le K_{11}/2, \\ -K_{22}/2 &< p_2 \equiv K_{23} \le K_{22}/2, \\ -(K_{11} \pm 2K_{12} + K_{22})/2 &< K_{23} \pm K_{13} \le (K_{11} \pm 2K_{12} + K_{22})/2. \end{aligned} \tag{37}$$

In view of $(32)_2$, the last condition actually yields

$$-(K_{11} - 2K_{12} + K_{22})/2 < K_{23} - K_{13} \le (K_{11} - 2K_{12} + K_{22})/2, \tag{38}$$

so that the metric K of $(\mathbf{e}_a, \mathbf{p})$ satisfies (32)–(33), that is, $K \in \mathcal{D}$. Recall that as we consider only $(\mathbf{e}_a, \mathbf{p})$ in $\mathcal{D}_{2,1}^{\rm ess}$ (that is, $K \in \mathcal{Q}_{2,1}^{\rm ess}$), some points in $\mathcal{W}(\mathbf{e}_a)$ in (35) are actually not allowed for $\mathbf{p}$ – see (13).

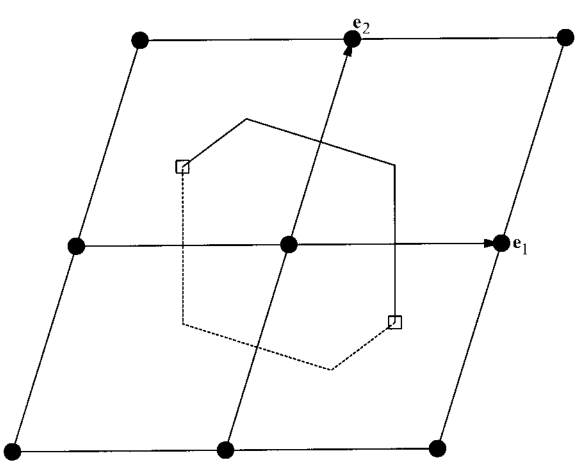

Figure 1
The Wigner–Seitz cell for a simple net of the rhombic type, in which $\|\mathbf{e}_1\| = \|\mathbf{e}_2\|$. The portion of the boundary of the cell that is included in $\mathcal{W}$ in (35) is indicated by solid lines. The hollow squares indicate that the two points in the boundary of $\partial\mathcal{W}$ are not included in $\mathcal{W}$. The symmetry axes and mirrors of $\mathcal{W}$ coincide with those of the lattice.

4.2. Fundamental domain for the action of $GL(2, \mathbb{Z})$ on $C^+(\mathcal{Q}_2)$

Let us consider in the six-dimensional space $\mathcal{Q}_3$ the subspace described by the first three coordinates K_{11}, K_{12}, K_{22}.

[10] See Pitteri (1985) for the case of general multilattices.
[11] We use this denomination because we consider all vectors in direct space, regardless of the basis used. However, as we define $\mathcal{W}$ in (35) through conditions on the covariant coordinates of its vectors, $\mathcal{W}$ may also be called the 'first Brillouin zone', as in Parry (1978). Notice that in definition (35) we do not consider all the boundary of the topological closure $\overline{\mathcal{W}}$ of $\mathcal{W}$. This is because a vector $\mathbf{p} \in \partial\overline{\mathcal{W}}$ is defined uniquely by (36) only if 'half' of $\partial\overline{\mathcal{W}}$ is counted, as in (35) – this is analogous to the classical discussion arising in reciprocal space for the wave-vectors $\mathbf{k}$ belonging to the boundary of the first Brillouin zone. Notice that the two points in the boundary of $\partial\mathcal{W}$ are not included in $\mathcal{W}$ – see Fig. 1.

The 'projection' of the fundamental domain $\mathcal{D} \subset \mathcal{Q}_{2,1}^{\rm ess}$ on such subspace gives a fundamental domain $\mathcal{D}'$, which is the one classically considered for the action (21) of $GL(2, \mathbb{Z})$ on the space $\mathcal{C}^+(\mathcal{Q}_2)$ of 1-net metrics (see Fig. 2):

$$\mathcal{D}' = \left\{ C \in \mathcal{C}^+(\mathcal{Q}_2) \,:\, 0 < C_{11} \leq C_{22},\ 0 \leq 2C_{12} \leq C_{11} \right\} \quad (39)$$

– compare with conditions (32) on the elements K_{ab} of the metrics $K \in \mathcal{D}$ $(a, b = 1, 2)$. The simple net metrics $C \in \mathcal{D}'$ are said to have the 'reduced form of Lagrange'; see Engel (1986); see also Michel (1995) and Figs. 1–2 therein.

5. Some useful lemmas

Having defined a fundamental domain $\mathcal{D}$ in $\mathcal{Q}_{2,1}^{\rm ess}$, we shall investigate the proper fixed sets having a nontrivial intersection[12] with $\mathcal{D}$ and analyse the conjugacy properties of their lattice groups. We shall do so by studying equation (22) for $K \in \mathcal{D}$ or, indeed, equations (28) for $(\mathbf{e}_a, \mathbf{p})$ such that (32) holds for $\mathbf{e}_a$ and $\mathbf{p} \in \mathcal{W}(\mathbf{e}_a)$ in (35). Before proceeding, we give some lemmas useful for these computations.

First, notice that $-\mathbf{1} \equiv {\rm diag}(-1, -1, -1) \in \Gamma_{2,1}$. This implies that all the (monoatomic) 2-nets are centrosymmetric. Furthermore, since $-\mathbf{1}$ trivially solves equation (22) for all $K \in \mathcal{Q}_{2,1}^{\rm ess}$, we have:

Lemma 1. The lattice groups (24) of monoatomic 2-nets all contain the matrix $-\mathbf{1} \in \Gamma_{2,1}$. Thus, for all $K \in \mathcal{Q}_{2,1}^{\rm ess}$, it follows that

$$\Lambda(K) = \Lambda(K)^+ \cup -\Lambda(K)^+, \quad (40)$$

where $\Lambda(K)^+$ is the subgroup of matrices μ in $\Lambda(K)$ such that $\alpha = 1$ [see (16)].

