Enantiomorphism of crystallographic groups in higher dimensions with results in dimensions up to 6

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This paper gives classification results for crystallographic groups in dimensions up to 6 which refine earlier enumeration results. Based on the classification data, the asymptotic growth of the number of space-group types is discussed. The classification scheme for crystallographic groups is revisited and a new classification level in between that of geometric and arithmetic crystal classes is introduced and denoted as *harmonic crystal classes*. Enantiomorphic pairs are determined on all classification levels from space-group types to crystal families and the enantiomorphic pairs of fixed-point-free space groups are given. A general algorithm to compute enantiomorphic pairs is described.

1. Introduction

The classification of crystallographic groups in dimensions beyond 3 has been motivated from many sources, ranging from incommensurate crystal phases and quasicrystals over snow crystals to biomacromolecules. An excellent overview of the different application areas is given by Janner (2001).

For the groups of four-dimensional space, information on the single groups has been tabulated in the book by Brown *et al.* (1978), but in comparison with *International Tables for Crystallography* (Hahn, 2002) the information is already heavily compressed. The rapid growth of the number of groups for increasing dimensions makes it obvious that for dimensions ≥ 5 an approach listing all the groups is not feasible. A new philosophy for dealing with crystallographic groups in higher dimensions was suggested by Opgenorth *et al.* (1998), namely the combination of a set of algorithms with a database containing crucial data from which further information can easily be computed. A system realizing this approach is the *CARAT* computer package described by Plesken *et al.* (1998), which is freely available at http://wwwb.math.rwth-aachen.de/carat/.

The power of a system like *CARAT* has been demonstrated by enumerating the crystallographic groups in dimensions 5 and 6 (Plesken & Schulz, 2000), as well as determining the fixed-point-free space groups in these dimensions (Cid & Schulz, 2001). The main advantage, however, lies in the capability to compute specific information without having to go through an enormous classification task. For example, for an interesting point group one is able to enumerate the space-group types in its geometric crystal class even if a full classification in the respective dimension is out of the question.

In the current paper, the results of Plesken & Schulz (2000) and Cid & Schulz (2001) are supplemented by determining enantiomorphic pairs on the different classification levels. An enantiomorphic pair is a pair of objects that are equivalent by an affine but not by an orientation-preserving transformation of the underlying Euclidean space. For example, two groups forming an enantiomorphic pair of space groups are isomorphic but have opposite handedness. The orbit of a point under one group is the mirror image of the orbit under the other group.

The paper is organized as follows: in §2 the terminology to describe the different classification levels is fixed (including the definition of a new level) and the notion of enantiomorphism is discussed in detail. §3 describes an algorithm to determine enantiomorphic pairs on the different classification levels. It also gives an example illustrating that geometric crystal classes in which all arithmetic crystal classes are enantiomorphic are not necessarily enantiomorphic themselves. The results obtained in dimensions 5 and 6 are presented in §4, together with a brief review of results in lower dimensions. As a byproduct of the classification, the smallest examples of crystal systems not containing a holohedry are presented. A short discussion on the asymptotic number of space-group types in higher dimensions concludes the paper.

2. Terminology and definitions

In this section, we will fix the terminology used throughout this paper, closely following the definitions of Opgenorth *et al.* (1998) and of Janssen *et al.* (1999, 2002).

2.1. Basic terminology

After fixing an origin and a basis of the lattice of translation vectors, the action of a crystallographic space group on the underlying Euclidean space is given by

$$R(P, v) := \left\{ \{g \mid v(g) + t\} := \begin{pmatrix} g & v(g) + t \\ 0 & 1 \end{pmatrix} \mid g \in P, t \in \mathbb{Z}^n \right\}$$

$\subseteq GL(n+1, \mathbb{R})$, where $P \leq GL(n, \mathbb{Z})$ is a finite integral matrix group and v is a *vector system*. This means that v is a map $v : P \rightarrow \mathbb{R}^n$ with $v(gh) = v(g) + g \cdot v(h) \pmod{\mathbb{Z}^n}$ for all $g, h \in P$. The group P is called the *point group* of $R(P, v)$, the matrix g is called the *linear part* of $\{g \mid v(g) + t\}$. We will always identify the translation group of a crystallographic space group with the corresponding lattice of translation vectors in the Euclidean space.

For a (metrical) lattice L with basis $(a_1, \ldots, a_n)$, the inner product on L is represented by the *metric tensor* F giving the inner products of the basis vectors, *i.e.* $F_{ij} = (a_i, a_j)$. If the point group is desired to consist of orthogonal matrices, the basis has to be chosen such that the metric tensor is the identity matrix. The base change from the lattice basis to an orthonormal basis then provides the link between integral matrices and orthogonal matrices for the point group.

For a set $\mathcal{F} \subseteq \mathbb{R}_{\text{sym}}^{n \times n}$ of metric tensors, the group

$$\mathcal{B}(\mathcal{F}) := \{g \in GL(n, \mathbb{Z}) \mid g^T F g = F \text{ for all } F \in \mathcal{F}\}$$

is called the *Bravais group of* $\mathcal{F}$. *Vice versa*, for an integral matrix group $G \leq GL(n, \mathbb{Z})$, the set

$$\mathcal{F}(G) := \{F \in \mathbb{R}_{\text{sym}}^{n \times n} \mid g^T F g = F \text{ for all } g \in G\}$$

is seen to be an $\mathbb{R}$-vector space and is called the *space of invariant tensors* of G. The positive definite tensors in $\mathcal{F}(G)$ represent the different metrics of lattices which are invariant under the action of G.

Finally, we combine the last two constructions and define for an integral matrix group G the *Bravais group of* G as

$$\mathcal{B}(G) := \mathcal{B}(\mathcal{F}(G)).$$

This is the group of common isometries of all the metric tensors left invariant by G. A group $G \leq GL(n, \mathbb{Z})$ is simply called a *Bravais group* if $G = \mathcal{B}(G)$.

2.2. The hierarchy of classification

We briefly recall the definitions for the various classification levels for crystallographic groups as given by Brown *et al.* (1978), Neubüser *et al.* (1981) and Janssen *et al.* (2002).

2.2.1. Space-group type. Crystallographic space groups are said to have the same *space-group type* if they are conjugate subgroups of the affine group. The Bieberbach theorems (Bieberbach, 1911) show that this is equivalent with the groups being isomorphic.

By a result of Zassenhaus (1948), two space groups $R(P, v)$ and $R(P, v')$ with the same point group P belong to the same space-group type if and only if the vector systems v and v' represent elements of the first cohomology group $H^1(P, \mathbb{R}^n/\mathbb{Z}^n)$, which lie in the same orbit under the action of the normalizer $N_{GL(n,\mathbb{Z})}(P)$ of P in $GL(n, \mathbb{Z})$.

2.2.2. Arithmetic crystal class. Two finite integral matrix groups belong to the same *arithmetic crystal class* if they are conjugate subgroups of $GL(n, \mathbb{Z})$, *i.e.* the class of $G \leq GL(n, \mathbb{Z})$ is the orbit of G under $GL(n, \mathbb{Z})$. In terms of space group, this means that two groups in the same class represent the action of the point group of a space group with

respect to different lattice bases of the lattice of translation vectors.

