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On the Definition and Classification of Bravais Lattices

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Dedicated to Professor J. L. Ericksen on his 70th birthday

Abstract

The number of *Bravais lattices* (or *lattice types*) in three-dimensional space is well known to be 14 if, as is usual, a lattice type is defined as the class of all simple lattices whose *lattice groups* (that is, *arithmetic holohedries*) belong to the same conjugacy class in $GL(3, \mathbb{Z})$. However, it is also common in the literature to introduce the lattice types using the original point of view of Bravais (and Cauchy), according to which a type collects all the lattices that can be connected by a continuous deformation along which the lattice symmetry does not decrease. It is shown that these two definitions are in fact *not* equivalent. Bravais' own criterion results in only 11 lattice types.

1. Introduction

It has long been accepted in crystallography that there are 14 distinct ways of arranging points in three-dimensional space so as to form a simple lattice. These 14 different lattice types are commonly called Bravais lattices because they were first correctly enumerated by Bravais in his well known 1850 memoir; Frankenheim had erroneously enumerated 15 types some years earlier (Frankenheim, 1842). However, it is not always very clear what the definition of a *lattice type* (or *Bravais lattice*) is, especially in the textbooks or papers that do not concern themselves with the more mathematical aspects of crystallography. In those that do, there are at least three formally different definitions.

(A) The first definition goes back to Bravais himself (and Cauchy, who presented Bravais' memoir to the Académie des Sciences). According to it, *"Deux Assemblages de la même classe appartiennent à des modes distincts de symétrie, lorsqu'en faisant varier d'une manière continue les espacements des Sommets de l'un des Assemblages, sans qu'il perde un seul instant ses axes de symétrie, on ne peut, malgré cela, le rendre que partiellement superposable avec l'autre Assemblage."* Also, *"Deux Assemblages appartiennent au même mode, lorsqu'une variation continue de leur paramètres pourra les rendre coincidents."* (see Bravais, 1850, p. 95); Bravais calls '*classe*' what is called today 'crystal system', while '*mode*' is what we call 'lattice type'. Therefore, two simple lattices in the same crystal system belong to the same lattice type if and only if there is a continuous deformation that brings the first lattice onto the second one without ever losing symmetry elements – see §3 for a detailed statement. A form of this criterion is adopted by Miller (1972, p. 43). A reference to this point of view for the classification of lattice types is also given by Bradley & Cracknell (1972, p. 82) or Farkas (1981, p. 541), among others.

(B) The second criterion is perhaps the one found most commonly in the literature on mathematical crystallography – see, for instance, Janssen (1973, p. 112) or Engel (1986, p. 128). It partitions lattices into types based on the arithmetic equivalence of their arithmetic holohedries, that is, of the integral representations in their lattice bases of their symmetry groups in $O(3)$. Again, see §3 for details.

(C) The third definition that can be found in the literature partitions simple lattices into types based on the affine conjugacy, which is equivalent to group isomorphism, of their *affine* symmetry groups (symmorphic space groups). See, for instance, Opechowski (1986, Section 8.3) or Schwarzenberger (1972).

Definitions (B) and (C) above are equivalent. See, for instance, Burckhardt (1947, Section 17) or Opechowski (1986, p. 221); Janssen (1973, p. 120) gives an elementary proof of this fact.

In the literature, definitions (A) and (B) are implicitly or explicitly understood to be equivalent and, as mentioned above, both are still used for defining lattice types. Bravais is also commonly credited with showing that the lattice types are exactly 14, and his construction is still often used as a proof.

Two remarks are necessary regarding this point. Firstly, it must be noticed that, while Bravais explicitly stated his definition (A) above, he never used it in his 1850 memoir to check whether his 14 lattice types were indeed all distinct; nor did he try to show that they are the only possible ones according to his definition.

Secondly, the criterion he chose needs to be clarified before it can be effectively used to establish an equivalence relation among lattices. Now, any orthogonal transformation applied to a lattice does not change its symmetry, and such 'deformations' must thus be included in those allowed by Bravais' definition (A). However, (A) seems to be based on the natural notion that there are also other deformations that do not change the symmetry of a lattice. Intuitively, these can for instance include the deformations that crystal lattices undergo under varying conditions of environmental temperature and pressure, for instance during thermal expansion *etc*.

In §3, we indicate the natural way to make the statement (A) precise: see definition (A'), which specifies that, during the deformation, the holohedry of the lattice should never decrease, up to conjugacy in $O(3)$. We show in §4 that Bravais' criterion (A') is *not* equivalent to the arithmetic criterion (B). This clarifies Bravais' own words and role regarding this fundamental issue in crystallography and points out a misunderstanding seemingly not appreciated in the literature.

On the one hand, based on the results of Niggli & Nowacki (1935), for instance, who enumerate all the three-dimensional arithmetic crystal classes (see also Burckhardt, 1947) or based on the results of Niggli (1928), who used the procedures proposed by Seeber (1831) to enumerate the reduced lattice bases (see Engel, 1986, pp. 46–59), it can be shown that the lattice types in three-dimensional space defined according to criterion (B) are indeed exactly 14, that is, the well known types indicated by Bravais (see also Michel, 1995).

On the other hand, we show that the classification of three-dimensional simple lattices according to Bravais' own criterion is in fact *strictly coarser* than the one based on (B), for (A') gives only 11 distinct lattice types.

The proof of these results is based on an analysis of the 'fixed sets' in the six-dimensional space $\mathcal{C}^+(\mathcal{Q}_3)$ of symmetric positive-definite 3×3 real matrices. The fixed sets in $\mathcal{C}^+(\mathcal{Q}_3)$ are the convex cones constituted by matrices stabilized by the natural action on $\mathcal{C}^+(\mathcal{Q}_3)$ of the lattice groups, that is, of the arithmetic holohedries of simple lattices.

The situation is similar in two dimensions. While this is an instructive example in itself, here we omit the details of the analysis, which can be easily derived from the three-dimensional case.