This lemma will be used to cut in half the computation of lattice groups deriving from (25) or $(28)_2$, because only the matrices in the subgroup $\Lambda(K)^+$ of any lattice group $\Lambda(K)$ need to be determined.[13] We shall thus consider equation $(28)_2$ only for $\alpha = 1$: any solution $(\mathbf{Q}, l^a)$ of $(28)_2$ found for a given $\mathbf{p}$ and $\alpha = 1$ then generates another solution $(-\mathbf{Q}, -l^a)$ for the same $\mathbf{p}$ and $\alpha = -1$ [notice that, given $\mathbf{p}$, $\mathbf{Q}$ solves (28) if and only if $-\mathbf{Q}$ does].

Let $\mathcal{W}^\circ(\mathbf{e}_a)$ denote the interior of the Wigner–Seitz cell defined in (35). The following results will help to reduce the computations in what follows:

Lemma 2. Let $\mathbf{e}_a$ be given, such that (32) holds for $K_{ab} = \mathbf{e}_a \cdot \mathbf{e}_b$, and let $\mathbf{Q} \in O(2)$ solve $(28)_1$ for $\mathbf{e}_a$ and some $m \in GL(2, \mathbb{Z})$.[14] In equation $(28)_2$, considered for $(\mathbf{e}_a, \mathbf{p})$ with $\mathbf{e}_a$ as above and $\mathbf{p} \in \mathcal{W}(\mathbf{e}_a)$, the following statements are true for $a = 1, 2$:

(i) if $\mathbf{p} \in \mathcal{W}^\circ$, then $l^a = 0$;

(ii) if $\mathbf{p} \in \partial\mathcal{W}$, then $l^a \in \{-1, 0, 1\}$.

Now, let us consider any set of descriptors $(\mathbf{e}_a, \mathbf{p})$ such that (32) holds for $\mathbf{e}_a$ and any solution $(\mathbf{Q}, m)$ of the related equation $(28)_1$ [that is, $\mathbf{Q} \in P(\mathbf{e}_a)$ with the corresponding matrix $m \in L(\mathbf{e}_a)$]. Also, let us denote by $M_{\mathbf{Q}}$ (mirror of $\mathbf{Q}$) the eigenspace of $\mathbf{Q}$ corresponding to the eigenvalue 1, if it exists. Then the following result is useful for checking whether $\mathbf{Q}$ can also solve equation $(28)_2$ for $\alpha = 1$:

Corollary 1. Let $\mathbf{e}_a$ satisfy (32) and $\pm\mathbf{1} \neq \mathbf{Q} \in P(\mathbf{e}_a)$ and $\pm 1 \neq m \in L(\mathbf{e}_a)$ satisfy $(28)_1$. Then, in checking whether $\mathbf{Q}$ also satisfies $(28)_2$ for $\mathbf{0} \neq \mathbf{p} \in \mathcal{W}(\mathbf{e}_a)$, $l^a \in \mathbb{Z}$ and $\alpha = 1$, the following cases arise (the case $\mathbf{Q} = \pm\mathbf{1}$ is trivial):

(i) $\mathbf{p} \in \partial\mathcal{W}$ $\Rightarrow$ any solutions of $(28)_2$ have $l^a \in \{-1, 0, 1\}$;

(ii) $M_{\mathbf{Q}}$ exists, $\mathbf{p} \in \mathcal{W}^\circ \cap M_{\mathbf{Q}} \Rightarrow (28)_2$ is solved by $l^a = 0$, that is, (25) is solved by

$$\left(\begin{array}{cc|c} \multicolumn{2}{c|}{\multirow{2}{*}{m}} & 0 \\ & & 0 \\ \hline 0 & 0 & 1 \end{array} \right);$$

(iii) if: $M_{\mathbf{Q}}$ exists, $\mathbf{p} \in \mathcal{W}^\circ \backslash M_{\mathbf{Q}}$, or $M_{\mathbf{Q}}$ does not exist, $\mathbf{p} \in \mathcal{W}^\circ$, then $(28)_2$ does not admit any solutions.

The proofs of these results are given in Appendix *A*.

6. The fixed sets intersecting the fundamental domain $\mathcal{D}' \subset \mathcal{C}^+(\mathcal{Q}_2)$ and their lattice groups

6.1. Solutions to $(28)_2$

As mentioned earlier, the determination of the fixed sets in $\mathcal{Q}_{2,1}^{\rm ess}$ that intersect the fundamental domain $\mathcal{D}$ is based on the analysis of equation (28) for $(\mathbf{e}_a, \mathbf{p})$ such that $\mathbf{e}_a$ satisfy (32) and $\mathbf{p} \in \mathcal{W}(\mathbf{e}_a)$, aided by the Lemmas in §5.

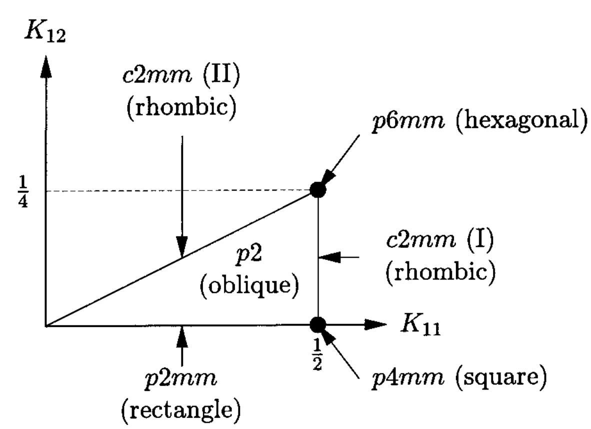

Figure 2
Two-dimensional section, in the plane $K_{11} + K_{22} = 1$, of the fundamental domain $\mathcal{D}'$ in the space (K_{11}, K_{22}, K_{12}) for two-dimensional simple lattices (Lagrange reduced forms for two-dimensional positive-definite quadratic forms); also indicated are the fixed sets intersecting $\mathcal{D}'$ listed in Table 1.

