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An emendatory discursion on defining crystal systems

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1. Introduction

The term 'crystal system' occurs very early in the description of crystal symmetry. It seems to have been introduced by Weiss in 1815 [15] and has been used since then to classify crystal lattices and/or crystallographic groups in three-dimensional space according to some common properties. Unfortunately the term has been given different meanings, of which at least three still persist.

There have been several attempts to give dimension-independent definitions which coincide with some of these different usages for three-dimensional space. Two of the present authors were involved in such attempts in [10] and [1]. The concept of 'crystal system', proposed in these publications, coincides with the usage in the International Tables for X-ray crystallography [9] (henceforth abbreviated IT), for dimensions 2 and 3 and is well-defined for dimension 4. However, a careful analysis of [10] by Ch. Leedham-Green (private communication) made us aware of the fact that the definition of 'crystal system' given in [10] and [1] breaks down for some higher dimensions. In part 6 of this paper we describe a situation in seven-dimensional space that shows that the definition given in [10] and [1] is not dimension-independent.

The main part of this paper is a modified proposal for (hopefully correct) dimension-independent generalizations of all three kinds of 'crystal system' presently in use. By discussing some of their properties and interrelations we also hope to clarify the background to the old discussion about what is the 'right' definition of this term.

Rather than basing classifications primarily on lattices, as e.g. Schwarzenberger [12] does, we start from the notions of 'crystal structure' and 'space group'. We have to refer the reader for our way of defining these concepts, as well as those of 'space-group type', '$\mathbb{Z}$-class'(or 'arithmetic crystal class'), '$\mathbb{Q}$-class'(or 'geometric crystal class'), 'Bravais $\mathbb{Z}$-class', 'lattice', 'lattice basis', and 'Bravais type of lattices' to [1]. There also the term 'Bravais flock' has been introduced. This definition hinges on the fact that to each $\mathbb{Z}$-class a unique Bravais $\mathbb{Z}$-class can be assigned, cf. [1], p.15. A proof of this fact is not given there, but the reader was referred to [3] and [12]. The first of these quoted papers contains a hint to the proof only, while in [12] the proof is contained in the proof of its Theorem 2.1. Though those statements in this theorem that were used in the definition of Bravais flocks are correct, other statements of that theorem are not, cf. [13]. We therefore start here with the definition of Bravais flocks, and include a proof of the facts used in the definition, as this concept will play an essential rôle in the sequel.

Notation

The notation follows closely the one of [1]. Italic letters n,.. denote numbers, capital italic letters X,.. denote matrices. Boldface small letters $\mathbf{e}$, $\mathbf{f}$,.. denote vectors, boldface capital letters $\mathbf{V}$, $\mathbf{L}$,.. denote sets of vectors or of matrices, where addition of these is essential, e.g. lattices and vectorspaces. Gothic letters $\mathcal{G}$, $\mathcal{H}$,.. denote groups of matrices (under matrix multiplication) while script letters G, H,.. denote equivalence classes of groups. Small greek letters α, φ,.. denote mappings, capital greek letters B, Γ,.. groups of affine mappings. $\mathbb{Z}$, $\mathbb{Q}$, $\mathbb{R}$ are the sets of integers, rational, and real numbers respectively; $\leq$, $<$ means subgroup and proper subgroup respectively, while $\subset$ stands for set-inclusion, $\cap$ for the intersection.

2. Bravais flocks

As explained in [1] there is a one-to-one correspondence between the $\mathbb{Z}$-classes of n-dimensional space groups, of n-dimensional space-group types, and of finite groups of unimodular $n\times n$ matrices (abbreviated f.u. groups). As in [1], we are going to work mainly with the latter.

With a lattice $\mathbf{L}$ in the Euclidean vector space $\mathbf{V}_n$ there is associated the group $B(\mathbf{L})$ of all isometric mappings of $\mathbf{V}_n$ that map the lattice $\mathbf{L}$ onto itself. Describing $B(\mathbf{L})$ with respect to all different lattice bases of $\mathbf{L}$ we obtain a full $\mathbb{Z}$-class of f.u. groups which is called the Bravais $\mathbb{Z}$-class of $\mathbf{L}$.

Not all $\mathbb{Z}$-classes of f.u. groups are Bravais $\mathbb{Z}$-classes, but to a $\mathbb{Z}$-class of f.u. groups, we can assign a unique Bravais $\mathbb{Z}$-class by virtue of the following

Theorem 2.1: Let A be a $\mathbb{Z}$-class of f.u. groups. Then there exists a unique Bravais $\mathbb{Z}$-class B such that each f.u. group in A is a subgroup of some f.u. group in B, but is not a subgroup of any f.u. group belonging to a Bravais $\mathbb{Z}$-class of smaller order.

To prove this claim, which is crucial for the definition of Bravais flocks, we introduce the spaces of real quadratic forms left invariant by an f.u. group, much as in [2]. (For some discussion of the geometric background of this prodecure, cf. [1], pp. 21,25)
By $\mathcal{GL}(n,\mathbb{Z})$ we denote the group of all unimodular $n\times n$ matrices.

