# CRYSTALLOGRAPHY AND COHOMOLOGY OF GROUPS

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**Introduction.** One imagines a crystal as an interlocking system of molecules (or balls connected by rods) that can be continued indefinitely in any direction filling up all of space (see Fig. 1). The essential feature that a mathematical treatment of crystals should abstract is the existence of a "small chunk" of the crystal pattern which acts as a building block for the whole structure. Of course, this building block must be of a very special nature so that the pieces will fit together.

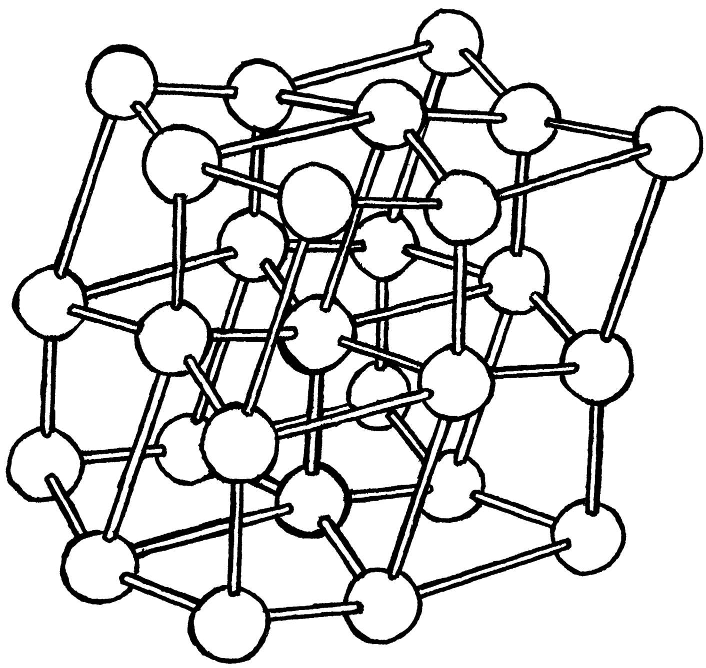

FIG. 1

The mathematical approach to this problem is to replace the crystal pattern by the group $G$ of rigid motions of Euclidean space $\mathbb{E}^n$ that preserve it. Such a group is called a **space group**. In this group $G$ there are $n$ linearly independent translations that correspond to the existence of the building block described above. These translations generate a subgroup $M$ of $G$ which is free abelian (i.e., is isomorphic to the sum of $n$ copies of the group $\mathbb{Z}$ of integers) and is called the **lattice** of $G$.

But there are also other symmetries the crystal system might possess (for example, rotations). If we consider the quotient group $G/M$, we obtain another algebraic invariant of the space group $G$ called the **point group** $H$.

Unfortunately these two invariants: the lattice $M$ and the point group $H$ are not enough to determine the space group $G$. We give an example in dimension 2, where a crystal pattern

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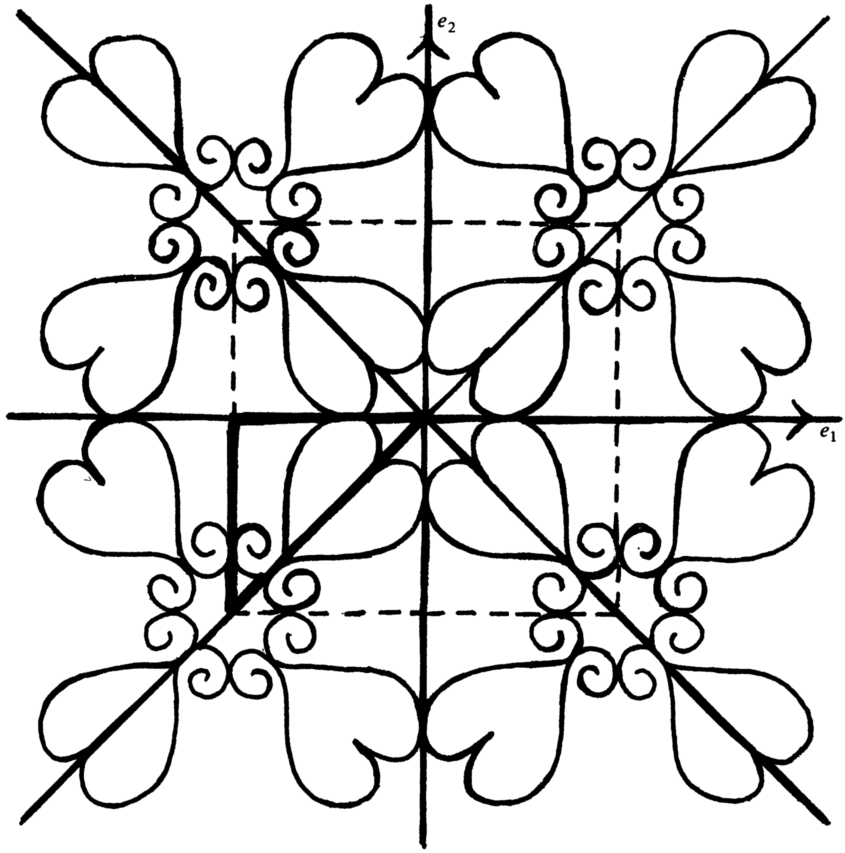


FIG. 2(a) G. The bold lines indicate reflections that are in the symmetry group. The boldly outlined triangle near the center is the fundamental domain for the symmetry group. The fundamental domain for the lattice generated by the translations in the directions $e_1$ and $e_2$ is the central dashed square. Rotation of 90° around the center is also in the symmetry group.

corresponds to a "tiling" of the plane. Consider the two tilings in Fig. 2.

Both symmetry groups $G, G'$ contain translations in the directions $\mathbf{e}_1$, $\mathbf{e}_2$, the standard basis vectors. It can also be shown that in both cases the point group $H$ is $D_4$, the symmetry group of a square, of order 8. (What are the 8 rigid motions that preserve a square ?) But these two tilings are not the same! The bold lines in the figures represent reflection mirrors. The group $G$ has a center of a 90° rotation that lies on the intersection of two reflection mirrors. The group $G'$ lacks such a center. Hence they cannot be the same.

The goal of this survey is to try to find the missing algebraic invariant that will determine the space group and then use this invariant to classify and enumerate space groups. The invariant is found in the cohomology of groups (see Section 5). This invariant plays a role in the modern solution to the eighteenth problem of Hilbert (see Section 7) namely a proof that in each dimension $n$ there are only finitely many space groups. Furthermore, the proof can be turned into an algorithm for enumerating space groups and hence gives a dimension-independent approach to the crystallographer's enumeration of the 219 crystals in dimension three.