We remark at the end of §4 that there is the possibility of a formal alternative interpretation of (A), imposing that the *arithmetic* holohedry of the lattice in $GL(3,\mathbb{Z})$ never be decreased during the deformation. While we show that this gives back the 'right' classification, we explain why it cannot correspond to Bravais' ideas. Also, the lattice deformations that we consider, following Bravais' words in (A), give paths in the space $\mathcal{C}^+(\mathcal{Q}_3)$ of lattice metrics on which several of the natural lattice parameters (lengths of lattice vectors and interaxial angles) may suitably change. If on such paths only one of the lattice parameters is allowed to vary, then the procedure results in 14 lattice types.* However, no restriction of this kind is mentioned by Bravais.

* We thank one of the referees for this observation.

Notice that if in definition (A) the requirement that there be no loss of symmetry elements along the lattice deformation is dropped, clearly all lattices belong to only *one* type because they can all be connected by means of deformations passing through suitable triclinic lattices. This is another way of stating the well known fact that from the affine point of view there is essentially only one simple lattice. On the other hand, if, unlike Bravais, *increased* symmetry is also prohibited along the deformation, the classification becomes strictly *finer* than the classical one given by (B), resulting in more than 14 lattice types; this is shown by Schwarzenberger (1972).

We mention that the complete picture of the topology of fixed sets in $\mathcal{C}^+(\mathcal{Q}_3)$ or, equivalently, of the group–subgroup relations among all the lattice groups in $GL(3,\mathbb{Z})$ is not necessary here. Schwarzenberger (1972), Engel (1986, pp. 46–59) and Michel (1995) all contain very useful information regarding the structure of $\mathcal{C}^+(\mathcal{Q}_3)$. As indicated by Ericksen, this is important for a better understanding of a variety of phenomena connected with phase transitions in crystals, whose investigation spurred the present work, as well as an increasing bulk of literature – see Ericksen (1979, 1980, 1989, 1993), Ball & James (1992), James (1992), Pitteri & Zanzotto (1996), and references quoted therein.

In §4, we exhibit the only three Bravais-type deformations connecting lattices that are inequivalent according to (B); they have been shown by Ericksen (1996) to be thermodynamically possible paths of equilibria for crystals undergoing solid-to-solid phase transitions while in contact with a heat bath with suitably controlled temperature and pressure. This theoretical possibility raises interesting questions, especially from the experimental point of view.

2. Preliminaries

In order to explain in detail the statements made in the *Introduction*, it is necessary to give some definitions.

For the purposes of this paper, it is sufficient to consider simple lattices in the three-dimensional inner-product vector space $\mathbb{R}^3$ rather than in the three-dimensional Euclidean affine space. Thus, we define a simple lattice $\mathcal{R}(\mathbf{E}_a)$ as follows:

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

where the three linearly independent vectors $\mathbf{E}_a$ in $\mathbb{R}^3$ ($a = 1,2,3$) are called the *lattice vectors* of $\mathcal{R}(\mathbf{E}_a)$ (or the *lattice basis*). In (1) and in what follows, the summation convention over repeated indices is understood. When there is no danger of confusion, $\mathcal{R}(\mathbf{E}_a)$ will be indicated by $\mathcal{R}$ only. The parallelepiped $\mathcal{P}(\mathbf{E}_a)$ spanned by $\mathbf{E}_a$ is called a *unit cell* of $\mathcal{R}$.

Following the notation of Michel (1995), we denote by $\mathcal{Q}_3$ the space of all symmetric 3×3 matrices and by $\mathcal{C}^+(\mathcal{Q}_3) \subset \mathcal{Q}_3$ the set of symmetric positive-definite matrices. Since any positive multiple of a matrix in $\mathcal{C}^+(\mathcal{Q}_3)$ is still in $\mathcal{C}^+(\mathcal{Q}_3)$, and any convex combination of elements of $\mathcal{C}^+(\mathcal{Q}_3)$ also belongs to $\mathcal{C}^+(\mathcal{Q}_3)$, the latter is a convex cone. The symmetric positive-definite matrix

$$C = (C_{ab}), \quad C_{ab} = \mathbf{E}_a \cdot \mathbf{E}_b \tag{2}$$

is the *lattice metric*. The volume of $\mathcal{P}(\mathbf{E}_a)$ is given by

$$\mathrm{vol}^2\, \mathcal{P}(\mathbf{E}_a) = \det C. \tag{3}$$

Clearly, the lattice $\mathcal{R}$ does not select its lattice vectors, for these are determined only up to transformations belonging to the group $GL(3,\mathbb{Z})$ of the 3×3 invertible (unimodular) matrices with integral entries. This can easily be seen by considering that any new basis $\mathbf{E}'_a$ of $\mathcal{R}$ is obtained from the old basis $\mathbf{E}_a$ by means of a linear transformation with integral coefficients:

$$\mathbf{E}'_a = m_a^b \mathbf{E}_b, \quad m_a^b \in \mathbb{Z}; \tag{4}$$

now, in order that $\mathbf{E}'_a$ be again a basis, the volume of $\mathcal{P}(\mathbf{E}'_a)$ must be the same as the volume of $\mathcal{P}(\mathbf{E}_a)$. Since, in obvious notation, under a transformation (4) the lattice metric transforms as

$$C' = m^t C m, \tag{5}$$

the equality of the volumes of the cells is possible if and only if the transformation matrix m in (4) is such that $\det m = \pm 1$, that is,

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

The (*geometric*) *holohedry* $P(\mathbf{E}_a)$ of $\mathcal{R}(\mathbf{E}_a)$ is the finite group of all the orthogonal transformations $\mathbf{Q}$ in $O(3)$ that leave $\mathcal{R}(\mathbf{E}_a)$ invariant, which are called the *symmetry operations* for $\mathcal{R}(\mathbf{E}_a)$. In view of (4), this can be defined as

$$P(\mathbf{E}_a) = \{\mathbf{Q} \in O(3) : \mathbf{Q}\mathbf{E}_a = m_a^b \mathbf{E}_b, m \in GL(3,\mathbb{Z})\}. \tag{7}$$