[12] That is, we shall determine all the fixed sets I in $\mathcal{Q}_{2,1}^{\rm ess}$ such that the intersection of their proper part I^* with $\mathcal{D}$ [see below (30)] has the full dimensionality of I^*: $\dim I^* = \dim I^* \cap \mathcal{D}$.

[13] We notice that if an operation $\mathbf{Q}$ of the point group $P(\varepsilon_\sigma)$ corresponds, through equations (25) or (28), to a matrix $\mu \in \Lambda(\varepsilon_\sigma)^+$, then, with the choice made in (1) for the origin O, the operation $(\mathbf{Q}|\mathbf{0})$ belongs to the space group $\mathcal{S}(\mathcal{M}(\varepsilon_\sigma))$ of the 2-net $\mathcal{M}(\varepsilon_\sigma)$. However, the operation $-\mathbf{Q}$, corresponding to the matrix $-\mu \in -\Lambda(\varepsilon_\sigma)^+$, gives the affine operation $(-\mathbf{Q}|\mathbf{p}) \in \mathcal{S}(\mathcal{M}(\varepsilon_\sigma))$, which involves also a translation $\mathbf{p}$.

[14] That is, $\mathbf{Q} \in P(\mathbf{e}_a)$ – the skeletal point group – and $m \in L(\mathbf{e}_a)$ – the skeletal lattice group (see at the end of §3.2).

The first step for this is giving a complete description of the solutions to equations $(28)_1$ under conditions (32) [or (34)] for $\mathbf{e}_a$, that is, in the fundamental domain $\mathcal{D}'$ in $\mathcal{C}^+(\mathcal{Q}_2)$ defined in §4.2. These are well known computations in crystallography, giving the (holohedral) point groups and lattice groups of the 1-nets with Lagrange-reduced metrics. One of their consequences is the description of the fixed sets in $\mathcal{C}^+(\mathcal{Q}_2)$ intersecting $\mathcal{D}'$ and the ensuing classical results about the Bravais types of 1-nets; we briefly discuss these results in §6.2 [see Engel (1986) or Michel (1995) for details].

We shall then proceed, in §7, to the analysis of equations $(28)_2$, which will give us explicitly the fixed sets in $\mathcal{Q}_{2,1}^{\rm ess}$ intersecting $\mathcal{D}$.

6.2. The fixed sets intersecting $\mathcal{D}'$ and the Bravais types of 1-nets

The conditions defining the fundamental domain $\mathcal{D}'$ for the action (21) of $GL(2, \mathbb{Z})$ on $\mathcal{C}^+(\mathcal{Q}_2)$ are given in §4.2. The subdivision of $\mathcal{D}'$ into fixed sets and their classification according to their Bravais net types (two-dimensional Bravais lattice types), *i.e.* to the conjugacy class in $GL(2, \mathbb{Z})$ of their lattice groups, is given in Table 1. There exist *five* such classes, that is, five Bravais net types, which are represented by *six* (portions of) fixed sets intersecting $\mathcal{D}' \subset \mathcal{C}^+(\mathcal{Q}_2)$. The same table lists the Bravais types, giving their International (Hermann–Mauguin) symbol, the equations for the related fixed sets intersecting $\mathcal{D}'$ and the corresponding lattice groups. Each matrix represents, with respect to the net basis, an orthogonal operation belonging to the (two-dimensional) point group of the net. See Fig. 2 for a geometrical representation of $\mathcal{D}'$ and Fig. 3(*a*) for a picture of the different net cells.

7. The fixed sets intersecting $\mathcal{D} \subset \mathcal{Q}_{2,1}^{\rm ess}$ and the corresponding lattice groups

From Table 1, we see that there are six 'classes' of solutions to equations $(28)_1$ for $\mathbf{e}_a$ satisfying (32); we now examine separately, aided by the results in §5, the solutions of $(28)_2$ for each such class,[15] with $\mathbf{p}$ belonging to the corresponding Wigner–Seitz cell $\mathcal{W}(\mathbf{e}_a)$. In each case, we have a set of $\mathbf{Q}$'s and m's to test in $(28)_2$; the solutions l^a and α will vary as the vector $\mathbf{p}$ varies in $\mathcal{W}(\mathbf{e}_a)$. This will tell us which groups of matrices μ – *i.e.* which lattice groups in $\Gamma_{2,1}$ – arise as K varies in the corresponding portions of $\mathcal{D}$. Recall that, by Lemma 1, we actually only need to check explicitly the case $\alpha = 1$.

7.1. The arithmetic types of monoatomic 2-nets

As the computations related to $(28)_2$ are somewhat cumbersome, only one example will be given explicitly in Appendix *B*. This analysis shows that *five* distinct arithmetic types of monoatomic 2-nets exist, represented by 13 fixed sets

[15] If we only wanted to determine the distinct arithmetic types in $\mathcal{Q}_{2,1}^{\rm ess}$, only five of these six classes of solutions of $(28)_1$ would have to be checked for $(28)_2$, because two fixed sets in Table 1 give the same skeletal type. However, we make the complete analysis so as to give an explicit description of the entire fundamental domain $\mathcal{D}$ in $\mathcal{Q}_{2,1}^{\rm ess}$.