The prerequisites for reading this article have been kept as minimal as possible. Nonetheless the reader should have seen some topological notions as in a course on advanced calculus, have a working knowledge of linear algebra, and some familiarity with basic group theory.

**1. Euclidean geometry.** We let $\mathbb{R}^n$ denote a real vector space of dimension $n$. A point in $\mathbb{R}^n$ is

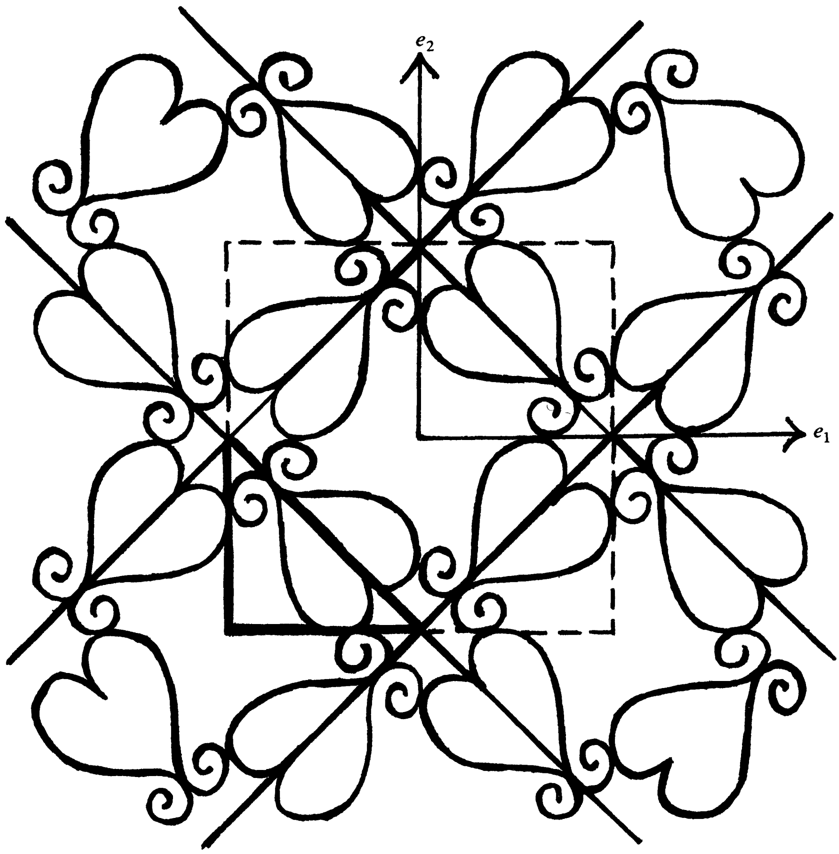


FIG. 2(b) G′

specified by an $n$-tuple $(x_1, \ldots, x_n)$ of real numbers. These points are added component-wise and can be multiplied component-wise by real numbers.

In order to do geometry we must equip this space with additional notions of length and angle. This can be done efficiently with the notion of the **inner** (or **dot**) product of two vectors. If $x$ and $y$ are in $\mathbb{R}^n$, we define the inner product

$$x \cdot y = \sum_{i=1}^{n} x_i y_i,$$

where $x = (x_1, \ldots, x_n)$ and $y = (y_1, \ldots, y_n)$. Now we can define the **length** of a vector $x$ as

$$\|x\| = (x \cdot x)^{1/2},$$

the **angle** between two non-zero vectors $x, y$ by

$$\theta = \arccos(x \cdot y / \|x\| \, \|y\|),$$

and the **distance** between $x$ and $y$ by $\|x - y\|$.

We refer to our space equipped with this additional structure as Euclidean space and denote it by $\mathbb{E}^n$. An **isometry** (or **rigid motion**) of $\mathbb{E}^n$ is a mapping $f: \mathbb{E}^n \to \mathbb{E}^n$ that preserves distance, i.e., $\|f(x) - f(y)\| = \|x - y\|$, for all $x, y$ in $\mathbb{E}^n$. It is not difficult to show that $f$ is necessarily bijective (see [**21**, Chap. 3]).

A good example of an isometry is an **orthogonal** mapping. This is an invertible linear mapping that preserves the inner product and, in particular, fixes the origin. The set of such mappings forms a subgroup $O(n)$ of the group of all real invertible linear mappings called the **orthogonal group**. If we identify a linear mapping $f$ with the matrix $A_f$ that represents it (say, with respect to the standard basis), then the orthogonality condition can be written $AA^t = I$, where $(\ )^t$ denotes the transpose of a matrix and $I$ is the identity matrix.

If, in addition, the linear mapping has determinant 1, we get a smaller subgroup written $\mathrm{SO}(n)$ and called the **special orthogonal group**. For example, if we choose a line (an axis) in $\mathbb{R}^n$ and rotate about it, we get an element of $\mathrm{SO}(n)$. If we choose a hyperplane in $\mathbb{R}^n$ and reflect through it, we get an element of $O(n)$ of determinant $-1$ (hence not in $\mathrm{SO}(n)$).

If we fix a vector $v$ in $\mathbb{E}^n$, the translation mapping $t(v)\colon \mathbb{E}^n \to \mathbb{E}^n$ that sends a vector $x$ to $x + v$ is also an isometry of $\mathbb{E}^n$. We write $V = \{t(v)\colon v \in V]$ for the vector space of translations (ignoring the inner product structure now) to distinguish it from the Euclidean space $\mathbb{E}^n$. Note that a translation determined by a nonzero vector is an example of an isometry that is not a linear mapping (as the origin is not even fixed).

The main result of Euclidean geometry (see [**21**, p. 101]) is the following assertion:

(1.0) THEOREM. *Every isometry can be written in a unique way as a composition $t(v)\circ\phi$, where $t(v)$ is the translation by $v$ and $\phi$ is an orthogonal mapping of $\mathbb{E}^n$.*

We can express this result very neatly in the language of group theory. Let us write $\mathrm{Isom}(\mathbb{E}^n)$ for the set of all isometries of $\mathbb{E}^n$. It is not difficult to check that under the operation of composition of mappings $\mathrm{Isom}(\mathbb{E}^n)$ is a group. It is called the **Euclidean group** or the **group of rigid motions** of $\mathbb{E}^n$. It is not difficult to check (see (1.1iii) below) that the vector space $V$ of translations is a normal subgroup of $\mathrm{Isom}(\mathbb{E}^n)$. It is a consequence of Theorem (1.0) that the quotient is isomorphic to the orthogonal group $O(n)$. This allows us to describe the elements of the isometry group and their composition in a very concrete fashion. Let $(v,\phi)$ denote the element $t(v)\circ\phi$ of $\mathrm{Isom}(\mathbb{E}^n)$ and note that the action of this element $(v,\phi)$ on a vector $x$ in $\mathbb{E}^n$ is given by

$$(v,\phi)(x) = t(v)(\phi(x)) = v + \phi(x).$$

Hence it is easy to figure out what the multiplication in $\mathbb{E}^n$ must be. We compute

$$\begin{aligned}(v,\phi)(v',\phi')(x) &= (v,\phi)(v' + \phi'(x))\\ &= v + \phi(v' + \phi'(x))\\ &= (v + \phi(v'), \phi\phi')(x).\end{aligned}$$

This forces that we define the multiplication in $\mathrm{Isom}(\mathbb{E}^n)$ by

$$(v,\phi)(v,',\phi') = (v + \phi(v'), \phi\phi').$$

It is now easy to check the following assertion:

(1.1) LEMMA. (i) *The identity element of* $\mathrm{Isom}(\mathbb{E}^n)$ *is* $(0,1)$.