It is immediately seen that the holohedry $P(\mathbf{E}_a)$ of $\mathcal{R}(\mathbf{E}_a)$ is independent of the lattice basis:

$$P(m_a^b \mathbf{E}_b) = P(\mathbf{E}_a) \quad \text{for all } m \in GL(3,\mathbb{Z}), \tag{8}$$

so that $P(\mathbf{E}_a)$ depends only on the lattice $\mathcal{R}(\mathbf{E}_a)$ itself. Furthermore, since $P(\mathbf{E}_a)$ describes some symmetry properties of $\mathcal{R}(\mathbf{E}_a)$ which should be considered equivalent in any lattice congruent to $\mathcal{R}(\mathbf{E}_a)$, and since

$$P(\mathbf{R}\mathbf{E}_a) = \mathbf{R}P(\mathbf{E}_a)\mathbf{R}^t \quad \text{for all } \mathbf{R} \in O(3), \tag{9}$$

it is customary to consider, rather than the holohedry $P(\mathbf{E}_a)$ itself, its conjugacy class in $O(3)$; the $O(3)$-conjugacy classes of the holohedries are called *crystal systems*. The lattices themselves are considered (geometrically) equivalent based on the fact that their holohedries are equivalent in $O(3)$, in which case they are said to belong to the same crystal system.

A well known result in crystallography states that there are seven crystal systems: triclinic, monoclinic, orthorhombic, tetragonal, trigonal or rhombohedral, hexagonal and cubic (see Table 1).

The matrices m appearing in (7) give a finite subgroup $L(\mathbf{E}_a)$ of $GL(3,\mathbb{Z})$ called the *lattice group*, or the *arithmetic holohedry*, of $\mathcal{R}(\mathbf{E}_a)$:

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

An orthogonal transformation does not change the lattice group:

$$L(\mathbf{R}\mathbf{E}_a) = L(\mathbf{E}_a) \quad \text{for all } \mathbf{R} \in O(3); \tag{11}$$

thus, $L(\mathbf{E}_a)$ can be equivalently defined as [see (2)]

$$L(\mathbf{E}_a) = \{m \in GL(3,\mathbb{Z}) : m^t C m = C\}. \tag{12}$$

Therefore, the lattice group $L(\mathbf{E}_a)$ is the stabilizer of the lattice metric C under the action of (5) and can be denoted by $L(C)$. The lattice group also determines a connected set in the space $\mathcal{C}^+(\mathcal{Q}_3)$, called the *fixed set* of $L(\mathbf{E}_a)$, denoted by $I(L(\mathbf{E}_a))$, consisting of all the metrics stabilized by $L(\mathbf{E}_a)$:

$$I(L(\mathbf{E}_a)) = \{C' \in \mathcal{C}^+(\mathcal{Q}_3) : m^t C' m = C' \text{ for all } m \in L(\mathbf{E}_a)\}. \tag{13}$$

A change of lattice basis does not change a lattice but changes its lattice group $L(\mathbf{E}_a)$ as follows:

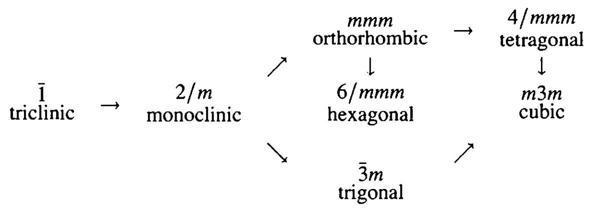
$$L(m_a^b \mathbf{E}_b) = m^{-1} L(\mathbf{E}_a) m, \quad m \in GL(3,\mathbb{Z}); \tag{14}$$

this leads to considering as (arithmetically) equivalent the lattice groups that are conjugate within $GL(3,\mathbb{Z})$.

3. Classification criteria

The (geometric) holohedry $P(\mathbf{E}_a)$ does give a description of the symmetry properties of a simple lattice $\mathcal{R}(\mathbf{E}_a)$; however, a sharper characterization of such properties is given by the arithmetic holohedry (lattice group) $L(\mathbf{E}_a)$. Indeed, a given holohedral group $P \subset O(3)$ does in general determine various arithmetically *inequivalent* lattice groups, depending on the basis $\mathbf{E}_a$ chosen among those for which $P = P(\mathbf{E}_a)$. This is because the same symmetry operation in $O(3)$ can be represented in different bases by integral matrices which need not be conjugate in $GL(3,\mathbb{Z})$: this makes conjugacy in $GL(3,\mathbb{Z})$ a stricter condition than conjugacy in $O(3)$

Table 1. *Diagram of the holohedries*



or in $GL(3,\mathbb{R})$. Therefore, based on (14), a natural equivalence relation is obtained for the bases of $\mathbb{R}^3$ and the lattices they generate, which is at the origin of criterion (B) stated in the *Introduction*. According to this point of view, two simple lattices $\mathcal{R}(\mathbf{E}_a)$ and $\mathcal{R}(\mathbf{E}'_a)$ are said to have the same *lattice type* or to belong to the same *Bravais lattice* if their lattice groups are arithmetically equivalent, that is, if

$$L(\mathbf{E}'_a) = m^{-1}L(\mathbf{E}_a)m \quad \text{for some } m \in GL(3,\mathbb{Z}). \quad (15)$$

From (4) and (14), this means that two simple lattices have the same symmetry type if and only if there are choices of their bases such that the associated lattice groups *coincide*. Since (15) remains true if we replace $\mathbf{E}_a$ and $\mathbf{E}'_a$ by equivalent triples of lattice vectors, the definition above does introduce an equivalence relation among the simple lattices themselves, which is criterion (B). As we recalled in the *Introduction*, according to this definition there are exactly 14 distinct types of lattice, that is, the classical ones indicated by Bravais. They are subdivided in the well known way into the seven crystal systems.