2.2.3. Geometric crystal class. Two finite rational matrix groups are said to lie in the same *geometric crystal class* if they are conjugate subgroups of $GL(n, \mathbb{Q})$, *i.e.* the class of $G \leq GL(n, \mathbb{Q})$ is the orbit of G under $GL(n, \mathbb{Q})$. In terms of space groups, this means that two groups in the same geometric crystal class represent the action of the point group of a space group with respect to different bases of the rational vector space spanned by the lattice of translation vectors. This classification level reflects the anisotropy of the macroscopic crystal structure in Euclidean space and is traditionally just called *crystal class*.

For the sake of brevity, we will omit the word *crystal* from the terms *arithmetic/geometric crystal class* throughout this paper.

2.2.4. Holohedry. For a lattice L with metric tensor F, the group of orthogonal transformations leaving L invariant is called the *holohedry of* L. Since with respect to a lattice basis of L all elements of the holohedry are represented by integral matrices, the holohedry of L can be identified with the Bravais group $\mathcal{B}(F)$, which is also called the *arithmetic holohedry* of L. The geometric class of a group G is called a *holohedry* if G is the holohedry of one of its invariant lattices.

2.2.5. Bravais flock. For a Bravais group B, the set of all integral matrix groups G with $\mathcal{B}(G)$ lying in the arithmetic class of B is called the *Bravais flock* of B. Crystallographic point groups in the same Bravais flock are said to be *Bravais equivalent*, their invariant lattices lie in the same *Bravais class*. Note that traditionally Bravais flocks are used to classify space groups (*cf.* Hahn, 2002), but the notion used here is equivalent, since all space groups with the same point group lie in one Bravais flock.

2.2.6. Bravais system. The union of Bravais flocks that have $GL(n, \mathbb{Q})$-conjugate Bravais groups is called a *Bravais system*. Clearly, the geometric class containing these Bravais groups is a holohedry and it is by definition the only holohedry in this Bravais system. Thus, there is a one-to-one correspondence between Bravais systems and holohedries. From the perspective of lattices, this definition means that two lattices belong to the same *lattice system* if their holohedries lie in the same Bravais system.

It is proved in §4 of Neubüser *et al.* (1981) that this definition of Bravais systems is equivalent with the alternative definition: A Bravais system is the union of all Bravais flocks intersecting the same set of geometric classes. Here, a Bravais flock is said to intersect a geometric class if there exists a matrix group that belongs both to the Bravais flock and to the geometric class. One therefore lists all the geometric classes for which representatives are found in a Bravais flock and joins those Bravais flocks into a Bravais system for which these lists coincide.

2.2.7. Crystal system. In analogy with the alternative definition of Bravais systems, the unions of all geometric classes intersecting the same set of Bravais flocks is defined to be a *crystal system* or *point-group system*. Amending the somewhat misleading Definition 14 of Janssen *et al.* (2002), this means

Bernd Souvignier · Enantiomorphism in higher dimensions   **211**

that two geometric classes belong to the same crystal system if for any representative of the first class there is a representative of the other class such that the representatives have $GL(n, \mathbb{Q})$-conjugate Bravais groups. Neubüser *et al.* (1981) show that a crystal system contains at most one holohedry and they give a (counter-)example in dimension 7 that illustrates that it does not necessarily contain one. Therefore, the number of crystal systems is greater than or equal to the number of Bravais systems.

The smallest examples for crystal systems not containing a holohedry are found in dimension 5 and in §4.3 one of them is discussed in detail. The definition for crystal systems as given by Brown *et al.* (1978) therefore is only valid in dimensions up to 4, where it coincides with the more general definition adopted here.

2.2.8. Crystal family. A *crystal family* is defined to be the smallest set of matrix groups that consists of full geometric classes and of full Bravais flocks. Since a Bravais system is the union of Bravais flocks intersecting the same set of geometric classes and a crystal system is the union of geometric classes intersecting the same set of Bravais flocks, the equivalence relation given by the classification into crystal families is the finest equivalence relation coarser than both the classification into crystal systems and into Bravais systems.

The dependencies between the different levels of classification are shown in Fig. 1. If two levels are connected by an edge, classes of the higher level consist of full classes of the lower level. The notion of a *harmonic crystal class* is explained below.

2.3. Harmonic crystal class

Even without considering the significance of the classification levels, reasons of symmetry in the classification scheme suggest the introduction of a new classification level, namely the intersection of geometric crystal classes with Bravais flocks and we call this a *harmonic crystal class*. In analogy with the crystal families being the finest equivalence classes coarser than both the crystal systems and the Bravais systems, this is the coarsest equivalence relation refining both the geometric

Figure 1
Hierarchy of classification.

crystal classes and the Bravais flocks. The name of this classification level is chosen to indicate that groups which are equivalent on this level are in a harmonic relation: if G is a representative with invariant lattice L, then all other groups in the harmonic crystal class of G are obtained as the action of G on sublattices of L that are isometric with L.

Besides completing the classification scheme with respect to unions and intersections, the significance of this new classification level is twofold: Arithmetic classes in a harmonic crystal class correspond to actions on isometric sublattices and thus indicate self-similar structures in a lattice which are not obtained by integral scalings. Such a type of self-similarity is an important feature in the description of the symmetry of an object. Secondly, the classification into harmonic crystal classes is almost as fine as that into arithmetic classes, but is computationally easier.

We will now describe properties of this new type of classification for crystallographic groups in more detail.

A harmonic crystal class is the intersection of a geometric class and a Bravais flock. Since two point groups G and H in one harmonic crystal class have Bravais groups that are conjugate subgroups of $GL(n, \mathbb{Z})$, we can assume that $\mathcal{B}(G) = \mathcal{B}(H)$ and therefore the spaces of invariant metric tensors $\mathcal{F}(G)$ and $\mathcal{F}(H)$ coincide. On the other hand, the groups lie in the same geometric class, hence there exists $y \in GL(n, \mathbb{Q})$ with $H = y^{-1}Gy$. Since in general we have $\mathcal{F}(y^{-1}Gy) = y^T\mathcal{F}(G)y$, we can therefore conclude that $y^T\mathcal{F}(G)y = \mathcal{F}(H) = \mathcal{F}(G)$, *i.e.* y acts on the space of invariant tensors.

There are different ways in which two groups in the same harmonic crystal class can be related algebraically. They are distinguished by the way in which the matrix y conjugating G to H transforms the Bravais group $\mathcal{B}(G)$.

(1) In the simplest case, $y^{-1}\mathcal{B}(G)y = \mathcal{B}(G)$, which means that $y \in N_{GL(n, \mathbb{Q})}(\mathcal{B}(G))$. In other words, the subgroups G and H of $\mathcal{B}(G)$ are interchanged by an automorphism of $\mathcal{B}(G)$, which can be realized as a rational matrix.

(2) A slightly more complicated situation occurs when $y^{-1}\mathcal{B}(G)y \neq \mathcal{B}(G)$ but the group $\langle y^{-1}\mathcal{B}(G)y, \mathcal{B}(G)\rangle$ generated by $y^{-1}\mathcal{B}(G)y$ and $\mathcal{B}(G)$ is still a finite group. By a suitable basis transformation, this group can be made an integral matrix group and therefore y is seen to lie in the rational normalizer of a conjugate of a larger Bravais group in the same crystal family.