Let $\mathcal{G}$ be a finite group of unimodular $n\times n$ matrices. The set of all symmetric real $n\times n$ matrices X (or, equivalently, n-dimensional quadratic forms) satisfying

$$G^{\mathrm{tr}}\, X\, G = X \text{ for all } G \in \mathcal{G}$$

forms an $\mathbb{R}$-vector space $\mathbf{S}(\mathcal{G})$ containing some positive definite matrix. Conversely, for any set $\mathbf{S}$ of real symmetric matrices, containing a positive definite matrix, the set of all unimodular $n\times n$ matrices H such that

$$H^{\mathrm{tr}}\, X\, H = X \text{ for all } X \in \mathbf{S}$$

forms an f.u. group $\mathcal{B}(\mathbf{S})$. If $\mathbf{S}$ consists of a single matrix X, we write $\mathscr{B}(X)$ instead. We shall abbreviate $\mathscr{B}(\mathbf{S}(\mathscr{G}))$ to $\mathscr{B}(\mathscr{G})$. Note that $\mathscr{G} \leq \mathscr{B}(\mathscr{G})$, $\mathbf{S}(\mathscr{B}(\mathscr{G})) = \mathbf{S}(\mathscr{G})$, and $\mathscr{B}(\mathscr{B}(\mathscr{G})) = \mathscr{B}(\mathscr{G})$. We first prove, following in essence Schwarzenberger [12]:

Theorem 2.2: Let $\mathscr{G}$ be an f.u. group, and let $\mathbf{S}(\mathscr{G})$ and $\mathscr{B}(\mathscr{G})$ be defined as above. Then there exists a positive definite form $X_o \in \mathbf{S}(\mathscr{G})$, such that $\mathscr{B}(\mathscr{G}) = \mathscr{B}(\mathbf{S}(\mathscr{G}))$ is equal to $\mathscr{B}(X_o)$. (Such a form X_o is called a generic form in $\mathbf{S}(\mathscr{G})$).

Proof: (i) As $\mathscr{GL}(n, \mathbb{Z})$ is a countable group it has only countably many subgroups of finite order. So, in particular, there exist at most countably many finite subgroups $\mathscr{U}$ of $\mathscr{GL}(n, \mathbb{Z})$ such that $\mathscr{B}(\mathscr{G}) \leq \mathscr{U}$.

(ii) For any f.u. group $\mathscr{U}$ with $\mathscr{B}(\mathscr{G}) \leq \mathscr{U}$ we have $\mathbf{S}(\mathscr{B}(\mathscr{G})) \geq \mathbf{S}(\mathscr{U})$. Moreover, $\mathbf{S}(\mathscr{B}(\mathscr{G})) = \mathbf{S}(\mathscr{U})$ implies $\mathscr{B}(\mathscr{G}) = \mathscr{B}(\mathbf{S}(\mathscr{B}(\mathscr{G})) = \mathscr{B}(\mathbf{S}(\mathscr{U})) = \mathscr{B}(\mathscr{U}) \geq \mathscr{U}$. Therefore for each f.u. group $\mathscr{U}$ for which $\mathscr{B}(\mathscr{G})$ is a proper subgroup of $\mathscr{U}$ we conclude that $\mathbf{S}(\mathscr{U})$ is a proper subspace of $\mathbf{S}(\mathscr{B}(\mathscr{G})) = \mathbf{S}(\mathscr{G})$. The set $\mathbf{P}$ of positive definite forms in $\mathbf{S}(\mathscr{G})$ is an open subset of $\mathbf{S}(\mathscr{G})$. Let $\mathbf{V}$ be the union of the subspaces $\mathbf{S}(\mathscr{U})$ belonging to the at most countably many subgroups $\mathscr{U}$ of $\mathscr{GL}(n, \mathbb{Z})$ properly containing $\mathscr{B}(\mathscr{G})$. Then $\mathbf{P} \cap \mathbf{V}$ is of measure zero in $\mathbf{P}$, and hence there exists an $X_o \in \mathbf{P}$, $X_o \notin \mathbf{P} \cap \mathbf{V}$. Now $\mathscr{B}(X_o) \geq \mathscr{B}(\mathbf{S}(\mathscr{G})) = \mathscr{B}(\mathscr{G})$, and as $X_o \notin \mathbf{S}(\mathscr{U})$ for any $\mathscr{U} \underset{\neq}{>} \mathscr{B}(\mathscr{G})$, we have $\mathscr{B}(X_o) = \mathscr{B}(\mathscr{G})$.

□

We are now ready to give the

Proof of Theorem 2.1

Let $\mathscr{G}$ be an f.u. group of A. We want to show that the $\mathbb{Z}$-class of $\mathscr{B}(\mathscr{G})$ (in the notation of theorem 2.2) is the unique Bravais $\mathbb{Z}$-class satisfying the conditions imposed on B in theorem 2.1. There exists a lattice $\mathbf{L}$ in $\mathbf{V}_n$, with lattices basis $\{ \mathbf{l}_1, \ldots, \mathbf{l}_n \}$, such that the matrix of the scalar products of the $\mathbf{l}_i$ is a matrix X_o with $\mathscr{B}(X_o) = \mathscr{B}(\mathscr{G})$, cf. Theorem 2.2. Then $\mathscr{B}(X_o)$ is an f.u. group from the Bravais $\mathbb{Z}$-class of $\mathbf{L}$. So the $\mathbb{Z}$-class of $\mathscr{B}(\mathscr{G})$ is a Bravais $\mathbb{Z}$-class B.

For $M \in \mathscr{GL}(n, \mathbb{Z})$ we have $\mathbf{S}(M^{-1} \mathscr{G} M) = M^{tr} \mathbf{S}(\mathscr{G}) M$, and therefore $\mathscr{B}(M^{-1} \mathscr{G} M) = M^{-1} \mathscr{B}(\mathscr{G}) M$, so each f.u. group in A is a subgroup of some f.u. group in B. On the other hand, let $\mathscr{G}$ (without loss of generality) be a subgroup of the f.u. group $\mathscr{C}$ from a Bravais $\mathbb{Z}$-class. Let $\mathbf{L}'$ be a lattice such that $\mathscr{C}$ represents $B(\mathbf{L}')$ with respect to a lattice basis $\mathbf{f}_1, \ldots, \mathbf{f}_n$ of $\mathbf{L}'$, and let X_1 be the matrix of the scalar products of the $\mathbf{f}_i$. Then $\mathscr{C} = \mathscr{B}(X_1)$ and as $X_1 \in \mathbf{S}(\mathscr{G})$ we have

$$\mathscr{C} = \mathscr{B}(X_1) \geq \mathscr{B}(\mathbf{S}(\mathscr{G})) = \mathscr{B}(\mathscr{G}).$$

In particular $\mathscr{G}$ is contained in no group from a Bravais $\mathbb{Z}$-class of smaller order than that of $\mathscr{B}(\mathscr{G})$.