(ii) *The inverse of an element of* $\mathrm{Isom}(\mathbb{E}^n)$ *is given by*

$$(v,\phi)^{-1} = (-\phi^{-1}(v), \phi^{-1}).$$

(iii) *The action of* $\mathrm{Isom}(\mathbb{E}^n)$ *on its subgroup $V$ is given by*

$$(v,\phi)(t,1)(v,\phi)^{-1} = (\phi(t),1).$$

*Proof*. The first part is completely trivial and for the second we have

$$(v,\phi)(-\phi^{-1}(v),\phi^{-1}) = (v + \phi(-\phi^{-1}(v)), \phi\phi^{-1}) = (0,1).$$

Finally, (iii) follows from

$$(v,\phi)(t,1)(v,\phi)^{-1} = (v + \phi(t), \phi)(-\phi^{-1}(v), \phi^{-1})$$

$$= \left(v + \phi(t) + \phi\left(-\phi^{-1}(v)\right), \phi\phi^{-1}\right)$$
$$= (\phi(t), 1).$$

Notice that the multiplication on $\mathrm{Isom}(\mathbb{E}^n)$ is **not** the usual direct product group structure. In the next section we develop the group theory that will clarify this new type of "product".

**2. Extensions of groups.** If $K$ and $H$ are two groups we can define a group structure on the set-theoretic product $K \times H$ by defining a multiplication pointwise. Namely

$$(k, h) \cdot (k', h') = (kk', hh').$$

This is the **direct product** of $K$ and $H$, which we write $K \times H$. By an **action** of $H$ on $K$ we mean a group homomorphism $\alpha$: $H \to \mathrm{Aut}(K)$. In particular, if $h$ is in $H$ and $k$ is in $K$, we can describe the action by

$$h \cdot k = \alpha(h)(k).$$

With such an action we can define the **semi-direct product** group structure $K \rtimes_\alpha H$ on the set-theoretic product $K \times H$ by the multiplication.

$$(k, h) \cdot_\alpha (k', h') = (k + \alpha(h)(k'), hh').$$

This may seem on the face of it to be a highly unmotivated construction, but if we compare it with our geometric situation it is perfectly natural. If we let $K = V$, $H = O(n)$ and let $\alpha$: $O(n) \to \mathrm{Aut}(V)$ be the natural inclusion then we can conclude from Section 1

$$\mathrm{Isom}(\mathbb{E}^n) = V \rtimes_\alpha O(n).$$

In fact, it is possible to give a more abstract characterization of semi-direct products. If $K$, $G$ and $H$ are groups, $K$ abelian, we say that the following diagram of groups and homomorphisms

$$K \xrightarrow{i} G \xrightarrow{p} H$$

is **exact** if the map $i$ includes $K$ as a normal subgroup of $G$ and $p$ is a surjection of $G$ onto $H$ that induces an isomorphism of groups $G/i(K) \cong H$. One also says that $G$ is an **extension** of $K$ by $H$.

There is an induced action of $H$ on $K$ by pulling-back and conjugating. More precisely, if $k$ is in $K$, then $h \cdot k = h^{\sim} k (h^{\sim})^{-1}$ in $K$, where $h^{\sim}$ is any element of $G$ satisfying $p(h^{\sim}) = h$. This definition is independent of the choice of $h^{\sim} \in G$, as the reader should check ($K$ is abelian). Hence in this situation it makes sense to ask if $G$ is the semi-direct product of $K$ by $H$ via this action. The answer is yes if and only if there exist a **splitting homomorphism** $\sigma$: $H \to G$, i.e., a group homomorphism for which $p \circ \sigma$ is the identity map on $H$. (There is always a set-theoretic map satisfying this condition but we are insisting that it be a homomorphism of groups.) Clearly such a map exists if $G = K \rtimes_\alpha H$ by taking $\sigma(h) = (1, h)$, where 1 is the identity element of $K$. We often say the sequence is **split** by $\sigma$.

Another example of a semi-direct product is the **affine group** $\mathrm{Aff}(\mathbb{E}^n)$ of Euclidean space $\mathbb{E}^n$. It can be written $\mathrm{Aff}(\mathbb{E}^n) = V \rtimes \mathrm{GL}(n, \mathbb{R})$, where $\mathrm{GL}(n, \mathbb{R})$ is the group of invertible $n \times n$ matrices with real entries. These affine mappings need not preserve distance.

The ideas from this section will play a crucial role in our algebraic understanding and classification of crystals.

**3. Space Groups.** The fundamental notion that relates the group theory of Section 2 with the geometric ideas of crystallography is the notion of a fundamental domain. This requires a certain familiarity with topological notions. If a group $G$ acts on a subset $X$ of $\mathbb{R}^n$, a **fundamental domain** for this action is an open subset $D$ of $X$ that satisfies two properties:

(a) $\cup\{\text{closure } (gD)\colon g \in G\} = X$,
(b) $D \cap gD = \varnothing$, for all $g \neq 1$ in $G$.

Consider $X = \mathbb{E}^2$ and $G = \mathbb{Z} \times \mathbb{Z} \subset V \subset \mathrm{Isom}(\mathbb{E}^2)$ acting on $\mathbb{E}^2$ as a group of translations. The open unit square $D = (0,1) \times (0,1)$ is a fundamental domain for this action as the reader can easily check.

Another way to view this is by considering the quotient of the action of $G$ on $X$. The action of $G$ on $X$ defines an equivalence relation $\equiv_G$ on $G$ by $x \equiv_G y$ if there exists a $g$ in $G$ satisfying $g \cdot x = y$. There is a (topological) quotient space $X/G = X/\equiv_G$. In the example described above the quotient $\mathbb{E}^2/\mathbb{Z} \times \mathbb{Z}$ is a torus. The vertical translation produces a cylinder and the horizontal translation identifies the two "ends" of this cylinder to produce a torus. The torus is compact. We come now to the fundamental definition:

(3.1) DEFINITION. A discrete subgroup $G$ of $\mathrm{Isom}(\mathbb{E}^n)$ is a **space group** (or **crystallographic group**) if the quotient space $\mathbb{E}^n/G$ is compact.