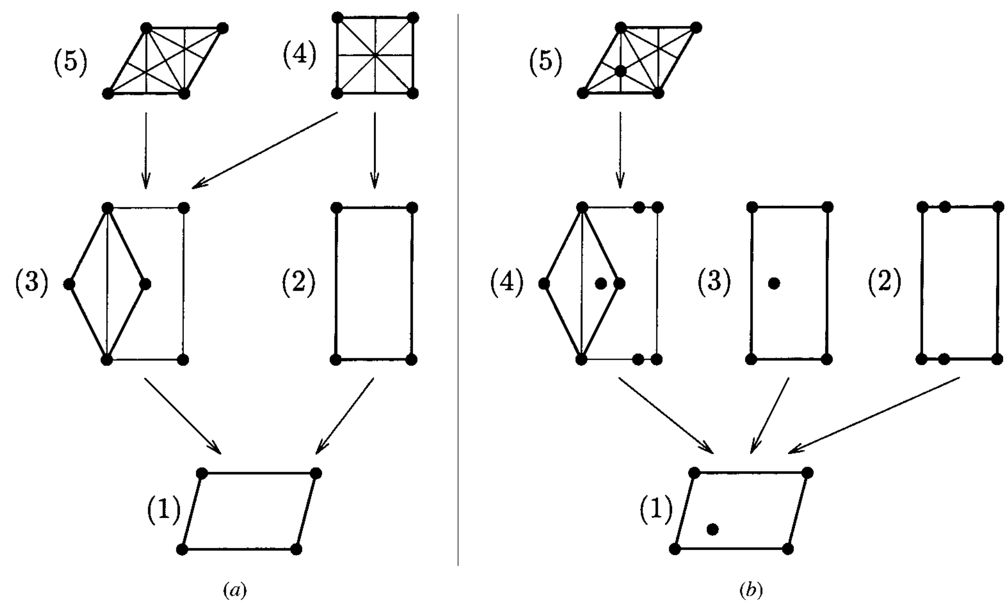

Figure 3
The unit cells of the distinct arithmetic types of monoatomic 1- and 2-nets, and their symmetry hierarchies. The numbering refers to the tables. The dots represent the lattice points in the unit cells, which are delimited by thick lines. (*a*) Schematic representation of the unit cells of the five distinct arithmetic types of simple nets (two-dimensional Bravais lattices). The primitive rectangular and centred-rectangular types belong to the same two-dimensional crystal system. The arrows indicate the group–subgroup relations of the lattice groups, up to $GL(2, \mathbb{Z})$ conjugacy. (*b*) Schematic representation of the unit cells of the five distinct arithmetic types of monoatomic 2-nets (two atoms per unit cell) – see Table 2. The arrows indicate the group–subgroup relations of the corresponding lattice groups, up to $\Gamma_{2,1}$ conjugacy.

intersecting $\mathcal{D}$ (see footnote **12**). The full results are summarized in Table 2, where for each type in $\mathcal{Q}_{2,1}^{\rm ess}$ we indicate the crystal class and the crystal system, the skeletal type, the plane group (two-dimensional space group) and the fixed sets intersecting $\mathcal{D}$, with their lattice groups. Fig. 3 represents schematically the 2-net cells of the five types and the group–subgroup relations among their lattice groups (up to $\Gamma_{2,1}$ conjugacy).

Here we only make some brief remarks about the arithmetic types listed in Table 2 (see Fig. 3).

(i) The 2-nets of the *oblique* type are generated by descriptors whose metric K is a generic element of $\mathcal{D}$, *not* belonging to any of the other fixed sets indicated below (that is, the corresponding proper fixed set is dense in $\mathcal{D}$); in this case, the lattice group is the trivial group Λ_{p2} in Table 2.

(ii) The 2-nets of the *side-rectangular* type have a skeleton with a primitive-rectangular mesh and extra atoms lying symmetrically on two opposite sides of the skeletal cell (hence the name); the two (conjugate) lattice groups Λ^1_{p2mm} and Λ^2_{p2mm} in Table 2 give two (proper) fixed sets belonging to this type and intersecting $\mathcal{D}$. This type has maximal symmetry in $\mathcal{Q}_{2,1}^{\rm ess}$, that is, no higher-symmetry monoatomic 2-net metric is contained in these fixed sets.

(iii) The 2-nets of the *axis-rectangular* type have a primitive-rectangular skeleton as the previous 2-nets, but the extra atom in the cell lies along one of the mirrors within the skeletal cell; in this case, there are again two conjugate lattice groups giving two (proper) fixed sets in this arithmetic type and intersecting the fundamental domain $\mathcal{D}$. Also, this type has maximal symmetry.

(iv) The *rhombic* 2-nets have a skeleton of the rhombic (*i.e.* centred-rectangular) Bravais type, and the extra atom on one of the mirrors within the unit cell [but in such a way not to meet the extra conditions giving a hexagonal 2-net as in point (v) below]. Six[16] proper fixed sets of this type intersect the fundamental domain $\mathcal{D}$, whose lattice groups are all conjugate. We notice explicitly that while there exist two distinct types of monoatomic 2-nets with a primitive-rectangular skeleton (see the two previous cases), only one type has a centred-rectangular skeletal net.

(v) The *hexagonal* 2-nets have a skeleton of the hexagonal Bravais type, with the second atom lying at the centre of the equilateral triangle giving a half unit cell. Two hexagonal fixed sets with conjugate lattice groups intersect $\mathcal{D}$. This type has maximal symmetry, achieved when the limit rhombic cases: $K_{11} = K_{22}$, $K_{12} = K_{11}/2$ with $K_{13} = K_{23} = K_{11}/2$, or with $K_{13} = 0$, $K_{23} = K_{11}/2$ are met.

[16] Besides the six rhombic fixed sets mentioned here, which are listed in Table 2, one can see that also three more rhombic fixed sets do intersect $\mathcal{D}$. However, such intersections only contain metrics of rhombic 2-nets with a hexagonal skeletal net as in point (v) below. These are thus cases of excess skeletal symmetry as discussed in point (i) of §8, that is, their intersections with $\mathcal{D}$ are lower-dimensional in the sense specified in footnote **12**. For this reason, such fixed sets are not listed in Table 2. The same happens with the intersection of some rhombic and rectangular fixed sets that meet $\mathcal{D}$ in lower-dimensional manifolds that contain 2-nets with square skeletal symmetry, and which do not give any square lattice group – see also footnote **20**.

8. Concluding remarks

The arithmetic criterion introduced in I for describing the symmetry of multilattices extends in a natural way the classical approach leading to the classification of simple lattices into Bravais lattice types. It also gives the most natural way of describing the symmetry changes occurring in deformable crystals and is at the basis of various recent models that allow for a detailed description of phase transitions in complex crystalline structures and related phenomena.