We can now state the following definition (taken from [1]):

Definition 2.3: The set of all $\mathbb{Z}$-classes to which a particular Bravais $\mathbb{Z}$-class B is assigned by the properties stated in theorem 2.1 is called the Bravais flock of B.

Theorem 2.1 guarantees that each $\mathbb{Z}$-class belongs to one and only one Bravais flock. So both Bravais flocks and $\mathbb{Q}$-classes form subdivisions of the set of all $\mathbb{Z}$-classes. The various definitions of crystal systems may be viewed as attempts to form coarser subdivisions of the set of all $\mathbb{Z}$-classes which respect the subdivision in Bravais flocks, $\mathbb{Q}$-classes, or both.

3. Crystal families

In one of the more often used conventions one distinguishes four 'crystal systems' (oblique, rectangular, square, and hexagonal) in the plane, and six (triclinic, monoclinic, orthorhombic, tetragonal, hexagonal, and cubic) in three-dimensional space, see, e.g. Buerger [4]. In [10] the name 'crystal family' has been introduced for the following dimension-independent classification that agrees with the one referred to above for dimensions 2 and 3:

Definition 3.1: A crystal family is the smallest set of space-group types containing, for any of its members, all space-group types of the Bravais flock, and all space-group types of the $\mathbb{Q}$-class, to which this member belongs.

Example: Space-group types $R3$ and $P6$ belong to the same crystal family, because $R3$ belongs to the same $\mathbb{Q}$-class as $P3$ and $P3$ belongs to the same Bravais flock as $P6$.

The classification of space-group types (and hence space groups) into crystal families also classifies $\mathbb{Z}$-classes, moreover it is the only one among the three discussed here that classifies both $\mathbb{Q}$-classes and Bravais flocks. Because of the first it may be thought of as a classification of crystals by their external shape, because of the second it is also a classification of lattices and Bravais types of lattices.

As in [1],p.16 the $\mathbb{Q}$-class to which a Bravais $\mathbb{Z}$-class of a lattice $\mathbf{L}$ belongs is called the holohedry of the lattice $\mathbf{L}$. In two dimensions all Bravais $\mathbb{Z}$-classes (and hence all lattices) in a crystal family belong to the same holohedry. In three-dimensional space, however, the rhombohedral lattices with holohedry $\bar{3}m$ and the hexagonal lattices with holohedry $6/mmm$ both belong to the same family. In four-dimensional space in eight of the twenty-three crystal families there exist two different holohedries each. In one family three different holohedries exist, and it is to be expected that in higher dimensions the situation is even more complicated. Among other reasons, it is the occurence of these cases that may be felt as a deficiency of the notion of crystal family and thus leads to the following classifications.

4. Bravais-flock systems (Bravais systems)

A second kind of 'crystal system', which for three-dimensional space has been used mainly by French crystallographers since Bravais, e.g. Friedel [5], will be called 'Bravais-flock system' or, for short, 'Bravais system' here. We shall first give a dimension-independent definition starting from a geometric aspect.

Definition 4.1: A Bravais-flock system (or, for short, Bravais system) consists of full Bravais flocks of space groups (or, equivalently, space-group types, or f.u. groups, or $\mathbb{Z}$-classes). Two Bravais flocks belong to the same Bravais system if the Bravais $\mathbb{Z}$-classes of these two Bravais flocks belong to the same geometric crystal class.

Bravais types of lattices and Bravais flocks of space groups are in one-to-one correspondence via their Bravais $\mathbb{Z}$-classes (cf. [1], p.15). Therefore lattices and Bravais types of lattices are classified into Bravais systems, too. A crystal family always contains full Bravais systems. In dimension two, Bravais systems and crystal families coincide. The same holds for the five non-hexagonal crystal families of three-dimensional space. The hexagonal family, however, splits into two Bravais systems, which are called the rhombohedral Bravais system (consisting of space-group types with Hermann-Mauguin symbols R ...) and the hexagonal Bravais system (consisting of space-group types with Hermann-Mauguin symbols P ...).

Each space-group type of the hexagonal Bravais system belongs to one of the twelve $\mathbb{Q}$-classes from 3 to $6/mmm$. Each space-group type of the rhombohedral Bravais system belongs to one of the five $\mathbb{Q}$-classes $3, \bar{3}$, 32, $3m$, and $\bar{3}m$ only. However, the Bravais systems do not provide a classification of the $\mathbb{Q}$-classes. The $\mathbb{Q}$-class 3, e.g., contains space-group type $R3$ which belongs to the rhombohedral Bravais system, and space-group type $P3$ belonging to the hexagonal Bravais system.

Definition 4.1 utilizes the distinguished rôle of the Bravais $\mathbb{Z}$-class in a Bravais flock. We shall now give another characterisation of the Bravais systems that completely avoids reference to this distinguished rôle. For the formulation of this and further concepts it will be convenient to use the term 'intersection' in its set-theoretical sense, i.e. we shall say that a $\mathbb{Q}$-class and a Bravais flock intersect if there is at least one space group common to both. If a $\mathbb{Q}$-class and a Bravais flock intersect they have, of course, a whole $\mathbb{Z}$-class of space groups - or, in the equivalent formulation using f.u. groups, a whole $\mathbb{Z}$-class of f.u. groups - in common.

Theorem 4.2: Let F and F' be Bravais flocks. If the Bravais $\mathbb{Z}$-classes of F and F' belong to the same $\mathbb{Q}$-class then F and F' intersect the same set of $\mathbb{Q}$-classes. Conversely, if F and F' intersect the same set of $\mathbb{Q}$-classes then the Bravais $\mathbb{Z}$-classes of F and F' belong to the same $\mathbb{Q}$-class.