Let us now consider Bravais' criterion (A). We already pointed out in the *Introduction* that, although he had listed his 14 lattice types in his 1850 memoir and had corrected an earlier list of Frankenheim, he actually never used his own definition (A) to show either that none of his 14 types are coincident or that there could be no more than those he enumerated. In order to effectively utilize Bravais' criterion (A) for distinguishing lattice types, it is necessary to phrase it in terms of the notions introduced in §2. Bravais' words are rather explicit; throughout his 1850 memoir, he clearly considers the holohedries of the lattices he constructs and states, on p. 94, that within each crystal system (that is, to within orthogonal transformations) the axes and planes of symmetry are the same: *"On a déja pu remarquer que, dans une même classe d'Assemblages, venaient se grouper des Assemblages à modes d'agencement des Sommets complétement distincts, quoique les axes et plans de symétrie fussent les mêmes de part et d'autre"*.

Here, as already recalled in (A), '*assemblage*' means 'lattice' and '*classe*' means 'system'. This point of view is undoubtedly shared by most present-day authors and, for instance, is reflected by the fact that in the literature the expression 'point group' is used to indicate, indifferently, either the finite subgroups of $O(3)$ or their conjugacy classes in $O(3)$. Since the symmetry of a lattice is unchanged by any orthogonal transformations, which are just particular 'deformations', from Bravais' own standpoint the way to phrase precisely his criterion (A) is the following:

(A') Two lattices $\mathcal{R}$ and $\mathcal{R}'$ in the same system have the same symmetry type if and only if there is a continuous deformation of lattices

$$\lambda \mapsto \mathcal{R}_\lambda, \quad \lambda \in [0,1], \quad \mathcal{R}_\lambda(0) = \mathcal{R}, \quad \mathcal{R}_\lambda(1) = \mathcal{R}' \quad (16)$$

such that the holohedry of $\mathcal{R}_\lambda$ contains that of $\mathcal{R}$ or $\mathcal{R}'$ for any λ, up to conjugacy in $O(3)$.

For brevity, a deformation between two lattices with the properties mentioned in this definition will be referred to as a *Bravais connection* between them.

A remark must be made about the existence of a Bravais connection between two lattices. Since lattices are referred to their bases, a connection between lattices can be given in terms of the lattice vectors. However, since lattices that differ by a rotation are trivially considered equivalent, the Bravais connections can be given in terms of the lattice metrics rather than lattice bases. This means that their existence can be investigated in the space $\mathcal{C}^+(\mathcal{Q}_3)$ and we will do so in the next section.

Also, it is important to notice that, if two lattices admit a Bravais connection, such a connection cannot in general be given in terms of *any* bases or metrics; in fact, only suitable bases, or metrics, will do. The reason is that a given lattice is represented in an infinite number of arithmetically equivalent ways – see (4) and (5) – in the space of lattice bases or in $\mathcal{C}^+(\mathcal{Q}_3)$, and this redundancy does not 'behave well' with respect to the existence of Bravais connections. This is clear if we think that even most pairs of distinct bases or metrics for the *same* lattice do not admit a Bravais connection.

Rather than introducing a formal 'space of lattices', for instance as a quotient $GL(3,\mathbb{R}) : GL(3,\mathbb{Z})$, with the consequent quotient topology, we will investigate the existence of Bravais connections directly in $\mathcal{C}^+(\mathcal{Q}_3)$, keeping track of the redundancies of the representation when necessary, and indicating 'suitable' representatives when they exist.

In the following lemma, we recall a number of properties of lattice groups and their fixed sets that are useful in the next section.

Lemma 3.1. (i) A subgroup of $GL(3,\mathbb{Z})$ is (a subgroup of) a lattice group if and only if it is finite.

(ii) 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.

(iii) The fixed set of any finite subgroup of $GL(3,\mathbb{Z})$ is a convex set.

(iv) The fixed sets of two finite subgroups of $GL(3,\mathbb{Z})$ have a non-empty intersection if and only if the two subgroups together generate a finite subgroup of $GL(3,\mathbb{Z})$, whose fixed set is the intersection of the given fixed sets.

For the proof of these statements, and for other information on lattice groups and their fixed sets, we direct the reader to Ericksen (1979) or to Michel (1995).

4. Classification of simple lattices according to Bravais' criterion

In this section we study the classification of simple lattices according to Bravais' criterion. In doing so, we take for granted the classification of lattices according to (B)* because the analysis of the existence of Bravais connections rests on the knowledge of the structure of the space $\mathcal{C}^+(\mathcal{Q}_3)$. The basic observation here is that the metrics belonging to the fixed set of any given lattice group all correspond to equivalent lattices according to (B), while the metrics of inequivalent lattices according to (B) never belong to the same fixed set. Thus, in a Bravais connection between two given lattices that are in the same system and are arithmetically inequivalent, the deformed lattice must leave its original fixed set by passing through the intersection with another fixed set. Such intersection is itself the fixed set of a lattice group that is strictly larger than the original ones, as a consequence of lemma 3.1. This means that Bravais connections necessarily go through a lattice of *strictly higher symmetry* than the given lattices.

Lemma 4.1. Criterion (A') is coarser than criterion (B).

Proof. This is an immediate consequence of lemma 3.1. Indeed, if any two given lattices are of the same type according to (B), then by hypothesis there exist suitable bases relative to which they have the same lattice group. This means that the corresponding lattice metrics belong to the same fixed set in $\mathcal{C}^+(\mathcal{Q}_3)$. Thus, so does the segment between these two metrics, and this gives a Bravais connection making the two given lattices equivalent according to (A').

We will now show that Bravais connections between arithmetically inequivalent lattices are possible, meaning that definition (A') is *strictly* coarser than definition (B).

Proposition 4.1. (Classification of simple lattices according to Bravais' criterion). There are exactly 11 different types of three-dimensional simple lattices according to definition (A'): triclinic, monoclinic, primitive orthorhombic, body-centered orthorhombic, primitive tetragonal, body-centered tetragonal, trigonal, hexagonal, primitive cubic, body-centered cubic, face-centered cubic.

Proof. According to definition (A') and to lemma 4.1, we only need to investigate separately the existence of Bravais connections among the lattice types that are already discriminated by definition (B) within each crystal system, which are well known; only the monoclinic, orthorhombic, tetragonal and cubic systems have more than one lattice type.