The reader should convince himself that this condition is equivalent to the compactness of the closure of the fundamental domain of $G$ acting on $\mathbb{E}^n$. The discreteness condition means that if $x_0$ is in $\mathbb{E}^n$ the set $\{g \cdot x_0 \colon g \in G\}$ has no accumulation point.

The study of such space groups was motivated in part by Hilbert's eighteenth problem (see section 7) and led Bieberbach to the following characterization.

(3.2) BIEBERBACH'S FIRST THEOREM. *A subgroup $G$ of* $\mathrm{Isom}(\mathbb{E}^n)$ *is a space group if and only if $G$ contains $n$ linearly independent translations.*

The crucial and difficult part of this result is the "only if" direction and a modern account of it can be found in Wolf's book [**30**]. A new and more informative proof has been recently discovered by M. Gromov. An exposition of his work can be found in [**7**].

The characterization of space groups provided by Bieberbach's First Theorem is not completely satisfying. It depends in an essential way on the realization of the elements of the group as isometries of $\mathbb{E}^n$. It would be preferable to have a purely algebraic (i.e., intrinsic) characterization of the class of space groups independent of their embedding inside $\mathrm{Isom}(\mathbb{E}^n)$. We have already made some progress in this direction by showing that $G$ fits into an exact sequence

$$M \to G \to H,$$

where $M$ denotes the free abelian group (isomorphic to the direct sum of $n$ copies of the group $\mathbb{Z}$ of integers) generated by the translations provided by Bieberbach's First Theorem. This group $M$ is often called the **lattice** of $G$ and $H = G/M$ is called the **point group** of $G$. It is possible (although not trivial) to show that the quotient $H$ is finite (see [**26**, pp. 26-27]). In fact, more is true. The group $H$ acts on $M$ by pulling an element $h$ in $H$ back to $h^{\sim}$ in $G$ and conjugating as in Section 2. One can show that this action is faithful (see [**26**, p. 30]). Finally we have the following assertion:

(3.3) THEOREM (Zassenhaus [**31**]). *An abstract group $G$ is isomorphic to an $n$-dimensional space group if and only if $G$ contains a finite index, normal, free abelian subgroup of rank $n$, that is also maximal abelian.*

The maximal abelian property is a direct reformulation of the faithfulness of the above action of $H$ on $M$. (Check this.) This Theorem provides the desired purely group-theoretic characterization of a space group. The problem remains to determine some practical set of algebraic data that specifies $G$ and can be used to enumerate space groups. We return to this problem in Section 4.

Now that we have a notion of space group, we must decide when we want to consider two such to be equivalent. One possibility is to consider two space groups identical if they are abstractly isomorphic as groups. This is apparently the point of view taken by Bieberbach [**10**] in his landmark paper on the subject in 1910. A year later Frobenius [**11**] suggested that perhaps a more intrinsic notion would be preferable. He considered two space groups to be equivalent if when viewed as subgroups of the Euclidean group $\mathrm{Isom}(\mathbb{E}^n)$ they are conjugate by an element of the somewhat larger affine group $\mathrm{Aff}(\mathbb{E}^n)$. This more geometric notion is called **affine equivalence**.

Soon after, Bieberbach published his second fundamental paper on the subject [4] and in fact showed the following result:

(3.4) BIEBERBACH'S SECOND THEOREM. *Any abstract isomorphism of space groups can be realized by conjugation by an affine motion of* $\mathbb{E}^n$.

Hence Bieberbach and Frobenius were using the same equivalence relation anyway. This basic fact (often referred to as "rigidity") will also turn up again in Section 5.

**4. Crystal classes.** Now that we feel comfortable deciding when two space groups should be considered the same, we can try to group them into naturally defined classes. The most obvious parameters for classifying space groups are the ones we have already introduced–namely the point group $H$, the lattice $M$, and the action of $H$ on $M$. For convenience we call these three pieces of structure together a **crystal class** and denote it simply $(H, M)$. The reader is warned that the notation is a bit sloppy in that mention of the action itself is suppressed.

The study of actions of finite groups on lattices ($\cong \mathbb{Z}^n$) is a rich and important subject in itself called **integral representation theory**. The standard reference is [**8**]. Sometimes the techniques and results of integral representation theory can be profitably brought to bear on problems in crystallography.

As in the previous section we are faced with the problem of deciding when to consider two crystal classes "equivalent". In contrast with our treatment of space groups we find that there are two reasonable notions of "equivalence" that are clearly not identical. Both of them will be useful in our treatment of the classification of space groups.

If we choose a free integral basis for $M$, a crystal class can be viewed as a one-to-one homomorphism $f\colon H \to \mathrm{Aut}(M) \cong \mathrm{GL}(n,\mathbb{Z})$, where $\mathrm{GL}(n,\mathbb{Z})$ denotes the general linear group of non-singular $n \times n$ integer entries and determinant $\pm 1$. (Recall from linear algebra that this last condition is equivalent to the condition that all the entries of the inverse matrix are integers.) So after choosing a basis for $M$, $H$ is embedded explicitly as a subgroup $f(H)$ of $\mathrm{GL}(n,\mathbb{Z})$. If $f'$: $H \to \mathrm{Aut}(M')$ is another crystal class, we say $(H, M)$ is **arithmetically equivalent** (or **$\mathbb{Z}$-equivalent**) to $(H, M')$ if there exists an isomorphism $\alpha\colon M \to M'$ so that

$$\alpha \cdot f(h) = f'(h) \cdot \alpha$$

for all $h$ in $H$. If we write this condition as $\alpha \circ f \circ \alpha^{-1} = f'$, we see that this is equivalent to insisting that the two corresponding subgroups $f(H), f'(H)$ are conjugate in $\mathrm{GL}(n,\mathbb{Z})$. If the two subgroups are conjugate in the larger rational general linear $\mathrm{GL}(n,\mathbb{Q})$ (where the matrix entries are rational numbers and the determinant is a nonzero rational numbet), then we say that the two crystal classes are **geometrically equivalent** (or **$\mathbb{Q}$-equivalent**). The resulting equivalence classes are the **arithmetic** and **geometric crystal classes**, respectively.