Proof: It is convenient to work with f.u. groups again. To prove the first assertion, let $\mathcal{G}$ be an f.u. group from some $\mathbb{Z}$-class in F. Then by the definition of a Bravais flock there exists an f.u. group $\mathcal{B}$ from the Bravais $\mathbb{Z}$-class B of F, such that $\mathcal{G} \leq \mathcal{B}$. Let X be a rational nonsingular matrix such that $X^{-1} \mathcal{B} X$ is contained in the Bravais $\mathbb{Z}$-class B' of F'. Then $X^{-1}\mathcal{G}X \leq X^{-1}\mathcal{B}X$ and so F' also intersects the $\mathbb{Q}$-class to which $\mathcal{G}$ belongs.

To prove the converse, let $\mathcal{B}$ and $\mathcal{B}'$ be f.u. groups from the Bravais $\mathbb{Z}$-classes B and B' of F and F' respectively. As F and F' are assumed to intersect the same set of $\mathbb{Q}$-classes, there exist rational non-singular matrices X and Y such that $X^{-1}\mathcal{B}X \leq \mathcal{B}'$ and $Y^{-1}\mathcal{B}'Y \leq \mathcal{B}$. Therefore the orders of $\mathcal{B}$ and $\mathcal{B}'$ must be equal and we have in fact $X^{-1}\mathcal{B}X = \mathcal{B}'$ as claimed.

□

As an immediate consequence of Theorem 4.2 we have that Definition 4.1 is equivalent to the following

Definition 4.3: A Bravais system consists of full Bravais flocks. Two Bravais flocks belong to the same Bravais system if both Bravais flocks intersect the same set of $\mathbb{Q}$-classes.

5. Crystal-class systems (Crystal systems)

In the last section, we have stressed the point that Bravais systems consist of whole Bravais flocks but not in all cases of whole $\mathbb{Q}$-classes. For the 'crystal systems', as used, e.g., in IT, the opposite is true: they consist of whole $\mathbb{Q}$-classes but not in all cases of whole Bravais flocks. More precisely: While the 'crystal systems' of IT coincide with the crystal families (and with the Bravais systems) for dimension 2 and for the five non-hexagonal families of three-dimensional space, the hexagonal family is subdivided into the trigonal crystal system consisting of the five $\mathbb{Q}$-classes 3, $\bar{3}$, 32, $3m$, and $\bar{3}m$ and the hexagonal crystal system consisting of the $\mathbb{Q}$-classes 6, $\bar{6}$, $6/m$, 622, $6mm$, $\bar{6}2m$, and $6/mmm$. Whereas a Bravais flock always determines uniquely its Bravais $\mathbb{Z}$-class (playing the rôle of a 'leading sheep' in the Bravais flock), there is in general no distinguished $\mathbb{Z}$-class within a $\mathbb{Q}$-class. This caused the difficulty (and the mistake in [10] and [1], see section 6) in finding a dimension-independent definition that generalizes this kind of subdivision.

However, Definition 4.3 lends itself to the formulation of a counterpart which will then join together whole $\mathbf{Q}$-classes, but not necessarily Bravais flocks.

Definition 5.1: A crystal-class system (or, for short, crystal system) consists of full $\mathbf{Q}$-classes. Two $\mathbf{Q}$-classes belong to the same crystal system if they intersect the same set of Bravais flocks.

This definition may be considered as a reformulation of the statement of I.T., p. 46, first section: "The grouping of the point groups according to the kind of lattice with which they can combine to form space groups is analogous to the grouping of three-dimensional point groups into 'systems'".

It is clear from the definition that a crystal family contains full crystal systems. It can be easily checked that for dimensions 2 and 3 the crystal systems defined by 5.1 coincide with the ones used in IT as described above. Definition 5.1 also yields the 33 four-dimensional crystal systems distinguished in [16] and [1]. Moreover, crystal systems, as defined by 5.1, have some useful properties that call for the adoption of this general definition.

As a first of these we show:

Theorem 5.2: A crystal system contains at most one holohedry.

Proof: By the definition of a holohedry, repeated above from [1], p. 16, one has to show that any two Bravais $\mathbf{Z}$-classes G and H contained in the same crystal system actually belong to the same $\mathbf{Q}$-class. By definition 5.1 the $\mathbf{Q}$-classes of G and H must intersect the same set of Bravais flocks, so in particular the $\mathbf{Q}$-class of G must intersect the Bravais flock of H and the $\mathbf{Q}$-class of H must intersect the Bravais flock of G. So for any two f.u. groups $\mathcal{G}$ and $\mathcal{H}$ from G and H, respectively, rational invertible matrices X_1 and X_2 exist such that

$$X_1^{-1} \mathcal{G} X_1 \leq \mathcal{H} \text{ and } X_2^{-1} \mathcal{H} X_2 \leq \mathcal{G}.$$

Then $\mathcal{G}$ and $\mathcal{H}$ have equal order and $X_1^{-1} \mathcal{G} X_1 = \mathcal{H}$, i.e. G and H belong to the same $\mathbf{Q}$-class.

□

Note that Theorem 5.2 does not claim that a crystal system does contain a holohedry (and hence a Bravais $\mathbb{Z}$-class) at all. In fact, while in dimensions 2, 3, and 4 this is the case, it is no longer true in some higher dimensions. In section 6 we shall describe some seven-dimensional groups which among other things will demonstrate the existence of a seven-dimensional crystal system without holohedry.

For dimensions in which all crystal systems contain a holohedry, it follows from Theorem 5.2 that the number of crystal systems is equal to the number of Bravais systems and that both can be characterized by their holohedries, while for higher dimensions there will in general be more crystal systems than Bravais systems.