In this paper, we have made a systematic investigation of the arithmetic symmetry of monoatomic 2-nets, describing a fundamental domain and determining their five distinct arithmetic types and their main properties (these results are summarized in Table 2 and Fig. 3). The following remarks may help clarify the results presented here.

(i) The fundamental domain $\mathcal{D}$ for the action (19) related to 2-nets has a more complex structure than the classical domain $\mathcal{D}'$ in (21) considered for simple nets (compare Tables 1 and 2). However, unlike what may have been intuitively expected, the number of distinct arithmetic types is the same for (monoatomic) 1- and 2-nets (see Figs. 3*a* and 3*b*). Partly, this is because often it is *not* possible for multilattices to have a skeleton that generically exhibits too high a symmetry. For instance, there are no generic (monoatomic) 2-nets with a square skeletal mesh, as any such 2-net gives an example of 'excess skeletal symmetry'. By this we mean skeletal symmetry relations not producing an increase of symmetry for the entire multilattice, *i.e.* not generating a larger lattice group.[17] This phenomenon, which is well known and rather common in multilattices, contributes to cut down the number of their arithmetic types relative to the number of Bravais types that are possible for the skeleton [*i.e.* it reduces the number of solutions of equation $(28)_2$ that constitute an actual fixed set, if compared to the possible solutions of $(28)_1$].

Physically, one expects a skeleton with 'excessive' symmetry not to be a stable feature of a multilattice, as pointed out for instance by Landau & Lifshitz (1959).[18] For instance, free thermal expansion should not maintain such a property, as, under varying temperature, the crystal descriptors are expected to vary generically within a given fixed set in the configuration space and not in some lower-dimensional submanifold of it, in which the skeleton has (too) high symmetry.

(ii) Fig. 3 shows schematically the unit cells of the 2-nets for each type described in §7; the figure indicates, moreover, the

[17] One can check that an extra atom in a square cell necessarily makes the lattice group shrink to a rhombic or rectangular group, if the second atom lies on one of the cell mirrors, or to the trivial group otherwise. Analogous are the various cases in which a 2-net has any non-oblique skeletal type but whose second atom is in a generic position at the interior of the Wigner–Seitz cell (not on a symmetry axis or a mirror of the net). Indeed, statement (iii) in Corollary 1 indicates that in this case there will not be nontrivial solutions to equation (28): thus, the corresponding 2-nets are actually of the oblique type in spite of their non-oblique skeleton. In Appendix *B*3, we show and briefly discuss an explicit example of solutions of $(28)_2$ with excess skeletal symmetry, which do not give an actual fixed set.

[18] From Landau & Lifshitz (1959), §130: '... Indeed it is physically highly improbable that the atoms of a crystal belonging to its Bravais lattice should be distributed more symmetrically than the symmetry of the crystal requires'.

Table 2
The arithmetic types of two-dimensional monoatomic 2-nets.

For each type, the (proper) fixed sets intersecting the fundamental domain $\mathcal{D}$ defined in (32)–(33) and (11)–(12) are indicated, with the corresponding lattice groups [only the elements of the subgroups Λ^+ in (40) are listed, with generators, marked by †, given first]. See Fig. 3(*b*) for the picture of the 2-lattice unit cells.

No.	Arithmetic type of 2-net	Skeletal type (see Table 1) Crystal system Crystal class		Fixed sets intersecting $\mathcal{D}$ (see also Table 1)	Symbol	Lattice group (subgroup Λ^+)	Plane group
1	Oblique	Oblique 2 2		Any $K_{13},\ K_{23}$	Λ_{p2}	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	*p*2
2	Side-rectangular	Primitive rectangular 2*mm* 2*mm*		$K_{13}=0$	Λ^1_{p2mm}	$\begin{pmatrix}-1&0&0\\0&1&0\\0&0&1\end{pmatrix}^\dagger, \begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	*p*2*mm*
				$K_{23}=0$	Λ^2_{p2mm}	$\begin{pmatrix}1&0&0\\0&-1&0\\0&0&1\end{pmatrix}^\dagger, \begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	
3	Axis-rectangular	Primitive rectangular 2*mm* 2*mm*		$K_{13}=K_{11}/2$	Λ^1_{p2mg}	$\begin{pmatrix}-1&0&-1\\0&1&0\\0&0&1\end{pmatrix}^\dagger, \begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	*p*2*mg*
				$K_{23}=K_{22}/2$	Λ^2_{p2mg}	$\begin{pmatrix}1&0&0\\0&-1&-1\\0&0&1\end{pmatrix}^\dagger, \begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	
4	Rhombic	Rhombic (centred-rectangular) 2*mm* 2*mm*	I	$K_{13}=K_{23}$	Λ^1_{c2mm}	$\begin{pmatrix}0&1&0\\1&0&0\\0&0&1\end{pmatrix}^\dagger, \begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	*c*2*mm*
				$K_{23}-K_{13}=K_{11}-K_{12}$	Λ^2_{c2mm}	$\begin{pmatrix}0&1&1\\1&0&-1\\0&0&1\end{pmatrix}^\dagger, \begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	
				$K_{13}=-K_{23}$	Λ^3_{c2mm}	$\begin{pmatrix}0&-1&0\\-1&0&0\\0&0&1\end{pmatrix}^\dagger, \begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	
			II	$K_{13}=2K_{23}$	Λ^4_{c2mm}	$\begin{pmatrix}1&1&0\\0&-1&0\\0&0&1\end{pmatrix}^\dagger, \begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	
				$K_{13}=K_{11}/2$	Λ^5_{c2mm}	$\begin{pmatrix}-1&-1&-1\\0&1&0\\0&0&1\end{pmatrix}^\dagger, \begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	
				$K_{13}=0$	Λ^6_{c2mm}	$\begin{pmatrix}-1&-1&0\\0&1&0\\0&0&1\end{pmatrix}^\dagger, \begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	
5	Hexagonal	Hexagonal 6*mm* 6*mm*		$K_{13}=K_{23}=K_{11}/2$	Λ^1_{p6mm}	$\begin{pmatrix}-1&-1&-1\\1&0&0\\0&0&1\end{pmatrix}^\dagger, \begin{pmatrix}0&1&0\\1&0&0\\0&0&1\end{pmatrix}^\dagger, \begin{pmatrix}-1&-1&-1\\0&1&0\\0&0&1\end{pmatrix}^\dagger,$ $\begin{pmatrix}1&0&0\\-1&-1&-1\\0&0&1\end{pmatrix}^\dagger, \begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}, \begin{pmatrix}0&1&0\\-1&-1&-1\\0&0&1\end{pmatrix}$	*p*6*mm*
				$K_{13}=0$ $K_{23}=K_{11}/2$	Λ^2_{p6mm}	$\begin{pmatrix}-1&-1&0\\1&0&-1\\0&0&1\end{pmatrix}^\dagger, \begin{pmatrix}0&1&1\\1&0&-1\\0&0&1\end{pmatrix}^\dagger, \begin{pmatrix}-1&-1&0\\0&1&0\\0&0&1\end{pmatrix}^\dagger,$ $\begin{pmatrix}1&0&0\\-1&-1&-1\\0&0&1\end{pmatrix}^\dagger, \begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}, \begin{pmatrix}0&1&1\\-1&-1&-1\\0&0&1\end{pmatrix}$	