As an example consider the following three matrices in $\mathrm{GL}(n,\mathbb{Z})$:

$$A_1 = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \quad A_2 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad A_3 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Since each has the property that $A^2 = 1$, they determine three crystal classes of the group $H = \mathbb{Z}_2$, the integers modulo 2. The matrix $A_1$ has eigenvalues $-1, -1$ and both $A_2$ and $A_3$ have eigenvalues $1, -1$ (compute it for $A_3$). Hence $A_1$ determines a different geometric crystal class than $A_2, A_3$. On the other hand we also have

$$\alpha A_2 \alpha^{-1} = A_3 \quad \text{where} \quad \alpha = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}.$$

So $A_2, A_3$ determine the same geometric crystal class. But since $\det(\alpha) = 2$, $\alpha$ is not in $\mathrm{GL}(2,\mathbb{Z})$ and $\alpha$ does **not** show that $A_2, A_3$ determine the same arithmetic crystal classes. We leave it as an exercise to show that $A_2$ and $A_3$, in fact, determine different arithmetic crystal classes.

We see from these samples that a single geometric crystal class can break up into two different arithmetic crystals classes. (Another example in dimension 2 is the group $H = D_3$, the symmetry group of the triangle with 6 elements; see Section 8 below). It is a consequence of a fundamental result of integral representation theory that a geometric crystal class can split up into at most finitely many arithmetic crystal classes. This is the Jordan-Zassenhaus theorem [**8**, Theorem 79.1] and is a key ingredient in the solution of Hilbert's eighteenth problem.

**5. Cohomology.** If $G$ is a space group, $G$ fits into a short exact sequence

$$(*) \qquad M \xrightarrow{i} G \xrightarrow{p} H,$$

where $M$ is free abelian, $H$ is finite and $H$ acts faithfully on $M$, so determines an arithmetic crystal class $(H, M)$ (again our notation is somewhat sloppy). We will also say that $G$ is **in the arithmetic crystal class** $(H, M)$. Although $G$ can be thought of as sitting inside the semi-direct product $V \rtimes_\alpha O(n) \cong \mathrm{Isom}(\mathbb{E}^n)$, (as in Section 2) there is no *a priori* reason to believe that $G$ itself is the semi-direct product of $H$ acting on $M$. In fact, this is the heart of our method for classifying space groups, seeing how far they differ from the semi-direct product. (The crystallographers call space groups that are semi-direct products **symmorphic**). We will see that Fig. 2 is a concrete geometric example of this phenomenon in dimension two.

By Bieberbach's First Theorem we can suppose that $G \subset V \rtimes_\alpha O(n)$ and that the map $p$: $G \to H$ is projection onto the second factor. Suppose $\tau$: $H \to G$ is a set-theoretic section to this map $p$: $G \to H$. This means that for each element $h$ in $H$, $p(\tau(h)) = h$. So $\tau(h) = (\sigma(h), h)$ for some set-theoretic map $\sigma$: $H \to V$. We will refer to this map $\sigma$ as a **section** to the exact sequence $(*)$ and dispense with $\tau$ altogether.

If $h$ happens to actually be in $G$, i.e., really is a symmetry of the crystal, then $\sigma(h)$ can be chosen to be any element of $M$, for example 0. But there are, for example, glide reflections (a reflection followed by a translation), for which $\sigma(h)$ cannot be chosen to be in $M$. We also know from Section 2 that if $\tau$ can be chosen to be a group homomorphism, then $G$ is necessarily the semi-direct product of $H$ acting on $M$.

Of course, such a section $\sigma$ is not unique. We can easily remedy this situation by composing with the natural projection $V \to V/M$. The resulting map $s$: $H \to V/M$ is then well defined. We indicate the proof. Suppose that $\sigma'$: $H \to V$ is another such section. Then:

$$\begin{aligned}(\sigma'(h), h)(\sigma(h), h)^{-1} &= (\sigma'(h), h)(-h^{-1}(\sigma(h)), h^{-1})\\ &= (\sigma'(h) - \sigma(h), 1).\end{aligned}$$

Hence the difference is in $M$ and the map $s$ makes perfect sense independent of the choice of $\sigma$. We also have the following result:

(5.1) PROPOSITION. *The map $s$ satisfies the following identities*:
(i) $s(1) = 0$ (*note*: 0 *denotes the* zero coset $M$ *in* $V/M$),
(ii) $s(xy) = s(x) + x \cdot s(y)$.

*Proof*. Firstly note that $H$ acts on $V/M$ because $M$ is invariant under $H$. This is the action on the right-hand side of equation (ii). Equation (i) merely asserts that $(0,1)$, the identity element, is in $G$. To show (ii) we need only observe that

$$(s(x), x)(s(y), y) = (s(x) + x \cdot s(y), xy).$$

We call (i) and (ii) the **cocycle identities** and $s$ a **1-cocycle**. The set of all such 1-cocycles forms an abelian group (because $V/M$ is) and is denoted $Z^1(H, V/M)$.

The procedure that we have just described that leads from $G$ to the 1-cocyle $s$ is reversible. The group $G$ can easily be reconstructed from the 1-cocyle by writing

$$G = \{(v, h) \in \mathrm{Isom}(\mathbb{E}^n)\colon h \in H \quad \text{and} \quad v \in s(h)\}.$$

(Remember that $s(h)$ is a coset of $M$ in $V$.) This assertion is easy to check. Hence instead of classifying space groups we are reduced to classifying 1-cocycles $s$: $H \to V/M$, i.e., functions satisfying certain identities, a seemingly more manageable task. Now we can invoke the second theorem of Bieberbach. Isomorphisms of space groups are detected by conjugacy of the space groups inside the affine group $\mathrm{Aff}(\mathbb{E}^n)$. What remains to do is understand the effect of conjugating by an element of $\mathrm{Aff}(\mathbb{E}^n)$ over in the realm of 1-cocycles. This is surprisingly easy and straightforward.

Firstly each element of $\mathrm{Aff}(\mathbb{E}^n) = V \rtimes \mathrm{GL}(V)$ is the composition of a translation $(a, 1)$, $a \in V$, and a linear mapping $(0, g)$, $g \in \mathrm{GL}(V)$. Hence it suffices to analyze the effect of conjugating a 1-cocycle by each of these separately.