Although, as pointed out, crystal systems need not contain holohedries they do have some nice 'coherence' properties. To derive them we first prove:

Lemma 5.3: Let $\mathcal{G}$ and $\mathcal{H}$ be f.u. groups with $\mathcal{G} \leq \mathcal{H}$. $\mathcal{G}$ and $\mathcal{H}$ belong to the same crystal family if and only if they belong to the same Bravais flock.

Proof: If $\mathcal{G}$ and $\mathcal{H}$ belong to the same Bravais flock they clearly belong to the same crystal family.

To show the converse we first note that the dimension of the $\mathbb{R}$-vector space $\mathbf{S}(\mathcal{G})$ (defined in section 2) is the same for all f.u. groups $\mathcal{G}$ in a family.
This is seen as follows:
If $\mathcal{G}$ and $\mathcal{H}$ are f.u. groups from the same Bravais flock, then $\mathbf{S}(\mathcal{G}) = \mathbf{S}(\mathcal{H})$. If on the other hand $\mathcal{G}$ and $\mathcal{H}$ are f.u. groups from the same $\mathbb{Q}$-class and X is a non-singular rational matrix with

$$X^{-1}\, \mathcal{G}\, X = \mathcal{H}, \text{ then } X^{tr}\, \mathbf{S}(\mathcal{G})\, X = \mathbf{S}(\mathcal{H}).$$

Therefore the dimension of the $\mathbb{R}$-vector space $\mathbf{S}(\mathcal{G})$ is a family-invariant.

Now let $\mathcal{G}$ and $\mathcal{H}$ be f.u. groups from the same crystal family and let $\mathcal{G} \leq \mathcal{H}$. Then $\mathbf{S}(\mathcal{H}) \leq \mathbf{S}(\mathcal{G})$ and $\dim \mathbf{S}(\mathcal{G}) = \dim \mathbf{S}(\mathcal{H})$ and thus $\mathbf{S}(\mathcal{G}) = \mathbf{S}(\mathcal{H})$. Therefore $\mathcal{G}$ and $\mathcal{H}$ belong to the same Bravais flock.

□

We further need:

Lemma 5.4: Let $\mathscr{G}$ and $\mathscr{H}$ be f.u. groups of the same Bravais flock such that $\mathscr{G} \leq \mathscr{H}$. Let G and H be the $\mathbb{Q}$-classes of $\mathscr{G}$ and $\mathscr{H}$, respectively. Then any Bravais flock that intersects H will also intersect G.

Proof: Let $\mathscr{H}'$ be any f.u. group in H and let X be a rational non-singular matrix with $X^{-1} \mathscr{H} X = \mathscr{H}'$.
Then $X^{-1} \mathscr{G} X \leq X^{-1} \mathscr{H} X = \mathscr{H}'$. Further as $\mathbf{S}(\mathscr{G}) = \mathbf{S}(\mathscr{H})$, we have

$\mathbf{S}(X^{-1}\mathscr{G} X) = X^{tr}\, \mathbf{S}(\mathscr{G})\, X = X^{tr}\, \mathbf{S}(\mathscr{H})\, X = \mathbf{S}(X^{-1} \mathscr{H} X)$, and thus $X^{-1} \mathscr{G} X$ belongs to the same Bravais flock as $X^{-1} \mathscr{H} X$.

□

From these two lemmas, which may also have some independent interest, we now obtain the desired coherence property of crystal systems:

Theorem 5.5: Let $\mathscr{G}$, $\mathscr{H}$, and $\mathscr{K}$ be f.u. groups with $\mathscr{G} \leq \mathscr{H} \leq \mathscr{K}$. If $\mathscr{G}$ and $\mathscr{K}$ belong to the same crystal system S then $\mathscr{H}$ also belongs to the crystal system S.

Proof: As $\mathscr{G}$ and $\mathscr{K}$ belong to the same crystal system they certainly belong to the same crystal family and thus by Lemma 5.3 to the same Bravais flock. As a direct consequence of the definition of a Bravais flock, $\mathscr{G}$, $\mathscr{H}$, and $\mathscr{K}$ therefore belong to the same Bravais flock. For an f.u. group $\mathscr{A}$ let $F(\mathscr{A})$ be the set of Bravais flocks intersecting the $\mathbb{Q}$-class of $\mathscr{A}$. Then by Lemma 5.4 we have

$F(\mathscr{K}) \subseteq F(\mathscr{H}) \subseteq F(\mathscr{G})$. However, as $\mathscr{G}$ and $\mathscr{K}$ belong to the same crystal system S, we have $F(\mathscr{K}) = F(\mathscr{G})$ and hence equality holds throughout, i.e. $\mathscr{H}$ also belongs to S.

□

6. An example and its consequences

In this section we shall describe some $\mathbb{Z}$-classes of finite groups of 7x7 unimodular matrices, which show that in seven-dimensional space the following situation exists, see Fig.1:

There is a $\mathbf{Q}$-class A of order $2^3\ 7$ consisting of nine $\mathbf{Z}$-classes $A_1, \ldots A_9$. These $\mathbf{Z}$ classes belong to seven Bravais flocks whose Bravais $\mathbf{Z}$-classes are D_1, D_2, D_3, E_3, E_4, F_1, and F_2. These belong to three different $\mathbf{Q}$-classes D, E, and F of orders $2^{11} \cdot 3^2 \cdot 5 \cdot 7$, $2^8 \cdot 3^2 \cdot 5 \cdot 7$, and $2^{10} \cdot 3^4 \cdot 5 \cdot 7$, respectively. D consists of D_1, D_2, and D_3, F consists of F_1 and F_2, while E contains not only E_3 and E_4, but also two $\mathbf{Z}$-classes E_1 and E_2 which are not Bravais $\mathbf{Z}$-classes.