(3) Finally, the group $\langle y^{-1}\mathcal{B}(G)y, \mathcal{B}(G)\rangle$ may happen to be an infinite group. This is for example the case if G and H are subgroups of a finite group B such that an automorphism α of B maps G to H, but α is not induced by a rational matrix. These three cases are illustrated in the following examples.

Examples:

(1) In dimension 2, there is only one harmonic crystal class that consists of more than one arithmetic class. The hexagonal crystal family contains two arithmetic classes of groups isomorphic to the dihedral group D_3 of order 6. The groups representing these classes are the symmetry groups of an equilateral triangle and are generated by a rotation by $2\pi/3$
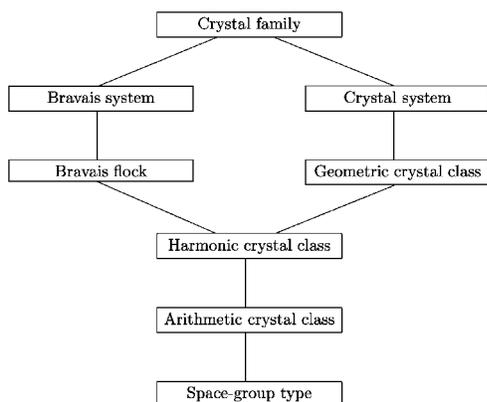
and a reflection. They are distinguished by the orientation of the invariant triangle with respect to the underlying hexagonal lattice as displayed in Fig. 2.

The first group, corresponding to the action on the solid triangle in Fig. 2, represents the arithmetic class with modified Hermann–Mauguin symbol $3m1p$ [following the notation recommended by de Wolff *et al.* (1985)] and is given by

$$G := \left\langle \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}, \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \right\rangle,$$

the second group, corresponding to the action on the dashed triangle in Fig. 2, represents the arithmetic class $31mp$ and is given by

$$H := \left\langle \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right\rangle.$$

The space of invariant tensors of both groups consists of the scalar multiples of

$$F := \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}$$

and their Bravais group is isomorphic to the dihedral group D_6 of order 12 and belongs to the arithmetic class $6mmp$.

A matrix conjugating the first group to the second is

$$y := \begin{pmatrix} 1 & -2 \\ -1 & -1 \end{pmatrix},$$

thus G and H belong to the same harmonic crystal class. We have $y \in N_{GL(2,\mathbb{Q})}(\mathcal{B}(G))$ and y induces the automorphism of D_6 which interchanges its two subgroups isomorphic to D_3.

In dimension 3, there are seven pairs of arithmetic classes that fall into one harmonic crystal class. Using again the modified Hermann–Mauguin symbol for arithmetic classes, these are: $mm2C$–$mm2A$, $\bar{4}2mP$–$\bar{4}m2P$, $\bar{4}m2I$–$\bar{4}2mI$, $312P$–$321P$, $3m1P$–$31mP$, $\bar{3}1mP$–$\bar{3}m1P$ and $\bar{6}m2P$–$\bar{6}2mP$. In all cases, the groups of each pair are conjugate by an element in the rational normalizer of the corresponding Bravais groups.

(2) Let L_1 be the four-dimensional lattice $\mathbb{Z}^4$ with metric tensor the four-dimensional identity matrix, *i.e.* a four-dimensional hypercubic lattice with Bravais type XXIII/I in

Figure 2
Different orientations of triangles in the hexagonal lattice.

the notation of Brown *et al.* (1978). The lattice L_2 generated by the columns of the matrix

$$y := \tfrac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}$$

is also a hypercubic lattice and is isometric with L_1. The group G_1 of orthogonal transformations of L_1 is the group of all matrices that have in each row and column precisely one entry unequal to 0 (which therefore has to be 1 or -1) and is called the *full monomial group* in $GL(4, \mathbb{Z})$. This group is isomorphic to the semidirect product $C_2^4 \rtimes S_4$ of order 384 and represents the arithmetic class 32/21/01 of Brown *et al.* (1978). If we transform G_1 to the lattice L_2, we obtain a non-integral matrix group $G_2 := y^{-1}G_1 y$, thus we see that $y \notin N_{GL(4,\mathbb{Q})}(G_1)$. The intersection H of G_1 and G_2 is an integral matrix group of order 192, representing the arithmetic class 32/19/01. We now observe that, up to conjugacy in G_1, H has four subgroups of order 32 having the same space of invariant tensors as G_1, which we denote by U_1, U_2, U_3 and U_4 and which represent the arithmetic classes 32/09/01, 32/09/01, 32/09/02 and 32/10/01, respectively. Conjugation with y interchanges U_1 and U_3 and fixes U_2 and U_4, therefore the groups U_1 and U_3 (and thus their arithmetic classes) lie in the same harmonic crystal class.

Finally, one sees that both G_1 and G_2 act on the hypercubic lattice

$$L := L_1 + L_2 = \langle a_1, a_2, a_3, \tfrac{1}{2}(a_1 + a_2 + a_3 + a_4) \rangle,$$

which has Bravais type XXIII/II and is isometric with the root lattice F_4 (up to a scaling by $2^{1/2}$). The group $B := \langle G_1, y^{-1}G_1 y \rangle$ turns out to be the full automorphism group of order 1152 of this lattice L and represents the arithmetic class 33/16/01. It is therefore conjugate to a Bravais group in the same crystal family but not in the same crystal system as G_1. The fact that $y^2 = 1$ shows that y is contained in the rational normalizer $N_{GL(4,\mathbb{Q})}(B)$ of B.

(3) Let L be the icosahedral lattice with metric tensor

$$F := \begin{pmatrix} 4 & -1 & -1 & -1 \\ -1 & 4 & -1 & -1 \\ -1 & -1 & 4 & -1 \\ -1 & -1 & -1 & 4 \end{pmatrix},$$

which has Bravais type XXII/I. The Bravais group $B := \mathcal{B}(F)$ represents the arithmetic class 31/07/01 and is isomorphic to the group $S_5 \times C_2$ of order 240. Up to conjugacy in B, B has two subgroups G_1, G_2 of order 20, which lie in the Bravais flock of B. These groups are isomorphic to the semidirect product $C_5 \rtimes C_4$ and represent the arithmetic classes 31/01/01 and 31/01/02, respectively. The groups G_1 and G_2 are given by
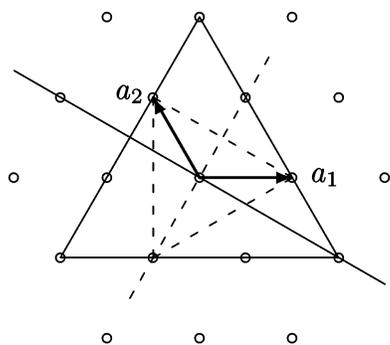
$$G_1 = \left\langle \begin{pmatrix} -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \\ -1 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & -1 & 0 & 0 \end{pmatrix} \right\rangle$$

$$G_2 = \left\langle \begin{pmatrix} -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \\ -1 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix} \right\rangle.$$

The inner automorphisms of B form a subgroup of index 2 in the full group of automorphisms of B and an outer automorphism interchanges G_1 and G_2 (mapping the two generating sets given onto each other). It can be checked that this outer automorphism is not induced by conjugation with an element from $GL(4, \mathbb{Q})$, hence the groups are not conjugate under the rational normalizer $N_{GL(4,\mathbb{Q})}(B)$ of B.