Suppose $a$ is an element of the vector space $V$ and the 1-cocycle $s$ is induced from $\sigma\colon V \to M$. Then we can compute

$$\begin{aligned}(a,1)(\sigma(h),h)(a,1)^{-1} &= (a,1)(\sigma(h),h)(-a,1)\\ &= (a+\sigma(h),h)(-a,1)\\ &= (a+\sigma(h)-h(a),h).\end{aligned}$$

Passing to the quotient $V \to V/M$, we see that conjugating by $(a,1)$ changes the 1-cocycle by adding another 1-cocycle of the form $b_a(h) = \alpha - h(\alpha)$, where $\alpha$ denotes $a$ mod $M$. That this function really is a 1-cocycle follows from the checking that $b_a(1) = \alpha - 1(\alpha) = 0$ and

$$b_a(hh') = \alpha - hh'(\alpha) = \alpha - h(\alpha) + h(\alpha) - hh'(\alpha) = b_a(h) + h(b_a(h')).$$

The 1-cocycles of this form are called **1-coboundaries** and form a subgroup of $Z^1(H, V/M)$ denoted $B^1(H, V/M)$. From the point of view of our study of space groups these 1-coboundaries should be considered trivial, so it is natural to consider the quotient group obtained by dividing out the 1-coboundaries: $Z^1(H, V/M)/B^1(H, V/M)$. This group is usually denoted $H^1(H, V/M)$ and is called the **1-dimensional cohomology group of** $H$ **with coefficients in** $V/M$.

It now remains to consider the effect of conjugating by $(0, g)$ where $g$ is an element of $\mathrm{GL}(V)$. So we compute

$$(0,g)(\sigma(h),h)(0,g)^{-1} = (0,g)(\sigma(h),h)(0,g^{-1}) = (g(\sigma(h)), ghg^{-1}).$$

This suggests defining the following action of $\mathrm{GL}(V)$ on the group of 1-cocycles. If $g$ is in $\mathrm{GL}(V)$ and s is in $Z^1(H, V/M)$, then

$$(g \cdot s)(h) = gs(g^{-1}hg).$$

Then the above computations can be summarized by saying that the effect of conjugating $s$ by $g$ in $\mathrm{GL}(V)$ is precisely $gs$. Hence if $g$ is in the normalizer $N(H, M)$ of $H$ in $\mathrm{Aut}(M)$, then the 1-cocycles should be identified. Putting this all together we obtain (see [**26**, p.35]) the main result:

(5.2) Main Theorem of Mathematical Crystallography. *There exists a one-to-one correspondence between space groups in the arithmetic crystal class* $(H, M)$ *and the orbits of* $N(H, M)$ *acting on the* 1-*dimensional cohomology group* $H^1(H, V/M)$.

Remark (for experts). More sophisticated readers might have expected to see the 2-dimensional cohomology group $H^2(H, M)$ play the pivotal role in the classification of space groups. In fact, using the long exact sequence associated to the coefficient sequence $O \to M \to V \to V/M \to O$ we get an isomorphism: $H^2(H, M) \cong H^1(H, V/M)$.

**6. An Example.** Not only is Theorem (5.2) a beautiful and powerful theorem, it also gives one a computational hold on classifying crystals. We return now to the examples of the introduction and show how these "tilings" can be distinguished with the use of cohomology of groups. We begin with an easy lemma:

(6.1) Lemma. *If* $s\colon H \to V/M$ *is a* 1-*cocycle and* $x$ *is in* $H$, *then*

$$s(x^k) = (1 + x + x^2 + \cdots + x^{k-1})s(x).$$

*Proof*. Induct on $k$.

The dihedral group $D_4$ of order 8 is generated by elements $R$ and $S$ subject to the relations

$$S^4 = 1 \qquad R^2 = 1 \qquad RSR = S^{-1}.$$

We will often write this last relation as $(SR)^2 = 1$. The group $D_4$ admits a unique arithmetic crystal class $(D_4, \mathbb{Z}e_1 \oplus \mathbb{Z}e_2)$ where $\{e_1, e_2\}$ is the standard basis and the action $D_4 \to \operatorname{Aut}(\mathbb{Z}e_1 \oplus \mathbb{Z}e_2) = \mathrm{GL}(2, \mathbb{Z})$ is given by

$$S \mapsto \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \qquad R \mapsto \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Geometrically $S$ is a rotation through an angle $\pi/2$ and $R$ is a reflection through the $y$-axis. We are going to apply (5.2) to this arithmetic crystal class $(H, M)$ to find the two-dimensional space groups with point group $D_4$.

To compute the cohomology group we begin by identifying the 1-cocycles $s\colon D_4 \to \mathbb{R}^2/\mathbb{Z}^2$. Certainly $s$ is determined by its values on $S$ and $R$. Let's suppose

$$s(S) = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}, \qquad s(R) = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix},$$

where we denote the elements of $\mathbb{R}^2/\mathbb{Z}^2$ by column vectors. By the first of the cocycle conditions, $s$ sends any relation into $\mathbb{Z}^2$. Hence by (6.1)

$$\begin{aligned} s(R^2) &= (1 + R)s(R) \\ &= \begin{pmatrix} 0 & 0 \\ 0 & 2 \end{pmatrix}\begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 2b_2 \end{pmatrix} \in \mathbb{Z}^2. \end{aligned}$$

So $b_2 \in (1/2)\mathbb{Z}$, a half-integer. Similarly,

$$\begin{aligned} s\big((SR)^2\big) &= (1 + SR)s(SR) \\ &= \left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}\right]s(SR) \\ &= \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}\left[\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} + \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} b_1 \\ b_2 \end{pmatrix}\right] \\ &= \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} a_1 - b_2 \\ a_2 + b_1 \end{pmatrix} \in \mathbb{Z}^2, \end{aligned}$$

or, equivalently, $a_1 - b_2 \equiv a_2 + b_1 \pmod{\mathbb{Z}}$. Since $1 + S + S^2 + S^3 = 0$, the condition $s(S^4) \in \mathbb{Z}^2$ places no restriction.

Now we determine the coboundaries. If

$$v = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \in \mathbb{R}^2,$$

then the 1-coboundary $b_v$ is given by $b_v(g) = v - gv = (1 - g)v$. We compute $b_v$ on the generators $S, R$:

$$\begin{aligned} b_v(S) &= (1 - S)v = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} v_1 + v_2 \\ v_2 - v_1 \end{pmatrix}, \\ b_v(R) &= (1 - R)v = \begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} 2v_1 \\ 0 \end{pmatrix}. \end{aligned}$$

To compute $H^1$ we begin by simplifying our given 1-cocycle $s$ by adding appropriate $b_v$'s. If we set

$$\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} \frac{1}{2}(a_1 - a_2) \\ \frac{1}{2}(a_1 + a_2) \end{pmatrix},$$

then clearly $(s - b_v)(S) = 0$ and

$$(s - b_v)(R) = \begin{pmatrix} b_1 - a_1 + a_2 \\ b_2 \end{pmatrix}.$$

The cocycle condition gives us

$$b_2 \in \left(\frac{1}{2}\right)\mathbb{Z}$$

and

$$b_1 + b_2 \equiv a_1 - a_2 (\operatorname{mod} \mathbb{Z}).$$

But since $s - b_v$ is also a cocycle with $a_1 = a_2 = 0$, we get

$$b_1 + b_2 \equiv 0 (\operatorname{mod} \mathbb{Z}).$$

Hence, mod $\mathbb{Z}$, we have only two possibilities:

$$\begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \equiv \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \equiv \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}.$$

Hence $H^1(D_4, V/M) \cong \mathbb{Z}_2$, the cyclic group with two elements.