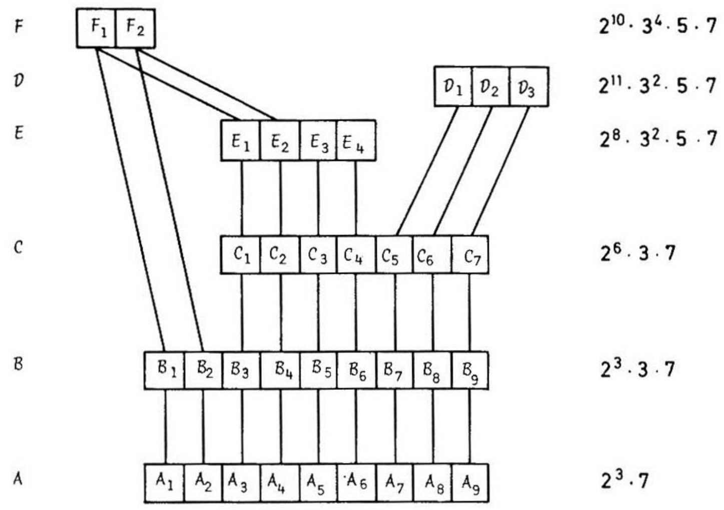

Fig.1 Some arithmetic classes of f.u. groups in seven-dimensional space

The crystal system to which A belongs contains no holohedry. It consists of eight $\mathbf{Q}$-classes, of which three (A , B, and C) are shown in Fig. 1.

The $\mathbf{Q}$-class A (or likewise B or C) provides an example that in [10] and [1] crystal systems were not well-defined independently of the dimension. In [10] the concept of crystal system was defined in the following way:

"2.9 Definition: Each holohedral crystal class (= holohedry) H determines a crystal system. We say that a (geometric) crystal class (= $\mathbf{Q}$-class) C belongs to the crystal system of H if each group of C is a subgroup of some group of H , but not a subgroup of a group of another holohedral geometric class (= holohedry) of smaller order."

The wrongly alledged property of $\mathbf{Q}$-classes is brought out even more clearly by the formulation on p. 16 of [1] :

"Not all $\mathbf{Q}$-classes of f.u. groups are holohedries. However, for any $\mathbf{Q}$-class C there is a unique holohedry H such that each f.u. group in C is a subgroup of some f.u. group in H but is not a subgroup of any f.u. group belonging to a holohedry of smaller order. Using this..."

This statement has been checked in dimensions 2, 3, and 4, but the example of the $\mathbf{Q}$-class A , mentioned above, shows, that it is not true for arbitrary dimensions. Therefore the definition of 'crystal system' in [10] and [1] breaks down in some higher dimensions, although it yields the same classification of $\mathbf{Q}$-classes as the new one, proposed in section 5, for dimensions 2, 3, and 4.

We shall now describe explicitly the seven-dimensional f.u. groups to whose existence we referred above. For the definition of the group-theoretic terms used in this section see, e.g., Huppert [8] .

Plesken and Pohst [11] derived the maximal finite irreducible subgroups of $\mathcal{GL}(7,\mathbf{Z})$. All of them turned out to be among the groups C. Hermann [6] had listed as the 'fully transitive' groups. They can be described as follows:

(1) Let $\mathbf{e}_1, \ldots, \mathbf{e}_7$ be an orthogonal basis of the seven-dimensional Euclidean vector space $\mathbf{V}_7$. Then the Bravais $\mathbb{Z}$-classes of the lattices

$$\mathbf{L}_1 = \{ \sum_{i=1}^{7} a_i \, \mathbf{e}_i \mid a_i \in \mathbb{Z} \} ,$$

$$\mathbf{L}_2 = \{ \sum_{i=1}^{7} a_i \, \mathbf{e}_i \mid a_i \in \mathbb{Z} , \sum_{i=1}^{7} a_i \equiv 0 (\mathrm{mod}\ 2) \}, \quad \text{and}$$

$$\mathbf{L}_3 = \{ \sum_{i=1}^{7} a_i \, \mathbf{e}_i \mid a_i \in \mathbb{Z} , a_1 \equiv a_i \ (\mathrm{mod}\ 2) \text{ for } i=2,\ldots,7 \}$$

form a complete $\mathbb{Q}$-class of order $2^7 \cdot 7! = 2^{11} \cdot 3^2 \cdot 5 \cdot 7$. In particular $B(\mathbf{L}_1)$ is represented by the full monomial group of degree 7 with respect to the basis $\mathbf{e}_1, \ldots, \mathbf{e}_7$ and so is isomorphic to the wreath product of a cyclic group of order 2 by the symmetric group of degree 7. The Bravais $\mathbb{Z}$-classes of $\mathbf{L}_1$, $\mathbf{L}_2$, and $\mathbf{L}_3$ are called $\mathcal{D}_1$, $\mathcal{D}_2$, and $\mathcal{D}_3$, respectively, in Fig.1 and its description above.

(2) Let $\mathbf{f}_1, \ldots, \mathbf{f}_8$ be vectors in $\mathbf{V}_7$ such that their scalar products satisfy

$$< \mathbf{f}_i, \mathbf{f}_j > = \begin{cases} 7 & \text{if } i = j = 1,\ldots,7 \\ -1 & \text{if } i \neq j, i,j = 1,\ldots,7 \end{cases}$$

Then $\mathbf{f}_1 + \ldots + \mathbf{f}_8 = \mathbf{o}$ and because of this property we can define four further lattices by:

$$\mathbf{L}^1 = \{ \sum_{i=1}^{8} a_i \, \mathbf{f}_i \mid a_i \in \mathbb{Z} \} ,$$

$$\mathbf{L}^2 = \{ \sum_{i=1}^{8} a_i \, \mathbf{f}_i \mid a_i \in \mathbb{Z} , \sum_{i=1}^{8} a_i \equiv 0 \ (\mathrm{mod}\ 2) \}$$

$$\mathbf{L}^3 = \{ \sum_{i=1}^{8} a_i \, \mathbf{f}_i \mid a_i \in \mathbb{Z} , \sum_{i=1}^{8} a_i \equiv 0 \ (\mathrm{mod}\ 4) \}$$

$$\mathbf{L}^4 = \{ \sum_{i=1}^{8} a_i \, \mathbf{f}_i \mid a_i \in \mathbb{Z} , \sum_{i=1}^{8} a_i \equiv 0 \ (\mathrm{mod}\ 8) \}$$