symmetry hierarchies existing among the five distinct types. These hierarchies are given by the group–subgroup relations (up to conjugacy in $\Gamma_{2,1}$) among the lattice groups of the distinct types, which we present in Fig. 3 without proof. Equivalently, by (30), such relations give the inclusion relations for the fixed sets pertaining to the various types. This knowledge allows one to describe the local structure (around any given point) of the configuration spaces for monoatomic 2-nets, that is, of the Ericksen–Pitteri neighbourhoods in $\mathcal{D}_{2,1}^{\rm ess}$ and $\mathcal{Q}_{2,1}^{\rm ess}$ (see for instance Ericksen, 1980, 1998, 1999*a*; Pitteri, 1984, 1985). A detailed description of the latter is left for further work. A complete study of the neighbourhoods for three-dimensional simple lattices can be found in Zanzotto (1999) and Pitteri & Zanzotto (2000). This information has proved very helpful in the investigation of phase transitions in crystalline materials, especially those involving small lattice distortions and a symmetry breakdown, and for the understanding of transformation twinning. The same approach will give valuable insight regarding these phenomena also in the case of multilattices; see James (1987), Bhattacharya *et al.* (1993) for some related work, and Ericksen (1997, 1999*b*) for recent novel ideas on this subject.

(iii) As was remarked at the end of §2, the results obtained in this paper about the lattice groups of monoatomic 2-nets carry through to the *diatomic* case, provided we only consider matrices μ with $\alpha = 1$, rather than $\alpha = \pm 1$, in (15)–(16) and in all the ensuing lattice groups. However, this is not sufficient to classify completely all the arithmetic types of diatomic 2-nets. The reason is that while the 'nonessential' positions of the shift $\mathbf{p}$ when $\varepsilon_\sigma \in \mathcal{D}_{2,1}\backslash\mathcal{D}_{2,1}^{\rm ess}$ must be excluded in the monoatomic case, because they give 1-nets rather than 2-nets, the latter positions cannot be excluded in the diatomic case as they do give admissible diatomic 2-nets. The complete analysis of diatomic 2-nets is left for future works.

Another natural research direction regards the arithmetic symmetry and neighbourhood structure for the other simplest kinds of multilattices, that is, the mono- and diatomic two-dimensional 3-nets and the three-dimensional 2-lattices. This should improve our understanding of the basic symmetry properties of complex crystalline materials, giving a fairly comprehensive kinematical background for the detailed modelling of crystal behaviour.

APPENDIX *A*
Some proofs

Proof of Lemma 2. Let us consider a vector $\mathbf{p} \in \mathcal{W}(\mathbf{e}_a)$ and an operation $\mathbf{Q}$ belonging to the point group $P(\mathbf{e}_a)$ of the skeletal basis $\mathbf{e}_a$ (see the end of §3.2). From the known invariance properties of $\mathcal{W}(\mathbf{e}_a)$ and its closure $\overline{\mathcal{W}}(\mathbf{e}_a)$, we have that

$$\begin{aligned} \mathbf{p} \in \mathcal{W}^\circ \ &\Rightarrow\ \mathbf{Qp} \in \mathcal{W}^\circ, \\ \mathbf{p} \in \partial\overline{\mathcal{W}} \ &\Rightarrow\ \mathbf{Qp} \in \partial\overline{\mathcal{W}}. \end{aligned} \tag{41}$$

Then statements (i) and (ii) of the Lemma follow from the following facts, which are immediate consequences of the definition and properties of the Wigner–Seitz cell $\mathcal{W}(\mathbf{e}_a)$:

$$\mathcal{W}^\circ(\mathbf{e}_a) + \mathcal{W}^\circ(\mathbf{e}_a) = 2\mathcal{W}^\circ(\mathbf{e}_a), \quad 2\mathcal{W}^\circ(\mathbf{e}_a) \cap \mathcal{L}(\mathbf{e}_a) = \{\mathbf{0}\}, \tag{42}$$

$$\begin{aligned} &\overline{\mathcal{W}}(\mathbf{e}_a) + \overline{\mathcal{W}}(\mathbf{e}_a) = 2\overline{\mathcal{W}}(\mathbf{e}_a), \\ &2\overline{\mathcal{W}}(\mathbf{e}_a) \cap \mathcal{L}(\mathbf{e}_a) \subset \mathcal{A}\mathbf{e}_1 \oplus \mathcal{A}\mathbf{e}_2, \quad \mathcal{A} = \{-1,\ 0,\ 1\}. \end{aligned} \tag{43}$$

Proof of Corollary 1. Statement (i) is an immediate consequence of (42) and (43) combined, applied to the vectors $\mathbf{p}$ and $\mathbf{Qp}$ for $\mathbf{p} \in \partial\mathcal{W}$. Statement (ii) follows immediately from statement (i) in Lemma 2 and the hypothesis that $\mathbf{p} \in M_{\mathbf{Q}}$. Statement (iii) follows from (42) applied to $\mathbf{p}$ and $\mathbf{Qp}$, for $p \in \mathcal{W}^\circ\backslash M_{\mathbf{Q}}$ (if $M_{\mathbf{Q}}$ exists).