The space groups $G$ and $G'$ of the introduction correspond to the trivial and non-trivial elements of this $H^1 \cong \mathbb{Z}_2$. Observe that the normalizer plays no role in this calculation since the normalizer permutes the nonzero elements of the cohomology group. The reader should study Fig. 2b to convince himself that although $R$ is not a symmetry of the "wallpaper", the element $((\frac{1}{2}, \frac{1}{2}), R) \in \operatorname{Isom}(\mathbb{E}^2)$ is.

**7. Finiteness.** In 1900 at the International Congress of Mathematicians in Paris, Hilbert gave a list of what he considered the outstanding, unsolved mathematical problems of the day. His inclusion of the following problem generated early interest in the mathematical approach to crystallography (see [**16**]):

"Is there in $n$-dimensional Euclidean space... only a finite number of essentially different kinds of groups of motions with a [compact] fundamental domain?"

Despite Hilbert's pessimism about a rapid solution of this problem, L. Bieberbach answered it affirmatively within the following decade.

(7.1) BIEBERBACH'S THIRD THEOREM. *For each $n$, there are only finitely many isomorphism classes of $n$-dimensional space groups.*

As we have already discussed in Section 2, one can replace "isomorphism class" by "affine conjugacy class" to get an apparently stronger statement.

After Bieberbach proved his First Theorem (see 3.2 above) the solution of Hilbert's problem followed from essentially known results. The strategy of the argument follows three steps.

1. For each $n$, there are only finitely many $n$-dimensional geometric crystal classes.

2. For each geometric crystal class, there are only finitely many arithmetic crystal classes geometrically equivalently to it.

3. For each arithmetic crystal class, there are only finitely many space groups in that class.

The final step is the easiest. According to the Main Theorem of Mathematical Crystallography (5.2), it suffices to check that $H^1(H, V/M)$ is finite. This is, in fact, an elementary fact from the theory of group cohomology (see [**6**]). An elementary and direct proof can be found in Schwarzenberger's book [**26**, p. 130].

The first step was given a group-theoretic proof by Minkowski [**18**] in 1905. It also follows from the so-called Minkowski-Siegel reduction theory [**17**] for positive-definite quadratic forms. A readable proof can be found in [**19**].

Finally the second step in the proof is a special case of the Jordan-Zassenhaus theorem of representation theory, a theorem we have already discussed in Section 4.

In 1948, Zassenhaus [**32**] observed that this proof could be turned into an effective algorithm for enumerating space groups. It was only in 1976 that this algorithm was fully implemented in dimension 4 and generated a complete list (with much additional data) of the 4783 (!) four-dimensional space groups.

The first step of the above strategy requires a listing of the conjugacy classes of finite subgroups of $\mathrm{GL}(n, \mathbb{Z})$. One begins this enumeration by finding the maximal finite subgroups of $\mathrm{GL}(n, \mathbb{Z})$. In fact, this has been worked out for $n \leqslant 7$ in the work of Dade [**9**] and Plesken-Pohst [**22**], [**23**]. All of the conjugacy classes of finite subgroups (i.e., arithmetic crystal classes) can then be found by applying certain "subgroup subroutines" to the list of maximal ones; this provides a count of the number of geometric crystal classes. Steps two and three then require writing down the integral representations of the groups, computing cohomology and normalizers and finally the set of orbits. More details on these procedures can be found in [**5**] as well as extensive computer printouts of the results.

Here is a table of some of the known statistics:

TABLE 1

| dimension | # geometric crystal classes | # arithmetic crystal classes | # space groups |
|---|---|---|---|
| 2 | 10 | 13 | 17 |
| 3 | 32 | 73 | 219 |
| 4 | 227 | 710 | 4783 |

Finally we mention that Schwarzenberger [**27**] (see also [**26**, p. 96]) has shown that if $s_n$ denotes the number of space groups in dimension $n$, then $s_n$ grows at least as fast as $2^{n^2}$ and conjectures that this is the exact asymptotic result.

**8. Wallpaper.** We began with our intuition about crystals in three-dimensional space. Historically this was also the starting point of mathematical crystallography. The possible point groups for the three-dimensional space groups were first determined by Hessel (1829); a modern readable account can be found in [**2**, Theorem 2.5.2.]. In an apparently surprising coincidence (but see [**26**, p. 132]) the crystals in three-dimensional space were classified independently and almost simultaneously by Fedorov (in Russia), Schoenflies (in Germany) and Barlow (in England) in the latter part of the nineteenth century. Their work built upon earlier contributions of Hessel, Bravais, Möbius, Jordan, and Sohncke. The methods they employed were *ad hoc* and directly geometric. A modern cohomological approach to the classification of the 219 crystals in the spirit of the techniques we have discussed can be found in [**26**] and [**14**].

REMARK. It should be mentioned that most crytallographers actually insist that there are 230 crystals. This discrepancy arises from 11 so-called enantiomorphic pairs—as in organic chemistry. These crystals differ by a mirror reflection (i.e., one is "left-handed" and the other "right-handed"). The mathematical explanation is that crystallographers use for their notion of equivalence of space groups the stronger one of conjugacy inside the special affine group $S\,\mathrm{Aff}(\mathbb{E}^n) = V \rtimes \mathrm{GL}^+(n, \mathbb{R})$, i.e., affine mappings with positive determinant (hence omitting the mirror reflections with determinant $-1$). A completely mathematical description of this phenomenon has been worked out by Maxwell [**15**].

Somewhat later it was realized that the same methods could be applied in the easier cases of dimensions 1 and 2. In dimension one, there are only three space groups contained in $\mathrm{Isom}(\mathbb{E}^1) = \mathbb{R} \rtimes \mathbb{Z}_2$. (What are they?) There are also 7 "frieze" patterns that can be viewed as the linear patterns that wind around Grecian urns. (Try finding 7 representative patterns and convincing yourself that these are all of them; see [**13**].)

The space groups in dimension 2 are usually called the **wallpaper groups**. There are 17 of them and they were first catalogued by Pólya [**24**] and Niggli [**20**] in the twenties. A completely elementary exposition of these results can be found in [**28**] (see also [**26**, Chap. 1]).

The reader is encouraged to apply the techniques of Sections 4–5 to check cohomologically the table of wallpaper groups given below. It is also instructive to compare this table with those that appear in Schattschneider's article [**25**].