On the other hand, G_2 is $\mathbb{Z}$-equivalent to the action of G_1 on the unique G_1-invariant sublattice of L of index 5^2, which has transformation matrix

$$y := \begin{pmatrix} 1 & 0 & -2 & 2 \\ 2 & -1 & -2 & 0 \\ 0 & -2 & -1 & 2 \\ 2 & -2 & 0 & 1 \end{pmatrix},$$

therefore y conjugates G_1 to a group in the arithmetic class of G_2. Thus, G_1 and G_2 lie in the same geometric class and hence also in the same harmonic crystal class.

In this example, we can already conclude that $\langle B, y^{-1}By \rangle$ is an infinite group, since there exists no larger Bravais group in this crystal family and thus case (2) cannot occur. But the fact that G_1 and G_2 are not conjugate by an element from the normalizer of a larger group can also be concluded by looking at the B-invariant sublattices of L: Since $y^{-1}L$ is invariant under $y^{-1}By$ and y has determinant 5^2, it is sufficient to look at sublattices of L with index a power of 5. The lattices invariant under B are of the form $5^m L$ or $5^m L'$ for some $m \in \mathbb{Z}$, where $L' \subseteq L$ is a B-invariant sublattice of index 5 in L. Thus, the B-invariant sublattices of L are of index 5^{4m} or 5^{4m+1} in L. Analogously, the lattices invariant under $y^{-1}By$ are of the form $y^{-1} \cdot 5^m L$ or $y^{-1} \cdot 5^m L'$. This shows that the sublattices of L invariant under $y^{-1}By$ have index 5^{4m+2} or 5^{4m+3} in L. Thus, there is no lattice on which both B and $y^{-1}By$ act and hence the group $\langle B, y^{-1}By \rangle$ generated by B and $y^{-1}By$ has to be an infinite group. In particular, the two groups cannot be conjugate by an element of the normalizer of any finite group they are contained in.

2.4. Fixed-point-free space groups

A crystallographic space group is called *fixed-point-free* if all group elements except the identity element leave no point of the underlying Euclidean space fixed. These are precisely the torsion-free space groups, since every element of finite order has fixed points: An element g of order n fixes the point

$$w := g \cdot v + g^2 \cdot v + \ldots + g^n \cdot v,$$

where v is an arbitrary point of the Euclidean space.

The fixed-point-free space groups are also called *Bieberbach groups* and play an important role in the classification of flat Riemannian manifolds (see Charlap, 1986). Of particular interest are Bieberbach groups with trivial center which correspond to manifolds with first Betti number 0.

The n-dimensional fixed-point-free space groups for $n = 1, 2, 3, 4$ are given in Brown *et al.* (1978) while Cid & Schulz (2001) list their numbers for dimensions 5 and 6 and describe a generic algorithm for arbitrary dimensions.

3. Enantiomorphism

The notion of enantiomorphism reveals a subtle difference in how crystallographic objects may be classified. Owing to the Bieberbach theorems, which state that abstract isomorphism of space groups is the same as equivalence under affine transformations, it is natural to regard objects as equivalent if they can be transformed into each other by an affine transformation. On the other hand, crystallography deals with objects in physical space and in some experimental situations the handedness plays a role. In this case, the orientation has to be respected by a symmetry operation (excluding for example reflections in three-dimensional space), which leads to the following refined classification scheme allowing only orientation-preserving affine transformations:

Two objects that are equivalent by an affine transformation but not by an orientation-preserving transformation are called an enantiomorphic pair, each member of an enantiomorphic pair is said to be enantiomorphic.

This general definition covers enantiomorphism of crystal structures with equivalence defined by the space-group types as well as enantiomorphism of point groups where equivalence is given by conjugacy.

A word of warning may be relevant at this point: While in three-dimensional space the relevance of enantiomorphism to describe handedness is clear, this is no longer true for higher-dimensional descriptions of objects like quasicrystals or incommensurately modulated crystals. The question is how transformations between objects in higher-dimensional space are related to the projections of these objects into three-dimensional space. For example, a fivefold screw in three-dimensional space is clearly enantiomorphic, but its five-dimensional description by integral matrices is found not to be enantiomorphic in the sense of the above definition. However, if enantiomorphism is found in higher dimensions, this indicates handedness for the projected objects as well. Thus, the mathematical notion adopted here may serve as a starting point for a better understanding of the handedness of objects with higher-dimensional descriptions.

Enantiomorphism can be defined on all levels of classification for crystallographic groups. In order to distinguish the equivalence classes under orientation-preserving transformations from those under arbitrary affine transformations, we will call the former *proper* classes.

For the space-group types, the arithmetic classes and the geometric classes, a common approach can be chosen to determine the enantiomorphic pairs.

3.1. Enantiomorphism of space-group types, arithmetic and geometric crystal classes

We assume that an equivalence class is given as the orbit of a member H of the class under a group $\mathcal{G}$ of transformations (as is the case for the space-group types, arithmetic classes and geometric classes). We denote the orbit of an element H under a group $\mathcal{G}$ by $H^{\mathcal{G}}$. If $\mathcal{G}$ contains a transformation r that does not preserve orientation, we can split $\mathcal{G}$ into the disjoint union of the two cosets with respect to the subgroup $\mathcal{G}^+$ of orientation-preserving transformations:

$$\mathcal{G} = \mathcal{G}^+ \,\dot{\cup}\, r \cdot \mathcal{G}^+.$$

The group H and its orientation-reversed transform $H' := r^{-1}Hr$ form an enantiomorphic pair if and only if H' is not contained in the orbit $H^{\mathcal{G}^+}$ of H under $\mathcal{G}^+$. We arrive at the following criterion:

A group H is enantiomorphic if and only if the stabilizer $\mathrm{Stab}_{\mathcal{G}}(H)$ of H in $\mathcal{G}$ is contained in $\mathcal{G}^+$.

This criterion is deduced as follows: assume that H and its transform H' do not form an enantiomorphic pair, then $H' \in H^{\mathcal{G}^+}$ and thus there exists $g_0 \in \mathcal{G}^+$ such that $g_0^{-1}Hg_0 = H' = r^{-1}Hr$. This shows that $r \cdot g_0^{-1} \in \mathrm{Stab}_{\mathcal{G}}(H)$ and since $r \cdot g_0^{-1} \notin \mathcal{G}^+$, we have $\mathrm{Stab}_{\mathcal{G}}(H) \not\subseteq \mathcal{G}^+$. On the other hand, if $\mathrm{Stab}_{\mathcal{G}}(H) \not\subseteq \mathcal{G}^+$, there exists $g_1 \in \mathrm{Stab}_{\mathcal{G}}(H)$ with $g_1 \notin \mathcal{G}^+$. We then have $g_1 \cdot r \in \mathcal{G}^+$ and $(g_1 \cdot r)^{-1}H(g_1 \cdot r) = r^{-1}(g_1^{-1}Hg_1)r = r^{-1}Hr = H'$, thus $H' \in H^{\mathcal{G}^+}$.