APPENDIX *B*
An example of computation of the fixed sets intersecting $\mathcal{D}$ and the corresponding lattice groups

Here we give an explicit example of how the results summarized in Table 2 are obtained. We recall that the main point here is the analysis of the solutions of equations $(28)_2$ for the six distinct cases listed in Table 1 for the skeletal metric $K_{ab} = \mathbf{e}_a \cdot \mathbf{e}_b$. We choose case 2 in Table 1, which refers to skeletal simple nets of the primitive-rectangular Bravais type. This is the most interesting example because the computations are not too cumbersome and because it is the only case in which two *distinct* arithmetic types of 2-nets with the *same* skeletal type are found. The other cases listed in Table 2 are treated in a similar way.

B1. Skeletal basis, Wigner–Seitz cell, and solutions to equations $(28)_1$

From Table 1, row 2, we see that the conditions on the skeletal reduced metric $K_{ab} = \mathbf{e}_a \cdot \mathbf{e}_b$, for $\mathbf{e}_a$ primitive-rectangular, are:

$$0 < K_{11} < K_{22}, \quad K_{12} = 0. \tag{44}$$

In this case, the solutions to equations $(28)_1$, which produce the point group $P(\mathbf{e}_a)$ and the lattice group $L(\mathbf{e}_a)$, are straightforwardly computed to be (see the last column of Table 1):

$$P(\mathbf{e}_a) = \{1,\ -1,\ M_{\mathbf{e}_1},\ M_{\mathbf{e}_2}\}, \tag{45}$$

$$L(\mathbf{e}_a) = \left\{ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\}. \tag{46}$$

In (45), the following notation is used, for $\mathbf{v} \in \mathbb{R}^2$:

$$\begin{aligned} M_{\mathbf{v}} &= 1 - 2\|\mathbf{v}\|^{-2}\mathbf{v} \otimes \mathbf{v} \\ &\equiv \text{mirror-symmetry operation whose mirror is} \\ &\qquad \text{orthogonal to } \mathbf{v}. \end{aligned} \tag{47}$$

This is very similar to the International (Hermann–Mauguin) notation for the operations in $P(\mathbf{e}_a)$; here we prefer the one in

(47) as it indicates more explicitly the direction of the mirrors and symmetry axes of $\mathcal{L}(\mathbf{e}_a)$, once the basis is given.

The Wigner–Seitz cell $\mathcal{W}(\mathbf{e}_a)$ in this case has a very simple rectangular shape. Explicitly, $\mathbf{p} = p^a\mathbf{e}_a \in \mathcal{W}$ when

$$-K_{aa}/2 < p_a = K_{a3} \leq K_{aa}/2 \quad \text{(not summed over } a\text{)}, \quad (48)$$

or, equivalently,

$$-\tfrac{1}{2} < p^a \leq \tfrac{1}{2}. \quad (49)$$

Recall that, for the descriptors $(\mathbf{e}_a, \mathbf{p})$ to belong to $\mathcal{D}^{\text{ess}}_{2,1}$, one needs to exclude the following $\mathbf{p}$'s from the cell $\mathcal{W}$ defined above – see (4) and (11)–(12):

$$(p^1, p^2) \notin \mathcal{N}, \quad \mathcal{N} = \{(0, 0), (\tfrac{1}{2}, 0), (0, \tfrac{1}{2}), (\tfrac{1}{2}, \tfrac{1}{2})\}. \quad (50)$$

B2. Solutions to equations $(28)_2$ for $\alpha = 1$

Among the solutions $\mathbf{Q}$ of $(28)_1$ listed in (45), we must now select those that also satisfy $(28)_2$ for $l^a \in \mathbb{Z}$ and (some) $\mathbf{p} \in \mathcal{W}(\mathbf{e}_a)$ in (48). Recall that by Lemma 1 we only need to check the case $\alpha = 1$ and that Corollary 1 can be used to simplify the computations. Hereafter, we list, in connection with each $\mathbf{Q} \in P(\mathbf{e}_a)$ in (45), the solutions $\mathbf{p}$ and l^a, if any, to $(28)_2$.

Remark. For all the indicated values of p^a below, recall the bounds (44) and (49) and the exclusions (50).

(i) $\mathbf{Q} = 1$, $m = 1$; in this case, we trivially get $l^a = 0$ for all $\mathbf{p} \in \mathcal{W}$.

(ii) $\mathbf{Q} = -1$, $m = -1$; in this case by Corollary 1 look for solutions of $(28)_2$ only for $\mathbf{p} \in \partial\mathcal{W}$. A straightforward analysis shows that solutions exist only for nonadmissible $\mathbf{p}$'s as in (50), which are thus not considered.

(iii)

$$\mathbf{Q} = M_{\mathbf{e}_1}, \quad m = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix};$$

in this case, the solutions to $(28)_2$ are as follows [see cases (i) and (ii) of Corollary 1]:

$$\begin{cases} l^1 = 0 \\ l^2 = 0 \end{cases} \text{for} \begin{cases} p^1 = 0 & (\textit{i.e.}\ \ p_1 = K_{13} = 0) \\ \text{any}\, p^2 & (\textit{i.e.}\ \ \text{any}\ \ p_2 = K_{23}) \end{cases}$$
$$\Rightarrow \mu = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix};$$
$$\begin{cases} l^1 = -1 \\ l^2 = 0 \end{cases} \text{for} \begin{cases} p^1 = \tfrac{1}{2} & (\textit{i.e.}\ \ p_1 = K_{13} = K_{11}/2) \\ \text{any}\, p^2 & (\textit{i.e.}\ \ \text{any}\ \ p_2 = K_{23}) \end{cases}$$
$$\Rightarrow \mu = \begin{pmatrix} -1 & 0 & -1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (51)$$