4.1. *Cubic system*

According to definition (B), in this system there are three distinct lattice types: primitive, body centered and face centered. There are no Bravais connections among them. To see this, recall that the cubic lattice groups are all finite maximal subgroups in $GL(3,\mathbb{Z})$; this property derives from the maximality of their conjugate copies as finite subgroups of $O(3)$. Maximality implies that any two distinct cubic lattice groups generate a subgroup of $GL(3,\mathbb{Z})$, which is infinite and thus cannot be a lattice group by lemma 3.1(i). This in turn means that the corresponding cubic fixed sets never intersect in $\mathcal{C}^+(\mathcal{Q}_3)$ by lemma 3.1(iv). A Bravais connection between any two cubic lattices of different type is thus impossible and therefore the three cubic types also remain distinct according to definition (A').

4.2. *Tetragonal system*

For the two tetragonal lattice types that are distinct according to definition (B), that is, the primitive and the centered ones, we prove that there are no Bravais connections. This leaves them distinct also according to definition (A').

In this case, we must show that there are no Bravais connections between any pairs of representatives in $\mathcal{C}^+(\mathcal{Q}_3)$, say C_p and C_c, of inequivalent tetragonal lattices. *A priori*, C_p can be chosen in any one of the infinitely many fixed sets, each corresponding to one of the arithmetically equivalent lattice groups of the tetragonal primitive type, and analogously for C_c and the fixed sets of the infinitely many equivalent lattice groups of the tetragonal centered type. If we suppose that a Bravais connection between the inequivalent metrics C_p and C_c exists, lemma 3.1(iv) specialized to this tetragonal case shows that such a connection must necessarily pass through a lattice whose metric, $\bar{C}$ say, belongs to the fixed set of a lattice group of one of the three inequivalent cubic types. Also, it can be concluded that $L(C_p) \subset L(\bar{C})$ and $L(C_c) \subset L(\bar{C})$. Thus, in order to show that no Bravais connections exist, we just need to check that no cubic lattice group can contain inequivalent tetragonal subgroups. To this end, it is enough to restrict ourselves to the subgroup of

* Notice that the lack of such preliminary knowledge would make it unclear how to proceed with this task. Bravais' own criterion (A) involving deformations indeed requires that the further notions regarding symmetry based on arithmetic equivalence be already established and fully utilized. As this point of view on symmetry was developed later than 1850, we may see one reason why Bravais did not actually use his own criterion (A) for classifying lattices in his famous memoir.

elements with positive determinant of any lattice group we will be considering. Here and in what follows, we will do so without changing the nomenclature and by adding a '+' to the symbols.

A check on the order of a cubic lattice group, $L^+(\bar{C})$ say, and of its possible tetragonal subgroups shows that the latter are necessarily three and are all conjugate within $L^+(\bar{C})$. This is an immediate consequence of the well known Sylow theorem – see, for instance, McLane & Birkhoff (1967). Since conjugacy in $L^+(\bar{C})$ clearly makes all the tetragonal subgroups arithmetically equivalent, there can never be inequivalent tetragonal lattice groups with a common cubic supergroup. Thus, Bravais connections between inequivalent tetragonal lattices cannot exist and the two lattice types in this system remain inequivalent also with respect to criterion (A').

Incidentally, we mention that it is possible to arrive at the same conclusion by analyzing the positions of the tetragonal fixed sets in the interior or on the boundary of the *fundamental region* in $\mathcal{C}^+(\mathcal{Q}_3)$, considered, for instance, by Opechowski (1986, p. 214), whose elements are the lattice metrics corresponding to the so-called (reduced) Dirichlet bases.

4.3. *Orthorhombic system*

In this system, there are four lattice types that are distinct according to definition (B): primitive, base-centered, body-centered and face-centered.

We first show that there are Bravais connections: (i) between the primitive and the base-centered types – this 'phase transition' was first discussed by Ericksen (1979); and (ii) between the body-centered and the face-centered types. We will then show that there are no further connections, so that *two* lattice types remain distinct in this system according to definition (A').

Inspection of the fixed sets of the orthorhombic system shows that Bravais connections exist between inequivalent metrics in the appropriate fixed sets: for simplicity, we only give the expressions of the corresponding metrics with their independent entries, without reference to the actual lattice bases, which can be seen in the figures.

In order to show the existence of a Bravais connection between primitive and base-centered orthorhombic lattices, consider the orthorhombic primitive metric (see Fig. 1a):

$$C = \begin{pmatrix} C_{11} & 0 & 0 \\ 0 & C_{22} & 0 \\ 0 & 0 & C_{33} \end{pmatrix}, \tag{17}$$

and the base-centered orthorhombic metric (see Fig. 1c)

$$\tilde{C} = \begin{pmatrix} \tilde{C}_{11} & 0 & 0 \\ 0 & \tilde{C}_{22} & \tilde{C}_{23} \\ 0 & \tilde{C}_{23} & \tilde{C}_{22} \end{pmatrix}. \tag{18}$$

By varying the lattice parameters in C and $\tilde{C}$ above, we obtain the fixed sets, I and $\tilde{I}$ say, of the lattice groups $L(C)$ and $L(\tilde{C})$, respectively. It is easy to see that I and $\tilde{I}$ intersect in the fixed set of a primitive tetragonal lattice group, whose typical element $\check{C}$ has the form (see Fig. 1b)

$$\check{C} = \begin{pmatrix} \check{C}_{11} & 0 & 0 \\ 0 & \check{C}_{22} & 0 \\ 0 & 0 & \check{C}_{22} \end{pmatrix}. \tag{19}$$

This is obtained from (17) for $C_{11} = \check{C}_{11}$, $C_{22} = \check{C}_{22} = C_{33}$ and from (18) for $\tilde{C}_{ii} = \check{C}_{ii}$, $i = 1, 2$, and $\tilde{C}_{23} = 0$. Thus, in this case, for any choice of $\check{C}$ as in (19), a Bravais connection between the two inequivalent orthorhombic lattices (17) and (18), passing through a primitive tetragonal lattice, can be given by the union of the segments

$$\lambda \mapsto \lambda C + (1 - \lambda)\check{C}$$

and

$$\lambda \mapsto \check{C} + (1 - \lambda)\tilde{C}, \quad \lambda \in [0, 1], \tag{20}$$

the first belonging to I and the second to $\tilde{I}$ by lemma 3.1(iii).