Since $\mathcal{G}^+$ is a subgroup of index 2 in $\mathcal{G}$, conjugation by elements of $\mathcal{G}$ fixes $\mathcal{G}^+$ and therefore conjugates of subgroups of $\mathcal{G}^+$ lie in $\mathcal{G}^+$. By our assumption, every group H_1 in the equivalence class of H is of the form $H_1 = g^{-1}Hg$ for some $g \in \mathcal{G}$, hence the stabilizer $\mathrm{Stab}_{\mathcal{G}}(H_1)$ of H_1 in $\mathcal{G}$ is $\mathrm{Stab}_{\mathcal{G}}(H_1) = g^{-1}\mathrm{Stab}_{\mathcal{G}}(H)g$. We therefore conclude that either none or all the groups in the class of H are enantiomorphic and in the latter case we call the equivalence class itself enantiomorphic.

3.1.1. Space-group types. The equivalence class of a crystallographic space group R is the orbit of R under the affine group $\mathcal{A}(n, \mathbb{R})$ and the orientation-preserving affine transformations are those for which the linear part has determinant > 0. For a space group $R = R(P, v)$ with point group $P \leq GL(n, \mathbb{Z})$, the point group of its stabilizer in $\mathcal{A}(n, \mathbb{R})$ lies in the normalizer $N := N_{GL(n, \mathbb{Z})}(P)$ of P in $GL(n, \mathbb{Z})$. Clearly, R is enantiomorphic if all elements of N have positive determinant, *i.e.* if $N \leq SL(n, \mathbb{Z}) := \{g \in GL(n, \mathbb{Z}) \mid \det(g) = 1\}$. But not every element of N is necessarily the linear part of a stabilizer element, hence the class of R may also be enantiomorphic in case $N \not\leq SL(n, \mathbb{Z})$. This is the case if the orbit under N of the vector system v of R splits into two orbits under $N^+ := N \cap SL(n, \mathbb{Z})$, since this implies that the point group of the stabilizer $\mathrm{Stab}_{\mathcal{A}(n, \mathbb{R})}(R)$ of R is contained in N^+.

3.1.2. Arithmetic crystal classes. The arithmetic class of an integral matrix group G is the orbit of G under $GL(n, \mathbb{Z})$, the orientation-preserving part of $GL(n, \mathbb{Z})$ is $SL(n, \mathbb{Z})$ and the stabilizer of G under the action of $GL(n, \mathbb{Z})$ is the normalizer $N_{GL(n, \mathbb{Z})}(G)$ of G in $GL(n, \mathbb{Z})$. Hence, the arithmetic class of G is enantiomorphic if and only if the normalizer $N_{GL(n, \mathbb{Z})}(G)$ is contained in $SL(n, \mathbb{Z})$.

Note that enantiomorphism of arithmetic classes can only occur in even dimensions, since $-I_n$, the negative of the identity matrix, is contained in the normalizer of every matrix group and has determinant -1 in odd dimensions. As a consequence, enantiomorphism on classification levels coarser than that of arithmetic classes can also only occur in even dimensions.

3.1.3. Geometric crystal classes. In analogy with the case of arithmetic classes, the geometric class of an integral matrix group G is enantiomorphic if and only if the normalizer $N_{GL(n, \mathbb{Q})}(G)$ of G in $GL(n, \mathbb{Q})$ is contained in $GL^+(n, \mathbb{Q}) := \{g \in GL(n, \mathbb{Q}) \mid \det(g) > 0\}$.

3.2. Enantiomorphism on other levels

Following Brown *et al.* (1978), we call a Bravais flock and a Bravais system enantiomorphic if all the arithmetic classes contained in them are enantiomorphic. Note that a Bravais flock is enantiomorphic if and only if the Bravais group contained in it is enantiomorphic, since the integral normalizer $N_{GL(n, \mathbb{Z})}(G)$ of a group G is contained in the normalizer $N_{GL(n, \mathbb{Z})}(\mathcal{B}(G))$ of its Bravais group. Thus, enantiomorphism of a Bravais group implies enantiomorphism of all arithmetic classes contained in its Bravais flock. Consequently, a Bravais system is enantiomorphic if and only if all Bravais groups contained in it are enantiomorphic.

Analogously, we define a harmonic crystal class to be enantiomorphic if all the arithmetic classes contained in it are enantiomorphic.

We would like to note that for the definition of enantiomorphism for crystal systems and crystal families one has to make a choice. One could either define them as enantiomorphic if all the arithmetic classes contained in them are enantiomorphic, or if all the geometric classes contained in them are enantiomorphic. Brown *et al.* (1978) remark (p. 15) that in dimension 4 it turns out that all the geometric classes in which all arithmetic classes are enantiomorphic are enantiomorphic themselves but that it is not known whether this is true in general. We will give a six-dimensional counterexample in §3.4, where a geometric class that is not enantiomorphic splits into three arithmetic classes that are enantiomorphic.

In view of the hierarchy of classification levels, it seems reasonable that enantiomorphism on a higher level should imply enantiomorphism on a finer level. We therefore suggest that crystal systems and crystal families be defined as enantiomorphic if all the geometric classes contained in them are enantiomorphic. Although this choice does not agree with the choice made in Brown *et al.* (1978), it does not lead to contradicting classification results in dimensions ≤ 6, since it turns out (*cf.* Tables 1 and 2) that the only dimension in which enantiomorphic crystal systems or families occur is dimension 4, and there the two definitions coincide (as noted before).

3.3. Algorithm to determine enantiomorphic pairs

In this section, we give an outline of an algorithm by which enantiomorphic pairs of crystallographic space groups, integral and rational matrix groups are determined. Enantiomorphism on the other classification levels is derived from these.

The algorithm uses the following simple observations:

(i) All arithmetic classes in an enantiomorphic geometric class are enantiomorphic, since $N_{GL(n,\mathbb{Z})}(G) = N_{GL(n,\mathbb{Q})}(G) \cap GL(n,\mathbb{Z})$.

(ii) An arithmetic class is enantiomorphic if and only if the corresponding symmorphic space-group type is enantiomorphic because, for a symmorphic crystallographic space group $R_0 = R(P, v_0)$, the point group of the stabilizer $\mathrm{Stab}_{\mathcal{A}(n,\mathbb{R})}(R_0)$ coincides with the integral normalizer $N_{GL(n,\mathbb{Z})}(P)$ of its point group P. In this case, any crystallographic space group R (*i.e.* not only the symmorphic ones) with point group in the arithmetic class of P is enantiomorphic, since the point group of the stabilizer $\mathrm{Stab}_{\mathcal{A}(n,\mathbb{R})}(R)$ is contained in the normalizer $N_{GL(n,\mathbb{Z})}(P)$, which in turn is contained in $SL(n,\mathbb{Z})$.

(iii) If an integral matrix group G contains an element g of determinant -1, the geometric class of G, the arithmetic class of G and all space-group types with point groups in the geometric class of G are not enantiomorphic, since g is contained in the rational and integral normalizers of G and since a space-group element with linear part g is a non-orientation-preserving element in the stabilizer of the space group.