$B(\mathbf{L}^1)$ permutes the vectors $\pm \mathbf{f}_1, \ldots, \pm \mathbf{f}_8$ since these are all vectors of norm 7 in $\mathbf{L}^1$. Using this, one concludes that $B(\mathbf{L}^1)$ is isomorphic to the direct product of a cyclic group of order 2 (corresponding to the point inversion) and the symmetric group of degree 8. $B(\mathbf{L}^1)$ also acts on the lattices $\mathbf{L}^2$, $\mathbf{L}^3$, and $\mathbf{L}^4$, hence is a subgroup of $B(\mathbf{L}^2)$, $B(\mathbf{L}^3)$, and $B(\mathbf{L}^4)$. In fact it can be seen that $B(\mathbf{L}^1) = B(\mathbf{L}^4)$ as the lattices $\mathbf{L}^1$ and $\mathbf{L}^4$ are 'dual' in the sense that there is a lattice basis $\mathbf{b}_1, \ldots, \mathbf{b}_7$ of $\mathbf{L}^4$ such that

$$< \mathbf{f}_i , \mathbf{b}_j > = \begin{cases} a & \text{if } i = j = 1, \ldots, 7 \\ 0 & \text{if } i \neq j, i, j = 1, \ldots, 7 \end{cases}$$

where $a \in \mathbb{R}$, $a \neq 0$ (and in this case $a = 8$).

Therefore, the Bravais $\mathbb{Z}$-classes of $\mathbf{L}^1$ and $\mathbf{L}^4$ belong to the same $\mathbb{Q}$-class.

However, as Hermann [6] remarked already, $\mathbf{L}^2$ and $\mathbf{L}^3$ have higher symmetry, namely $B(\mathbf{L}^3)$ turns out to be the Weyl group of the root system E_7, which is a reflection group of order $2^{10} \cdot 3^4 \cdot 5 \cdot 7$, cf., e.g. [7]. Since also $\mathbf{L}^2$ and $\mathbf{L}^3$ are dual in the above sense, the Bravais $\mathbb{Z}$-classes of $\mathbf{L}^2$ and $\mathbf{L}^3$ again belong to the same $\mathbb{Q}$-class.

In Fig. 1 and the accompanying description the Bravais $\mathbb{Z}$-classes of $\mathbf{L}^1$ and $\mathbf{L}^4$ are denoted by E_3 and E_4, respectively and the Bravais $\mathbb{Z}$-classes of $\mathbf{L}^2$ and $\mathbf{L}^3$ by F_1 and F_2.

Plesken and Pohst [11] have proved that $\mathbf{L}_1$, $\mathbf{L}_2$, $\mathbf{L}_3$, $\mathbf{L}^1$, $\mathbf{L}^2$, $\mathbf{L}^3$, $\mathbf{L}^4$ constitute a set of representatives of the Bravais types of lattices with irreducible Bravais $\mathbb{Z}$-class in 7-dimensional space. As the groups of the seven Bravais $\mathbb{Z}$-classes belonging to the lattices $\mathbf{L}_1, \ldots, \mathbf{L}^4$ are complex irreducible, the corresponding form spaces are one-dimensional. Each of them can, therefore, be characterized by the matrix of the scalar products of a particular lattice basis. For completeness we include for each of the lattices a lattice basis such that the matrix of the scalar products is particularly simple.

$\mathbf{L}_1$: $\mathbf{e}_1; \dots; \mathbf{e}_7$

$\mathbf{L}_2$: $\mathbf{e}_1+\mathbf{e}_2; \mathbf{e}_2+\mathbf{e}_3; \mathbf{e}_3+\mathbf{e}_4; \mathbf{e}_4+\mathbf{e}_5; \mathbf{e}_5+\mathbf{e}_6; \mathbf{e}_6+\mathbf{e}_7; \mathbf{e}_7+\mathbf{e}_1$

$\mathbf{L}_3$: $2\mathbf{e}_1; 2\mathbf{e}_2; 2\mathbf{e}_3; 2\mathbf{e}_4; 2\mathbf{e}_5; 2\mathbf{e}_6; \mathbf{e}_1+\mathbf{e}_2+\mathbf{e}_3+\mathbf{e}_4+\mathbf{e}_5+\mathbf{e}_6+\mathbf{e}_7$

$\mathbf{L}^1$: $\mathbf{f}_1; \mathbf{f}_2; \mathbf{f}_3; \mathbf{f}_4; \mathbf{f}_5; \mathbf{f}_6; \mathbf{f}_7;$

$\mathbf{L}^2$: $\mathbf{f}_1+\mathbf{f}_2; \mathbf{f}_2+\mathbf{f}_3; \mathbf{f}_3+\mathbf{f}_4; \mathbf{f}_4+\mathbf{f}_5; \mathbf{f}_5+\mathbf{f}_6; \mathbf{f}_6+\mathbf{f}_7; \mathbf{f}_7+\mathbf{f}_1$

$\mathbf{L}^3$: $-\mathbf{f}_1+\mathbf{f}_2; \mathbf{f}_3-\mathbf{f}_4; \mathbf{f}_1-\mathbf{f}_5; +\mathbf{f}_4+\mathbf{f}_5+\mathbf{f}_6+\mathbf{f}_7; -\mathbf{f}_3-\mathbf{f}_4-\mathbf{f}_6-\mathbf{f}_7; -\mathbf{f}_1-\mathbf{f}_2-\mathbf{f}_5-\mathbf{f}_6; \mathbf{f}_6-\mathbf{f}_7;$

or $\mathbf{f}_1+\mathbf{f}_2+\mathbf{f}_3+\mathbf{f}_4; \mathbf{f}_2+\mathbf{f}_3+\mathbf{f}_4+\mathbf{f}_5; \mathbf{f}_3+\mathbf{f}_4+\mathbf{f}_5+\mathbf{f}_6; \mathbf{f}_4+\mathbf{f}_5+\mathbf{f}_6+\mathbf{f}_7;$