For a face-centered orthorhombic lattice, the metric can be given the form

$$C = \begin{pmatrix} C_{11} & \frac{1}{2}C_{11} & \frac{1}{2}C_{11} \\ \frac{1}{2}C_{11} & C_{22} & \frac{1}{4}C_{11} \\ \frac{1}{2}C_{11} & \frac{1}{4}C_{11} & C_{33} \end{pmatrix}, \tag{21}$$

and, for a body-centered orthorhombic lattice, the form

$$\tilde{C} = \begin{pmatrix} \tilde{C}_{11} & \frac{1}{2}\tilde{C}_{11} & \frac{1}{2}\tilde{C}_{11} \\ \frac{1}{2}\tilde{C}_{11} & \tilde{C}_{22} & \tilde{C}_{23} \\ \frac{1}{2}\tilde{C}_{11} & \tilde{C}_{23} & \tilde{C}_{22} \end{pmatrix}. \tag{22}$$

Again, by varying the parameters in C and $\tilde{C}$, we obtain the fixed sets, I and $\tilde{I}$ say, of the lattice groups $L(C)$ and $L(\tilde{C})$, respectively, which intersect in the fixed

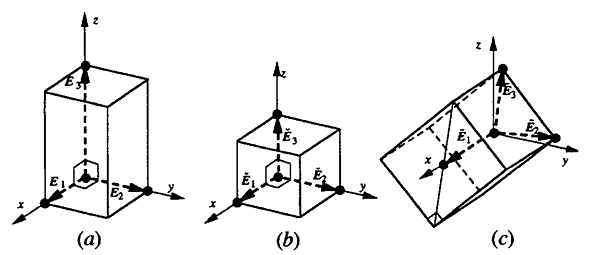


Fig. 1. Lattice bases used for the Bravais connection given in (17)–(19). (a) The primitive orthorhombic basis. (b) The primitive tetragonal basis. (c) The base-centered orthorhombic basis.

set of a centered tetragonal lattice group, whose typical element $\check{C}$ has the form (see Fig. 2*b*)

$$\check{C} = \begin{pmatrix} \check{C}_{11} & \frac{1}{2}\check{C}_{11} & \frac{1}{2}\check{C}_{11} \\ \frac{1}{2}\check{C}_{11} & \check{C}_{22} & \frac{1}{4}\check{C}_{11} \\ \frac{1}{2}\check{C}_{11} & \frac{1}{4}\check{C}_{11} & \check{C}_{22} \end{pmatrix}. \qquad (23)$$

This can be obtained from (21) for $C_{22} = \check{C}_{22} = C_{33}$, $C_{11} = \check{C}_{11}$, and from (22) for $\tilde{C}_{11} = \check{C}_{11}$, $\tilde{C}_{22} = \check{C}_{22}$, $\tilde{C}_{23} = \frac{1}{4}\check{C}_{11}$. Therefore, in this case, a Bravais connection between the two inequivalent orthorhombic lattices, passing through a centered tetragonal lattice, can again be given by the union of the segments in (20), with the choices (21), (22) and (23) for C, $\tilde{C}$ and $\check{C}$, respectively.

Henceforth, *inequivalent* orthorhombic types will refer for brevity to the lattice types in the orthorhombic system and to their lattice groups or fixed sets, which are still inequivalent according to (A') after having given the Bravais connections (17)–(20) and (20), (21)–(23).

In order to show that there are no Bravais connections between the inequivalent orthorhombic types, we proceed in a way that is analogous to the tetragonal case.

First, we show that no Bravais connections are possible that pass directly through the intersection of fixed sets of inequivalent orthorhombic lattice groups. As we have seen above, this amounts to showing that no two such groups admit any lattice group as a common supergroup. The latter, if it existed, would necessarily be a tetragonal, a cubic or a hexagonal group, owing to lemma 3.1(iv). No other cases are possible because the cubic and hexagonal lattice groups are maximal finite subgroups of $GL(3, \mathbb{Z})$.

The case of a hexagonal supergroup is strictly analogous to the cubic tetragonal case considered above. In fact, the orders of the hexagonal and the orthorhombic groups are such that the Sylow theorem can again be applied so that there are three necessarily conjugate, and hence equivalent, orthorhombic subgroups in any hexagonal lattice group. Thus, there cannot be Bravais connections between inequivalent orthorhombic lattices through any hexagonal lattice.

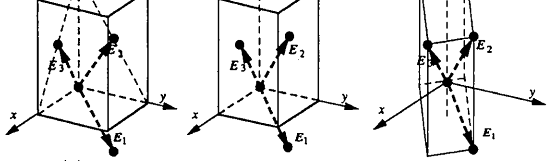


Fig. 2. Lattice bases used for the Bravais connection given in (21)–(23). (*a*) The face-centered orthorhombic basis. (*b*) The centered tetragonal basis. (*c*) The body-centered orthorhombic basis.

For the cubic and tetragonal supergroups, the analysis is slightly more complex. It is convenient to examine both these cases at once and to do so preliminarily in $O(3)$. Consider any cubic lattice basis $\mathbf{E}_a$. From the theory of finite groups, it is well known that the cubic holohedry $P^+(\mathbf{E}_a)$, which is isomorphic to the group S_4 of permutations of four objects, admits the three conjugate tetragonal subgroups T_i, $i = 1, 2, 3$, mentioned earlier, and four orthorhombic subgroups; three of them, O_i, $i = 1, 2, 3$, say, are conjugate in $P^+(\mathbf{E}_a)$ and the remaining one, O_4 say, is normal in $P^+(\mathbf{E}_a)$ and thus is not conjugate in $P^+(\mathbf{E}_a)$ to any one of the O_i. Each O_i is a subgroup of one and only one of the (conjugate) tetragonal subgroups T_i in $P^+(\mathbf{E}_a)$ and O_4 is a subgroup of all the T_i.