The algorithm proceeds in four steps:

(1) For representatives G of each geometric class, check whether $G \leq SL(n, \mathbb{Q})$. If so, compute representatives $G_1, \ldots, G_m$ for the arithmetic classes in the geometric class of G. Otherwise, G contains an element of determinant -1 and therefore this geometric class, all arithmetic classes therein and all space-group types with point group therein are not enantiomorphic.

(2) For representatives $G \leq SL(n, \mathbb{Z})$ of the arithmetic classes obtained in step (1) compute the normalizer $N := N_{GL(n,\mathbb{Z})}(G)$. If $N \leq SL(n, \mathbb{Z})$, then the arithmetic class of G and all space-group types with point groups in this class are enantiomorphic. Otherwise, the symmorphic space group with this point group is not enantiomorphic but non-symmorphic space groups may be. In that case, compute the vector systems $V(G, \mathbb{Q}^n/\mathbb{Z}^n)$ for G and the orientation-preserving part $N^+ := N \cap SL(n, \mathbb{Z})$ of the normalizer.

(3) For a group G with normalizer N and vector systems $V(G, \mathbb{Q}^n/\mathbb{Z}^n)$ obtained in step (2), compute the orbits of N and N^+ on $V(G, \mathbb{Q}^n/\mathbb{Z}^n)$, respectively. If an orbit o under the action of N splits into two orbits o^+ and o^- under the action of N^+, then the space groups $R(G, v^+)$ and $R(G, v^-)$ with vector systems v^+ and v^- lying in o^+ and o^-, respectively, form an enantiomorphic pair. Otherwise, if an orbit o is the same under N and N^+, the space groups with vector system in o are not enantiomorphic.

(4) For geometric classes in which all arithmetic classes are enantiomorphic, compute the rational normalizer $N_{GL(n,\mathbb{Q})}(G)$ for a representative G. If $N_{GL(n,\mathbb{Q})}(G) \leq GL^+(n, \mathbb{Q})$ then the geometric class is enantiomorphic, otherwise it is not.

The rational normalizer $N_{GL(n,\mathbb{Q})}(G)$ of a group $G \leq GL(n, \mathbb{Z})$ is computed in two stages: First the rational centralizer

$$C_{GL(n,\mathbb{Q})}(G) := \{c \in GL(n, \mathbb{Q}) \mid cg = gc \text{ for all } g \in G\}$$

of G in $GL(n, \mathbb{Q})$ is determined and is checked for being contained in $GL^+(n, \mathbb{Q})$. In the second stage, additional normalizer elements are computed that form a set of coset representatives of $\langle C_{GL(n,\mathbb{Q})}(G), N_{GL(n,\mathbb{Z})}(G) \rangle$ in $N_{GL(n,\mathbb{Q})}(G)$. One possibility to find such a set of elements is to inspect the action of G on the G-invariant sublattices of $\mathbb{Z}^n$. Suppose that y_1 and y_2 are basis transformations such that $L_1 = y_1 \cdot \mathbb{Z}^n$ and $L_2 = y_2 \cdot \mathbb{Z}^n$ are G-invariant sublattices of $\mathbb{Z}^n$ and such that the actions of G on L_1 and L_2 are $\mathbb{Z}$-equivalent. Then there exists $x \in GL(n, \mathbb{Z})$ with $x^{-1}(y_1^{-1}Gy_1)x = y_2^{-1}Gy_2$ and therefore $y_1 x y_2^{-1} \in N_{GL(n,\mathbb{Q})}(G)$. A second possibility to find $N_{GL(n,\mathbb{Q})}(G)$ is to compute the abstract automorphism group $\mathrm{Aut}(G)$ of G and to check which of the (finitely many) automorphisms are induced by conjugation with a rational matrix. The so-obtained elements of $N_{GL(n,\mathbb{Q})}(G)$ form a set of coset representatives of $C_{GL(n,\mathbb{Q})}(G)$ in $N_{GL(n,\mathbb{Q})}(G)$.

3.4. Enantiomorphism for geometric crystal classes

It is pointed out by Brown *et al.* (1978) that in dimension 4 all geometric classes which fulfil the necessary condition that all arithmetic classes contained in them are enantiomorphic turn out to be enantiomorphic themselves. In dimension 6, the situation is precisely the opposite, namely none of the three geometric classes that contain only enantiomorphic arithmetic classes is enantiomorphic. The members of the three geometric classes in question all have the property that their rational representation is absolutely irreducible, hence the rational centralizer consists only of scalar matrices. One of the groups is isomorphic to $C_2 \times S_5$ acting on a six-dimensional hypercubic lattice, one is isomorphic to $\mathrm{PSL}(2, 7)$ and the third is isomorphic to $C_2 \times \mathrm{PSL}(2, 7)$. To split the geometric class into arithmetic classes is easy in these cases, because up to scalings by a rational constant there are only finitely many G-invariant lattices. For the example $G \cong C_2 \times S_5$ with G given by

$$G := \left\langle \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \right\rangle,$$

the lattice of G-invariant sublattices (up to scalings) is displayed in Fig. 3.

The geometric class of G splits into three arithmetic classes, represented by the action of G on the lattices L_1, L_2 and L_3, the arithmetic classes represented by the actions of G on L_4,

Table 1
Summary of classification results in dimensions up to 4.

Classification level	Number of classes in dimension			
	1	2	3	4
Crystal families	1	4	6	23 (+6)
Bravais systems	1	4	7	33 (+7)
Crystal systems	1	4	7	33 (+7)
Bravais flocks	1	5	14	64 (+10)
Geometric crystal classes	2	10	32	227 (+44)
Harmonic crystal classes	2	12	66	551 (+63)
Arithmetic crystal classes	2	13	73	710 (+70)
Space-group types	2	17	219 (+11)	4783 (+111)
Fixed-point-free space groups	1	2	10 (+3)	74
with trivial center	0	0	1	4

L_5 and L_6 are found to be $\mathbb{Z}$-equivalent to those on L_1, L_2 and L_3, respectively. If we denote the basis transformation matrix from L_1 to L_4 by y and the action of G on L_1 by G_1, then the action of G on L_4 is given by $G_4 := yG_1y^{-1}$. Since G_1 and G_4 are found to be $\mathbb{Z}$-equivalent, there is a matrix $x \in GL(6, \mathbb{Z})$ such that $G_4 = x^{-1}G_1x$, hence $xy \in N_{GL(6,\mathbb{Q})}(G_1)$. One finds that $\det(xy) = -125$, thus the geometric class containing G is not enantiomorphic although the arithmetic classes represented by the action of G on L_1, L_2 and L_3, respectively, are enantiomorphic.

4. Results

4.1. Review of results in dimensions up to 4

Although the results for dimensions up to 4 are already summarized in Brown *et al.* (1978), we would like to redisplay them, augmented with the new classification level of harmonic crystal classes and to add a few remarks. The rows in Table 1 give the numbers of equivalence classes on the different classification levels, the numbers of enantiomorphic pairs are added in parentheses in the case where they are different from 0. The number of equivalence classes under orientation-preserving transformations is thus obtained as the sum of the two numbers given, *e.g.* there are $230 = 219 + 11$ proper
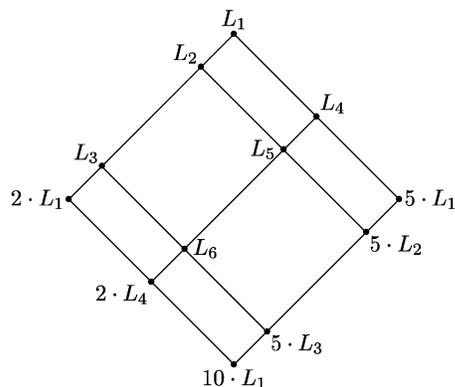

Figure 3
Lattice of *G*-invariant sublattices.

space-group types in dimension 3 and $271 = 227 + 44$ proper geometric crystal classes in dimension 4.