The fact that the groups listed in the first column below are the only possible point groups is a fact usually attributed to Leonardo Da Vinci (for example, see Weyl [**29**]). For an elementary proof see [**2**].

TABLE 2. Wallpaper groups.

| point group | acc | # $H^1(H, V/M)$ | # space groups | notation |
|---|---|---|---|---|
| e | $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ | 1 | 1 | p1 |
| $\mathbb{Z}_2$ | $\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$ | 1 | 1 | p2 |
| $\mathbb{Z}_3$ | $s_3 = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$ | 1 | 1 | p3 |
| $\mathbb{Z}_4$ | $s_4 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ | 1 | 1 | p4 |
| $\mathbb{Z}_6$ | $s_6 = \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}$ | 1 | 1 | p6 |
| $D_1$ | $r = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$ | 2 | 2 | pm, pg |
| | $\begin{pmatrix} 1 & 1 \\ 0 & -1 \end{pmatrix}$ | 1 | 1 | cm |
| $D_2$ | $\pm\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$ | 4 | 3 | pmm, pmg, pgg |
| | $\pm\begin{pmatrix} 1 & 1 \\ 0 & -1 \end{pmatrix}$ | 1 | 1 | c2mm |
| $D_3$ | $r \quad s_3$ | 1 | 1 | p3m1 |
| | $\begin{pmatrix} -1 & 0 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} -1 & -1 \\ 1 & 0 \end{pmatrix}$ | 1 | 1 | p31m |
| $D_4$ | $r \quad s_4$ | 2 | 2 | p4m, p4g |
| $D_6$ | $r \quad s_6$ | 1 | 1 | p6m |

The book of Schwarzenberger [**26**] is a natural source for further details and elaborations of the results described here. The more ambitious reader might consult the book of Wolf [**30**] where the ideas of crystallography are extended to the other non-Euclidean geometries—spherical and hyperbolic. The spherical case is fairly well understood (although the required group-theoretic labors were substantial) while the hyperbolic case is still something of a mystery. The two-dimensional hyperbolic situation was studied extensively by Fricke and Klein [**10**] in the latter part of the nineteenth century in the context of their work on automorphic functions. The reader should browse through the book of Magnus [**12**] (or a catalogue of Escher drawings) to see what wallpaper in hyperbolic 2-space looks like.

**9. Epilogue: Flat Manifolds.** In Section 3 we introduced the fundamental notion of a space group by examining the quotient space $\mathbb{E}^n/G$. If we consider the simple case of a cyclic point group, say $\mathbb{Z}^2 \rtimes \mathbb{Z}_3$ acting on $\mathbb{E}^2$ by a 120° rotation, the resulting quotient space $\mathbb{E}^2/\mathbb{Z}^2 \rtimes \mathbb{Z}_3$ has a nasty singularity (or corner) at the origin.

Mathematicians generally find such singularities unpleasant so it is natural to ask whether there are space groups $G$ for which the quotient $\mathbb{E}^n/G$ is without singularities, i.e., is a **manifold**. We call such a group a **Bieberbach group**. We already saw such an example back in Section 3 where we considered $\mathbb{Z} \oplus \mathbb{Z}$ acting by translations on $\mathbb{E}^2$. The quotient was seen to be a **torus** which is a compact surface, a two-dimensional manifold. Of course this example generalizes to any dimension, since $\mathbb{E}^n/\mathbb{Z}^n$ is an $n$-dimensional torus. In this family of examples the point group $H$ (now called the **holonomy group**) is trivial. In general one has that $\mathbb{E}^n/G$ is a manifold if and only if no element of $G$ fixes a point in $\mathbb{E}^n$. In such a case we call the action of $G$ on $\mathbb{E}^n$ a **free** action. For example, a pure rotation could not be in $G$ if we want $\mathbb{E}^n/G$ to be a manifold. In fact one has the following general algebraic criterion:

(9.1) PROPOSITION. *A space group $G \subset \operatorname{Isom}(\mathbb{E}^n)$ is a* **Bieberbach group** *if and only if it is torsion-free.*

Recall that a group is **torsion-free** if it has no elements of finite order. In particular, a Bieberbach group is never a semi-direct product, because in that case the holonomy group $H$ would inject into $G$ via any map that splits $G$ (see Section 2). In fact we can re-express the criterion of (9.1) by saying that the short exact sequence defining $G$ does not split over any subgroup of $H$. This can then be expressed as a condition on the 1-dimensional cohomology class defining $G$.

The manifolds that arise as quotients of Euclidean space have certain special differential-geometric properties. They are precisely the **flat manifolds**. These are Riemannian manifolds that have zero curvature. (For the precise definition of curvature see [**21**]. They are also the Riemannian manifolds whose Riemannian universal covering spaces are Euclidean space $\mathbb{E}^n$.) In dimension two there are precisely 2 flat manifolds: the torus and the Klein bottle. The second example arises from the unique non-trivial class in $H^1(\mathbb{Z}_2, \mathbb{R}^2/\mathbb{Z}^2)$, where $\mathbb{Z}_2$ acts by flipping the factors (it is not orientable). In dimension 3 there are 10 flat manifolds among the 219 crystals, and in dimension 4 there are 75 flat manifolds among the 4783 crystals. It is unknown how many 5-dimensional flat manifolds there are, but Schwarzenberger [**26**] has shown that there are at least 9806 space groups with point group $(\mathbb{Z}_2)^5$.

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# THE PARTIAL ORDER OF ITERATED EXPONENTIALS

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**1. Introduction.** Which is larger, $\pi^e$ or $e^\pi$? Before the advent of hand calculators, this was a more interesting exercise in calculus texts than at present. But even with current technology, try finding the larger of

$$e^{e^{\pi^{e^{\pi^{\pi}}}}} \quad \text{and} \quad e^{\pi^{e^{\pi^{e^{\pi}}}}}$$

by computing the decimal approximations.

Here is a more general question: let $e \leq x_1 \leq x_2 \cdots \leq x_n$, and for each permutation $(y, z, \dots, w)$ of the $x_i$'s, let $T(y, z, \dots, w)$ be the "iterated exponential":

$$T(y, z, \dots, w) = y^{z^{\cdot^{\cdot^{\cdot^{w}}}}}.$$

Such an expression is called a *tower* with levels $1, 2, \dots, n$; level 1 is at the base, and association is always to the upper right:

Barry Brunson received the Ph.D. from Indiana University under the direction of Victor Goodman. His mathematical interests are broad, and include martingales with unusual index sets, analysis, foundations, and combinatorics. Among perceived ills of the world, he sees the misuse and abuse of statistics as causing much social harm. He entered both the professoriate and parenthood 18 years after high school, and spends considerable time with children Cory and Nicole, whose ages have a sum of five and a product of four.