Let us consider the 'pure stretches' $\bar{\mathbf{V}}_i = \bar{\mathbf{V}}_i^t > 0$, $i = 1, 2, 3$, and $\bar{\mathbf{U}} = \bar{\mathbf{U}}^t > 0$, having the form

$$\begin{aligned} \bar{\mathbf{V}}_1 &= \eta_1(\mathbf{k}_1 - \mathbf{k}_2) \otimes (\mathbf{k}_1 - \mathbf{k}_2) \\ &\quad + \eta_2(\mathbf{k}_1 + \mathbf{k}_2) \otimes (\mathbf{k}_1 + \mathbf{k}_2) + \eta_3 \mathbf{k}_3 \otimes \mathbf{k}_3, \\ &\qquad \eta_1 \neq \eta_2, \\ \bar{\mathbf{V}}_2 &= \mathbf{R}^{\pi/2}(\mathbf{k}_1)\bar{\mathbf{V}}_1[\mathbf{R}^{\pi/2}(\mathbf{k}_1)]^t, \\ \bar{\mathbf{V}}_3 &= \mathbf{R}^{\pi/2}(\mathbf{k}_2)\bar{\mathbf{V}}_1[\mathbf{R}^{\pi/2}(\mathbf{k}_2)]^t, \\ \bar{\mathbf{U}} &= \eta_1 \mathbf{k}_1 \otimes \mathbf{k}_1 + \eta_2 \mathbf{k}_2 \otimes \mathbf{k}_2 + \eta_3 \mathbf{k}_3 \otimes \mathbf{k}_3, \\ &\qquad \eta_1 \neq \eta_2 \neq \eta_3 \neq \eta_1, \end{aligned} \qquad (24)$$

where the real numbers η_1, η_2, η_3 are all positive; the $\mathbf{k}_a$ are the three orthonormal vectors along the axes of the three fourfold elements of $P^+(\mathbf{E}_a)$ and $\mathbf{R}^\theta(\mathbf{k})$ denotes the rotation by the angle θ about the axis $\mathbf{k}$. We then have

$$O_i = P^+(\bar{\mathbf{V}}_i\mathbf{E}_a), \quad i = 1, 2, 3, \quad O_4 = P^+(\bar{\mathbf{U}}\mathbf{E}_a); \qquad (25)$$

furthermore, the three conjugate tetragonal subgroups T_i in $P^+(\mathbf{E}_a)$ are given by

$$T_i = P^+(\bar{\mathbf{U}}_i\mathbf{E}_a), \qquad (26)$$

where $\bar{\mathbf{U}}_i$ has the same form as $\bar{\mathbf{U}}$ in (24) with the further condition that only the ith eigenvalue is different from the two other ones. The group–subgroup relations are summarized in the diagram in Fig. 3, where the horizontal lines indicate conjugacy in $P^+(\mathbf{E}_a)$.

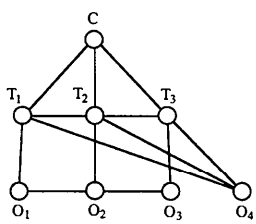


Fig. 3. Diagram of the group–subgroup relations among the cubic, tetragonal and orthorhombic holohedries; the horizontal lines mean conjugacy in the cubic group.

The same group–subgroup relations clearly hold for the lattice groups representing the above holohedries relative to their own bases. Now, it is not difficult to check that:

(i) If $\mathbf{E}_a$ is a basis for a primitive cubic lattice, then $\bar{\mathbf{U}}_i\mathbf{E}_a$ are all bases for tetragonal primitive lattices, $\bar{\mathbf{U}}\mathbf{E}_a$ generates a primitive orthorhombic lattice and $\bar{\mathbf{V}}_i\mathbf{E}_a$ are all bases for base-centered orthorhombic lattices.

(ii) If $\mathbf{E}_a$ is a basis for a body-centered cubic lattice, the $\bar{\mathbf{U}}_i\mathbf{E}_a$ are all bases for body-centered tetragonal lattices, $\bar{\mathbf{U}}\mathbf{E}_a$ generates a body-centered orthorhombic lattice and the $\bar{\mathbf{V}}_i\mathbf{E}_a$ are all bases for face-centered orthorhombic lattices.

(iii) If $\mathbf{E}_a$ is a basis for a face-centered cubic lattice, the $\bar{\mathbf{U}}_i\mathbf{E}_a$ all generate face-centered tetragonal lattices (which are indeed equivalent to the body-centered ones obtained in the previous case), $\bar{\mathbf{U}}\mathbf{E}_a$ generates a face-centered orthorhombic lattice and the $\bar{\mathbf{V}}_i\mathbf{E}_a$ are all bases for body-centered orthorhombic lattices.

Clearly, all these statements are true regardless of the cubic basis $\mathbf{E}_a$ chosen at the beginning from all those geometrically equivalent to any given one.

It can be verified that the analysis above allows one to retrieve the Bravais connections given in (17)–(20) and in (20), (21)–(23). At the same time, it also shows why inequivalent orthorhombic lattices, that is, lattices belonging to fixed sets of primitive or base-centered types on the one hand and to face-centered or body-centered types on the other hand, do not admit any Bravais connection through the intersection of their fixed sets, for they do not admit any common finite supergroup.