(iv)

$$\mathbf{Q} = M_{\mathbf{e}_2}, \quad m = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix};$$

the solutions to $(28)_2$ are as follows:

$$\begin{cases} l^1 = 0 \\ l^2 = 0 \end{cases} \text{for} \begin{cases} \text{any}\, p^1 & (\textit{i.e.}\ \ \text{any}\ \ p_1 = K_{13}) \\ p^2 = 0 & (\textit{i.e.}\ \ p_2 = K_{23} = 0) \end{cases}$$
$$\Rightarrow \mu = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix};$$
$$\begin{cases} l^1 = 0 \\ l^2 = -1 \end{cases} \text{for} \begin{cases} \text{any}\, p^1 & (\textit{i.e.}\ \ \text{any}\ \ p_1 = K_{13}) \\ p^2 = \tfrac{1}{2} & (\textit{i.e.}\ \ p_2 = K_{23} = K_{22}/2) \end{cases}$$
$$\Rightarrow \mu = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & -1 \\ 0 & 0 & 1 \end{pmatrix}. \quad (52)$$

B3. Determination of the fixed sets and lattice groups

The analysis of the solutions to $(28)_2$ in the preceding sections shows that for $\mathbf{e}_a$ as in (44) and $\mathbf{p} \in \mathcal{W}(\mathbf{e}_a)$, the following five possibilities arise:[19]

(i) For $\mathbf{p}$ such that $p^1 = 0$ and any $p^2 \notin \{0, \tfrac{1}{2}\}$:

$$\Lambda^1_{p2mm} = \left\{ \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \right\}. \quad (53)$$

(ii) For $\mathbf{p}$ such that $p^2 = 0$ and any $p^1 \notin \{0, \tfrac{1}{2}\}$:

$$\Lambda^2_{p2mm} = \left\{ \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \right\}. \quad (54)$$

(iii) For $\mathbf{p}$ such that $p^1 = \tfrac{1}{2}$ and any $p^2 \notin \{0, \tfrac{1}{2}\}$:

$$\Lambda^1_{p2mg} = \left\{ \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & -1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 1 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \right\}. \quad (55)$$

[19] When computing the lattice groups, recall that the analysis of equation $(28)_2$ in the previous section only refers to the case $\alpha = 1$. By Lemma 1, each solution $(\mathbf{Q}, l^a)$ of $(28)_2$ with $\alpha = 1$ generates a solution $(-\mathbf{Q}, -l^a)$ for $\alpha = -1$, which must also be counted in the lattice group for any given $\mathbf{p}$. Also the exclusions (50) must be recalled.

(iv) For $\mathbf{p}$ such that $p^2 = \frac{1}{2}$ and any $p^1 \notin \{0, \frac{1}{2}\}$:

$$\Lambda^2_{p2mg} = \left\{ \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & -1 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & -1 \end{pmatrix} \right\}. \quad (56)$$

(v) For any other $\mathbf{p} \notin \mathcal{N}$ [see (50)]:

$$\Lambda^3_{p2mm} = \left\{ \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right\} = \Lambda_{p2}. \quad (57)$$

Now, in order to find the actual fixed sets intersecting $\mathcal{D} \subset \mathcal{Q}^{\rm ess}_{2,1}$ and related to 2-nets with a primitive-rectangular skeleton [*i.e.* satisfying (44)], we must check through (22) that each of the lattice groups indicated above does indeed produce the fixed set indicated by (44) and the corresponding conditions on p^a. This check is necessary because in some cases the above conditions on $\mathbf{e}_a$ and $\mathbf{p}$ do not give the entire fixed set of the corresponding lattice group, but only a portion of it; in other words, that lattice group has a (larger) fixed set that actually pertains to a lower-symmetry 2-net type and appears here only as a case of 'excess of skeletal symmetry', as discussed in point (i) of §8. A check with (22) shows that the first four cases above are actual fixed sets intersecting $\mathcal{D}$, with their own lattice groups. These are consequently listed in Table 2. On the other hand, the descriptors $(\mathbf{e}_a, \mathbf{p})$ of case (v), as is perhaps obvious from their trivial lattice group, do not constitute an entire fixed set, but only a subdimensional portion of the oblique fixed set in Table 2, which generically contains metrics of 2-nets with an *oblique* (and not rectangular) skeleton. The descriptors in case (v) only happen to satisfy some special relations that are *not* connected to an actual change in multilattice symmetry.[20]

B4. Conjugacy classes of lattice groups and distinct arithmetic types

Now that we have established that four distinct fixed sets with primitive-rectangular skeletal type intersect $\mathcal{D}$, we need to establish the number of distinct $\Gamma_{2,1}$ conjugacy classes to which their lattice groups belong. A check on the conjugacy conditions with a $\mu \in \Gamma_{2,1}$ on the set of generators of each pair of lattice group (53)–(56) shows that the two groups Λ^1_{p2mm} and Λ^2_{p2mm} are indeed $\Gamma_{2,1}$ conjugate, as are Λ^1_{p2mg} and Λ^2_{p2mg}; however, Λ^1_{p2mm} and Λ^1_{p2mg} are *not* conjugate in $\Gamma_{2,1}$. This means that there exist *two* distinct arithmetic types of 2-nets with primitive rectangular skeleton, as is indicated in Table 2. Fig. 3(*b*) illustrates the different arrangements of the atoms in their unit cells. A check shows that the plane groups of these two types are distinct (notice that the axis-rectangular type has a nonsymmorphic plane group): thus, unlike for the general case, for 2-nets the arithmetic symmetry is equivalent to the plane-group symmetry.

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[20] In this case, in order to pass from the lowest-symmetry generic 'oblique' 2-nets in Table 2 to those belonging to the higher-symmetry 'rectangular' ones, the net descriptors must come to satisfy simultaneously two relations, that is $K_{12} = 0$ and, for instance, $K_{13} = 0$ [see (51)–(52)]. The descriptors in case (v) above satisfy only $K_{12} = 0$, which is not enough to generate new symmetries in the multilattice, *i.e.* it does not enlarge its lattice group.

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