Remarks on dimension 4:

(i) The number of enantiomorphic space-group types given by Brown *et al.* (1978) has to be corrected from 112 to 111. There, the space-group type 08/01/01/002 in the hexagonal monoclinic crystal family VII is erroneously claimed to be enantiomorphic. Consequently, there is no enantiomorphic fixed-point-free space group in dimension 4. [The corrections that have to be made to the tables in Brown *et al.* (1978) are announced in Neubüser *et al.* (2002).]

(ii) All but six enantiomorphic space-group types have enantiomorphic point groups. Two of these six classes lie in the ditetragonal orthogonal crystal family XIV (space-group types 18/04/03/006 and 18/04/05/007) and four in the hyper-cubic family XXIII (space-group types 32/10/02/004, 32/10/02/007, 32/12/02/002 and 32/12/02/004).

(iii) All but one enantiomorphic arithmetic classes lie in enantiomorphic geometric classes. The only exception is the class 29/03/03 in the diisohexagonal crystal family XXI, where only one of the five arithmetic classes in the geometric class is enantiomorphic.

(iv) All geometric classes in which all arithmetic classes are enantiomorphic are enantiomorphic themselves.

(v) The enantiomorphism of the six crystal families VIII, IX, XII, XIII, XVIII and XX implies the enantiomorphism of six of the seven enantiomorphic crystal systems and Bravais systems, since these are already full crystal families. The remaining enantiomorphic crystal and Bravais systems are due to the enantiomorphic geometric class 21/04 in the dihexagonal orthogonal crystal family XVI, which splits into the two arithmetic classes 21/04/01 and 21/04/02. The first of these arithmetic classes consists of Bravais groups whereas the Bravais groups of groups in the second class lie in the arithmetic class 23/11/01, which is not enantiomorphic.

(vi) Of the 710 arithmetic classes, 416 form a harmonic crystal class on their own, 118 harmonic crystal classes consist of two arithmetic classes, 10 harmonic crystal classes consist of three arithmetic classes and 7 harmonic crystal classes consist of four arithmetic classes.

4.2. Results in dimensions 5 and 6

Table 2 gives the numbers of equivalence classes on the various classification levels for dimensions 5 and 6. Again, the numbers of enantiomorphic pairs are given in parentheses.

Remarks on dimension 5:

(i) The small number of enantiomorphic space-group types comes as a surprise.

(ii) The only class of enantiomorphic fixed-point-free space groups is represented by a space group $R(P, v)$ for which the point group P lies in the crystal family of the direct product of the cubic crystal family in dimension 3 and the rectangular crystal family in dimension 2. The point group P of order 24 is

Table 2
Summary of classification results in dimensions 5 and 6.

	Number of classes in dimension	
Classification level	5	6
Crystal families	32	91
Bravais systems	57	220
Crystal systems	59	251
Bravais flocks	189	841
Geometric crystal classes	955	7104
Harmonic crystal classes	3990	41915 (+26)
Arithmetic crystal classes	6079	85311 (+30)
Space-group types	222018 (+79)	28927922 (+7052)
Fixed-point-free space groups	1060 (+1)	38746 (+218)
with trivial center	101	5004 (+18)

isomorphic to S_4 and belongs to the geometric class of a subdirect product of $\bar{4}3m \perp m$ which, following the recommendations of Janssen *et al.* (1999), has symbol $\bar{4}3m(m1m)$. The group P is given as $P = \langle g, h \rangle$ with

$$g := \begin{pmatrix} 1 & -1 & 0 & 0 & 0 \\ 0 & -1 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad h := \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix},$$

the vector system v is given by the vectors $v(g) := (0, 0, 0, 0, 2/3)$ and $v(h) := (0, 0, 1/2, 0, 0)$.

(iii) As suspected in Neubüser *et al.* (1981), the distribution of Bravais systems and crystal systems in the crystal families becomes more complicated in higher dimensions. Only 13 of the 32 crystal families contain a unique holohedry and therefore consist of a single Bravais and a single-crystal system, 16 of the families contain two holohedries and two crystal systems and one family contains three holohedries and three crystal systems. The remaining two crystal families contain three holohedries and four crystal systems, and six holohedries and seven crystal systems, respectively. Therefore, these crystal families provide examples of crystal systems that do not contain a holohedry and one of these is described in detail in §4.3.

(iv) Only 2588 of the 6079 arithmetic classes form a harmonic crystal class on their own, the number of arithmetic classes in one harmonic crystal class goes up to 8.

Remarks on dimension 6:

(i) In contrast to the situation in dimension 4, there are very few symmorphic groups amongst the enantiomorphic space-group types. Only 110 of the 7052 enantiomorphic space-group types have enantiomorphic point groups.

(ii) Although there are 30 enantiomorphic arithmetic classes and 26 enantiomorphic harmonic crystal classes, there are no enantiomorphic classes on coarser classification levels. Of the 26 enantiomorphic harmonic crystal classes, 22 consist of a single arithmetic class and 4 consist of two arithmetic classes.

(iii) There are three geometric classes in which all the arithmetic classes are enantiomorphic. All three fail to be

enantiomorphic themselves. One of these cases has been discussed in more detail in §3.4.

(iv) The distribution of Bravais systems and crystal systems in the crystal families is even more complicated than in dimension 5. Only 29 of the 91 crystal families contain a unique holohedry, 28 crystal families contain two holohedries, 19 families contain three, 5 contain four, 5 contain five, 3 contain six, 1 family contains seven and 1 crystal family contains eight holohedries. There are 18 crystal families that contain crystal systems without holohedries. 13 of them contain one such crystal system, 1 of them contains two, 1 contains three, 2 contain four and 1 crystal family contains five different crystal systems without a holohedry. The number of Bravais systems in a single crystal family runs up to 8, the number of crystal systems even up to 11.

(v) Only 20850 of the 85311 arithmetic classes form a harmonic crystal class on their own, the number of arithmetic classes in one harmonic crystal class goes up to 30.

4.3. Crystal systems without holohedry

As mentioned earlier, the non-existence of crystal systems without holohedries in dimensions up to four led to a definition of crystal systems that is based on a holohedry contained in a crystal system. An example in seven-dimensional space (due to C. R. Leedham-Green) where this definition fails is discussed in Neubüser *et al.* (1981) and led to the adjusted definition of crystal systems adopted here. As a byproduct of the classification of crystallographic groups in five-dimensional space, two examples for this situation were found which are therefore the smallest ones. We will discuss one of these here in some detail.

Let G be the group generated by the four matrices

$$\begin{pmatrix} 1 & -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$
$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix},$$

then $G \cong D_6 \times C_2 \times C_2$ lies in the arithmetic class with symbol $6mm \perp 2 \perp mP_5$ [following the recommendations of Janssen *et al.* (2002)]. The crystal family of G contains three Bravais systems (consisting of two Bravais flocks each) but four crystal systems.