In principle, 'indirect' Bravais connections that do not pass directly through the intersection of the fixed sets of two given inequivalent orthorhombic lattices are still a possibility. Let C_0 and C_1 be the metrics of two such lattices and let us suppose that there exists an indirect Bravais connection $\lambda \mapsto C(\lambda)$, $\lambda \in [0, 1]$ between them. When leaving the fixed set $I_0 = I(L(C_0))$, of which C_0 is an element, C_λ must enter the intersection of I_0 with some intermediate fixed set, say I_2, which by hypothesis is different from $I_1 = I(L(C_1))$. We have seen above that $I_0 \cap I_2$ is then the fixed set of a tetragonal, hexagonal or cubic lattice group containing $L(C_0)$. Clearly, I_2 must not be an orthorhombic fixed set equivalent to I_0 or the deformation would be trivial. This immediately excludes the possibility that $I_2 \cap I_0$ be either a tetragonal or a hexagonal fixed set, owing to the previous analysis of thc subgroups of the tetragonal or hexagonal supergroups of any orthorhombic lattice group. Thus, $I_2 \cap I_0$ would have to be cubic. However, this case also does not allow for indirect Bravais connections between C_0 and C_1. Indeed, if $I_2 \cap I_0$ is cubic, I_2 must be tetragonal (it could in principle be orthorhombic but necessarily equivalent to I_0, a case we excluded as trivial). Again from the analysis of the tetragonal subgroups of the cubic groups, we see that from I_2 it would be impossible for $C(\lambda)$ to reach any inequivalent orthorhombic fixed set because inequivalent orthorhombic lattice groups only admit inequivalent tetragonal supergroups [we have seen from (i), (ii) and (iii) above that no tetragonal lattice group is a subgroup of two distinct cubic lattice groups containing inequivalent orthorhombic lattices].

This concludes the proof that there are two distinct lattice types in the orthorhombic system, according to (A').

4.4. *Monoclinic system*

The primitive and the face-centered monoclinic lattices are known to be the only two types in this system that are distinct according to definition (B). An analysis of the intersections of the monoclinic fixed sets is naturally possible also in this case through the study of the group–subgroup relations of the monoclinic lattice groups with the 'larger' lattice groups. This shows that Bravais connections between the inequivalent monoclinic lattices are indeed possible. Here we only give an example and omit the general analysis. The inequivalent monoclinic lattices admit the following metrics:

primitive monoclinic (see Fig. 4*a*)

$$C = \begin{pmatrix} C_{11} & 0 & 0 \\ 0 & C_{22} & C_{23} \\ 0 & C_{23} & C_{33} \end{pmatrix}; \qquad (27)$$

base-centered monoclinic (see Fig. 4*c*)

$$\tilde{C} = \begin{pmatrix} \tilde{C}_{11} & \tilde{C}_{12} & 0 \\ \tilde{C}_{12} & \tilde{C}_{22} & \frac{1}{2}\tilde{C}_{33} \\ 0 & \frac{1}{2}\tilde{C}_{33} & \tilde{C}_{33} \end{pmatrix}. \qquad (28)$$

As the lattice parameters are varied arbitrarily in C and $\tilde{C}$, we obtain the fixed sets of the lattice groups $L(C)$ and $L(\tilde{C})$, respectively, which have a non-empty intersection consisting of the following metrics (see Fig. 4*b*):

$$\check{C} = \begin{pmatrix} \check{C}_{11} & 0 & 0 \\ 0 & \check{C}_{22} & \frac{1}{2}\check{C}_{33} \\ 0 & \frac{1}{2}\check{C}_{33} & \check{C}_{33} \end{pmatrix}. \qquad (29)$$

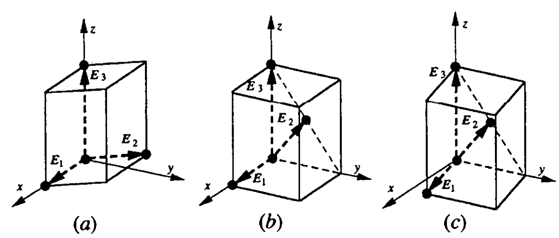


Fig. 4. Lattice bases used for the Bravais connection given in (27)–(29). (*a*) The primitive monoclinic basis. The twofold axis is *x*. (*b*) The base-centered orthorhombic basis. (*c*) The base-centered monoclinic basis. The twofold axis is *z*.

This is the fixed set of the lattice group of a base-centered orthorhombic lattice, which is obtained from (27) for $C_{ii} = \check{C}_{ii}$, $i = 1, 2, 3$, and $C_{23} = \frac{1}{2}\check{C}_{33}$, and from (28) for $\tilde{C}_{ii} = \check{C}_{ii}$, $i = 1, 2, 3$, and $\tilde{C}_{12} = 0$. Thus, in this case, a Bravais connection between two inequivalent monoclinic lattices, passing through a base-centered orthorhombic lattice, can be given by the union of the segments (20) with the choices (27), (28) and (29) for C, $\tilde{C}$ and $\check{C}$, respectively.

This shows that there is only one lattice type in the monoclinic system according to definition (A') and it completes the proof of proposition 4.1.

4.5. *Other interpretations of* (A)

Proposition 4.1 makes it interesting to consider other interpretations of (A), which, although less adherent to Bravais' own spirit, can give the same classification as (B). One possibility is to consider that in (A) the axes or planes of symmetry are intended to be 'material' during the lattice deformation. The notion of material lines or planes in a family of deformations for a body is classical in continuum mechanics and it refers to lines or planes that are 'in the matter', that is, pass through the same material points (in this case lattice points) during the deformation considered. In this interpretation, the axes or planes of symmetry mentioned in (A) necessarily have constant indices with respect to any given lattice basis $\mathbf{E}_a$ of the deforming lattice and are thus determined by the matrices (m_a^b) belonging to the lattice group $L(\mathbf{E}_a)$. The requirement in (A) that there be no loss of symmetry elements corresponds to assuming that in (16), for any λ, the lattice group of $\mathcal{R}_\lambda$ contains that of $\mathcal{R}$ or $\mathcal{R}'$ and the lattice groups of $\mathcal{R}$ and $\mathcal{R}'$ coincide.

It is easy to see from this definition and the arguments used for lemma 4.1 that, in this interpretation, (A) is equivalent to (B); indeed, since by hypothesis for the end lattices $\mathcal{R}$ and $\mathcal{R}'$ there are bases such that the corresponding lattice groups coincide, $\mathcal{R}$ and $\mathcal{R}'$ are necessarily equivalent according to (B).

However, this interpretation of (A) cannot be regarded to reflect Bravais' ideas because the equivalence with (B) rests only on the assumed properties of the end lattices and not on the properties of the deformation, any mention of which becomes inessential.

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