$\mathbf{f}_5+\mathbf{f}_6+\mathbf{f}_7+\mathbf{f}_1; \mathbf{f}_6+\mathbf{f}_7+\mathbf{f}_1+\mathbf{f}_2; \mathbf{f}_7+\mathbf{f}_1+\mathbf{f}_2+\mathbf{f}_3$

$\mathbf{L}^4$: $\mathbf{f}_1-\mathbf{f}_8; \mathbf{f}_2-\mathbf{f}_8; \mathbf{f}_3-\mathbf{f}_8; \mathbf{f}_4-\mathbf{f}_8; \mathbf{f}_5-\mathbf{f}_8; \mathbf{f}_6-\mathbf{f}_8; \mathbf{f}_7-\mathbf{f}_8.$

We shall now exhibit in a way slightly different from [11] the existence of the $\mathbf{Q}$-class A of Fig.1, that plays such a crucial part in the discussion above. B and C can be obtained by similar arguments.

Let G be a permutation group of degree 8, generated by $\alpha = (1234567)(8)$ and $\beta = (18)(24)(37)(56)$. G has order 56 and can be viewed as the affine group on the line over the Galois field of eight elements, cf. Sims [14]. In particular G has a normal subgroup N of order 8 generated by the elements conjugate to β. N is a direct product of three cyclic subgroups of order 2.

(1) Since G acts as a permutation group of degree 8, we can embed it into S_8 and let it act on the lattice $\mathbf{L}^1$ where it permutes the vectors $\mathbf{f}_1, \dots \mathbf{f}_8$. Hence G yields a subgroup Γ of $B(\mathbf{L}^1)$, and Γ acts also on $\mathbf{L}^2$, $\mathbf{L}^3$, and $\mathbf{L}^4$, as $B(\mathbf{L}^1)$ does.

(2) Since the index of N in G is 7, we can induce any representation $\delta: N \to \{\pm 1\}$ of N to G and get a monomial representation $\Delta : G \to \mathcal{GL}(7, \mathbb{Z})$. If we choose δ different from the trivial representation, Δ is faithful, and hence we get a group $\Gamma' \cong G$ acting on the lattice $\mathbf{L}_1$. Since $B(\mathbf{L}_1)$ acts also on $\mathbf{L}_2$ and $\mathbf{L}_3$, Γ' also does.

(3) As G has only eight irreducible characters, one of degree 7, and seven of degree 1, any faithful representation of G of degree 7 must be irreducible, therefore Γ and Γ' act irreducibly. Moreover these actions are rationally equivalent, i.e. all f.u. groups obtained from Γ and Γ', respectively, by choosing lattice bases for $\mathbf{L}_1,\dots,\mathbf{L}_3,\mathbf{L}^1,\dots,\mathbf{L}^4$ belong to the same $\mathbb{Q}$-class.

(4) Let $\mathcal{G}$ be the f.u. group obtained from Γ by choosing a lattice basis for $\mathbf{L}_1$. Then all f.u. groups in the $\mathbb{Q}$-class G of $\mathcal{G}$ will be irreducible and therefore also the groups $\mathcal{B}(\mathcal{H})$ for all $\mathcal{H} \in G$. As, in seven-dimensional space, the Bravais $\mathbb{Z}$-classes of the lattices $\mathbf{L}_1, \mathbf{L}_2, \mathbf{L}_3, \mathbf{L}^1, \mathbf{L}^2, \mathbf{L}^3$, and $\mathbf{L}^4$ are the only Bravais $\mathbb{Z}$-classes consisting of irreducible groups, we see that all the groups $\mathcal{B}(\mathcal{H})$ as above must belong to these 7 Bravais $\mathbb{Z}$-classes. This suffices to show that the $\mathbb{Q}$-class A lies in a crystal system without holohedry. The further details, shown in Fig.1, have been obtained by computer calculations using the methods of Plesken and Pohst [11].

7. Conclusion

The relations between the concepts $\mathbb{Z}$-class; $\mathbb{Q}$-class and Bravais flock; crystal system and Bravais system; and finally crystal family may be summarized in Fig.2, where downward connection means that the classification below is a subdivision of that above. By comparison with Fig.1 of [10] the greater symmetry of the new one reflects the fact that the definitions proposed in sections 2, 3, 4, and 5 of this paper give more balance to the viewpoints of classification by lattice symmetry and by symmetry of macroscopic shape.

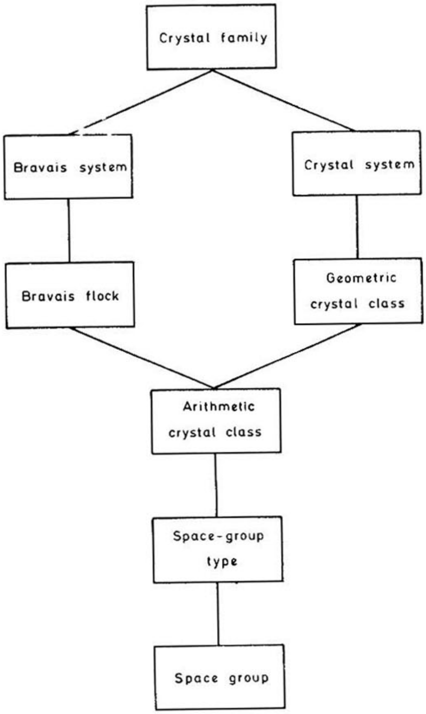

Fig.2 Relations between main crystallographic classifications

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