The arithmetic classes in the crystal family of G that are relevant to explain the existence of a crystal system not containing a holohedry are displayed in Fig. 4. Shown are the arithmetic classes of those groups for which either the

geometric class of the group or the geometric class of a subgroup intersects all six Bravais flocks in the crystal family.

The boxes in the figure represent the arithmetic classes, boxes that are directly joined together horizontally represent arithmetic classes in the same geometric class and the boxes with thick boundaries are the Bravais classes. The six Bravais flocks in the crystal family are thus represented by the Bravais groups G_{34}, G_{56}, H_1, H_2, H'_7 and H'_8. Two boxes are joined by an edge if the class of lower order contains a maximal subgroup of a group in the class of higher order. The indices for the names of the groups are chosen such that they reflect the inclusion relations. The Bravais flocks can be read off the diagram by following down the edges starting from a Bravais group. For example, the Bravais flock of G_{34} consists of the arithmetic classes of G_{34}, H_3, H_4, H'_3, H'_4, U_3, U_4, M_3, M_4, M'_3 and M'_4.

Since groups in one Bravais system intersect the same set of geometric classes, one sees that the Bravais flocks of G_{34} and G_{56}, those of H_1 and H_2 and those of H'_7 and H'_8 form the three Bravais systems. On the other hand, the geometric class of G_{34} intersects the Bravais flocks of G_{34} and G_{56}, the geometric class of H_1 intersects the Bravais flocks of G_{34}, G_{56}, H_1 and H_2 and the geometric class of H'_8 intersects the Bravais flocks of G_{34}, G_{56}, H'_7 and H'_8. This shows that the geometric classes of G_{34}, H_1 and H'_8 form three different crystal systems. Finally, the geometric classes of U_1, M_1 and M'_1 intersect all six Bravais flocks and therefore lie in a crystal system that is different from those containing the geometric classes of the Bravais groups. In particular, the crystal system containing the geometric classes of U_1, M_1 and M'_1 and indicated by the oval frame in Fig. 4 does not contain a holohedry.

4.4. Asymptotic behaviour in higher dimensions

It is stated by Schwarzenberger (1980, p. 34) that typically there are few very large arithmetic classes (in the sense of containing many space-group types) together with a rather large number of small arithmetic classes. In order to obtain an
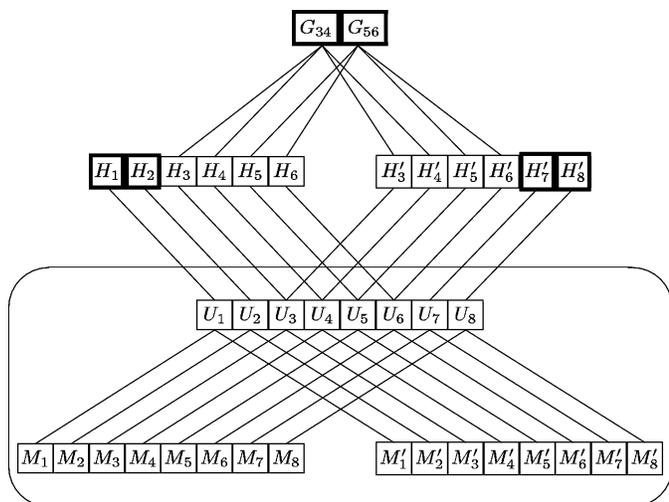

Figure 4
Crystal system without holohedry.

idea of the number of space-group types in higher dimensions, it may therefore be worthwhile to inspect arithmetic classes that are known to be large and whose size can be explicitly determined. One candidate already examined in Schwarzenberger (1980) is the group D of diagonal matrices of order 2^n. The normalizer $N := N_{GL(n,\mathbb{Z})}(D)$ of D in $GL(n, \mathbb{Z})$ is the full monomial group, *i.e.* the semidirect product $D \rtimes G$ of D with the group $G \cong S_n$ of permutation matrices. Since D acts trivially on the vector systems $V(D, \mathbb{Q}^n/\mathbb{Z}^n)$, the space-group types with point groups in the arithmetic class of D correspond to the orbits of G on the vector systems. This action can be described explicitly as the conjugation action of the permutation matrices on the set

$$\mathcal{X} := \{M \in (\mathbb{Z}/2\mathbb{Z})^{n \times n} \mid M_{ii} = 0 \text{ for } 1 \leq i \leq n\}$$

of matrices over $\mathbb{Z}/2\mathbb{Z}$ with zeros on the diagonal, since $\mathcal{X}$ represents the $2^{n(n-1)}$ elements of $H^1(D, \mathbb{Q}^n/\mathbb{Z}^n)$. The fixed-point lemma by Burnside–Cauchy (see Burnside, 1955, Section 145) states that the group order multiplied by the number of orbits of a group action equals the sum over the fixed points of each element, *i.e.*

$$\text{orb}(G) = \frac{1}{|G|} \sum_{g \in G} |\text{Fix}(g)|,$$

where $\text{orb}(G)$ denotes the number of orbits of G. The right-hand side of this formula is dominated by the term $2^{n(n-1)}/n!$ contributed by the identity element and a closer analysis for this special situation shows that

$$\lim_{n \to \infty} \text{orb}(G) \cdot \frac{n!}{2^{n(n-1)}} = 1.$$

Thus, $2^{n(n-1)}/n!$ is the asymptotic value for the number of space-group types in the arithmetic class of the group of diagonal matrices.

Some results that indicate that the arithmetic class of the group of diagonal matrices contains a substantial (and possibly growing) portion of all space-group types are displayed in Table 3. The first three rows of the table give the total number of space-group types and the numbers of space-group types in the two largest arithmetic classes. In dimensions 4 and 5, the group of diagonal matrices lies in the second largest class, in the other dimensions it lies in the largest class. The fourth row gives the estimate for the number of space-group types in the arithmetic class containing the group of diagonal matrices as derived above from the Burnside–Cauchy lemma. The fifth row gives the portion of space-group types that is found in the largest arithmetic class and the last row the ratio between the estimated class size and the actual size of the largest class.

One may expect that the estimate for the largest class becomes more and more accurate for higher dimensions. If one now assumes that the portion of space-group types in the largest arithmetic class is roughly the same for dimensions differing only by 1, moving from dimension n to dimension $n + 1$ gives an increase of space-group types by a factor of $[2^{(n+1)n}/(n + 1)!] \times [n!/2^{n(n-1)}] = 2^{2n}/(n + 1)$. Extrapolating from the figures for dimensions 5 and 6, one would therefore

Table 3
Asymptotic results.

Dimension	2	3	4	5	6
Space-group types	17	219	4783	222018	28927922
Largest arithmetic class	3	16	272	11456	1540944
Second largest arithmetic class	2	16	218	9608	1432608
$\lceil 2^{n(n-1)}/n! \rceil$	2	11	171	8739	1491309
In largest arithmetic class	17.6%	7.3%	5.7%	5.2%	5.3%
Estimated/actual size	0.67	0.69	0.61	0.76	0.97

expect about 1.7×10^{10} space-group types in dimension 7 and 3.5×10^{13} space-group types in dimension 8.

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