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book reviews

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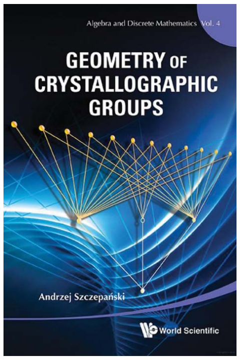

Geometry of Crystallographic Groups. By Andrzej Szczepański. World Scientific, 2012. Pp. 208. Price (hardcover) GBP 51.00. ISBN 978-981-4412-25-4.

The crystallographic groups are critical elements of any crystallographer's toolkit. As the subject is extended and refined, the resulting tools become more powerful and useful. This book is an introduction to the theoretical foundations of the subject.

It is a text for a second-year graduate course in mathematics, so it is a mathematically advanced introduction as well as a snapshot of (part of) the current state of the subject. Although most practicing crystallographers will probably not be interested in investing in this book, it does provide a useful update on developments in mathematical (particularly geometric) crystallography. So this review will focus on what this book tells us about how mathematicians view the crystallographic groups.

The book begins at the geometric core of crystallography with the three fundamental results of Ludwig Bieberbach, published from 1910 to 1912, that summed up the nineteenth-century construction of the crystallographic groups. Bravais, Schoenflies, Federov and others had developed tables of 219 – or 230, depending on how you counted them – classes of crystallographic space groups on three-dimensional space. In 1900, David Hilbert challenged the mathematical community with 23 questions, and the 18th consisted of three parts (Milnor, 1974). The first part of the Eighteenth Question was whether it was true that for every integer n, there were finitely many 'isomorphism classes' of crystallographic groups on n-dimensional space.

Here is a little background. Let's focus on three-dimensional space. One starts with the notion of an *isometry*, a function f from 3-space onto itself such that for any two points $\mathbf{x}$ and $\mathbf{y}$, the distance from $\mathbf{x}$ to $\mathbf{y}$ is the same as the distance from $f(\mathbf{x})$ to $f(\mathbf{y})$. It is a standard exercise in (graduate) linear algebra that an isometry is *affine*: in vector notation, there exists a matrix M and a vector $\mathbf{b}$ such that for any vector $\mathbf{x}$ in 3-space, $f(\mathbf{x}) = M\mathbf{x} + \mathbf{b}$. During the nineteenth century, crystallographers proposed that a given crystal would have a *group G* of *isometries* that act as symmetries of the crystal: for a symmetry g and a point $\mathbf{x}$ in 3-space, there would be an atom at $\mathbf{x}$ if and only if there was an atom at $g(\mathbf{x})$. Such a group of symmetries of a given crystal should have the following properties:

(i) There would be a fixed positive distance, call it d, such that given atoms at the distinct points $\mathbf{x}$ and $\mathbf{y}$, the distance from $\mathbf{x}$ to $\mathbf{y}$ is at least d.

(ii) If there was an atom at $\mathbf{x}$, then the set of all positions $g(\mathbf{x})$, for g in G, is the *orbit* of $\mathbf{x}$. That is, the orbit is the set of points occupied by atoms of the same 'kind' as the original atom at $\mathbf{x}$ (in terms of placement in the crystal). For a crystal, one would want all the atoms distributed into finitely many orbits (*e.g.* one orbit for the carbon atoms in diamond, two orbits for the silicon and oxygen atoms in quartz, and so on).

(iii) The crystal would extend in all directions, in the following sense. If there was an atom at a point $\mathbf{x}$, then for any plane there would be an atom at a point on the opposite side of the plane from $\mathbf{x}$.

Such a group of symmetries is called *crystallographic*.

In 3-space, Bieberbach's three results become:

(1) If G is a crystallographic group, then it has a 'lattice' subgroup L generated by translations in three independent axial directions. Recalling that the group consists of affine functions, *i.e.*, of the form $f(\mathbf{x}) = M\mathbf{x} + \mathbf{b}$, Bieberbach also showed that there were only finitely many matrices M in the 'point' group of G.

(2) Two groups G and H are *isomorphic* if they have the same addition or multiplication table. For example, any two lattice groups in 3-space are isomorphic, even if they share no translations: there is a one-to-one correspondence between the two groups from which one can derive the same addition table. Although there are infinitely many crystallographic groups, they fall into finitely many *isomorphism classes* (where any two groups in the same isomorphism classes are *isomorphic*).

(3) Finally, he proved that for any two isomorphic crystallographic groups, there is an affine function of 3-space that is also an isomorphism from one group to the other. This is what makes the diagrams of the (isomorphism classes of) crystallographic groups possible.

This much is the first half of the core of the book. Chapters 1 and 2 concern preliminaries and the Bieberbach results, respectively. In Chapter 2, Szczepański follows the presentation in Joseph Wolf's classic *Spaces of Constant Curvature* (Wolf, 1974). The rest of the book falls into two parts. Chapters 3, 4 and 5 concern the generation and classification of the crystallographic groups; Szczepański concentrates on the classification methods of Hans Zassenhaus, of Eugenio Calabi, and that of Louis Auslander and Alphonse Vasquez. Chapters 6, 7, 8 and 9 make up a sample of recent topics. Let us look at the second half of the core of the book, Chapters 3, 4 and 5.

Suppose that one desired to generate, for a given n, a catalog of the (isomorphism classes of the) n-dimensional crystallographic groups. Or at least some nice subcollection of these groups. The 219 three-dimensional crystallographic groups were obtained during the late nineteenth century, and Hans Zassenhaus employed modern techniques to obtain the 4783 four-dimensional crystallographic groups (Brown *et al.*, 1948). Here is the idea.

Suppose that one has something that is difficult to count – like the collection of four-dimensional crystallographic groups. It may be helpful to find some easily enumerated set that can be put into a correspondence with the collection, and in enumerating that set one enumerates the collection. To this end, Szczepański employs a popular workhorse, the *cohomology group*. For a point group G, the ('second') cohomology group of G has some elements for each crystallographic space group of point group G, and cohomology groups are easier to enumerate. The Zassenhaus approach is perhaps the most popular enumeration algorithm and, for example, is the mechanism underlying the program *CARAT* (Opgenorth *et al.*, 1998; http://wwwb.math.rwth-aachen.de/carat/), a package within the *Groups, Algorithms, and Programming* (*GAP*) system (The GAP Group, 2013). Szczepański uses *CARAT* for several of his computations.

The other two methods in these three chapters concentrate on *torsion-free* crystallographic groups: a crystallographic group is torsion-free if, given any of its elements f and any positive integer k, f^k is not the identity. For example, the wallpaper group *pg*, which consists of translations and glide reflections, is torsion-free for the following reason. Repeating a glide any number of times, or repeating a translation any number of times, will not result in the identity. On the other hand, the wallpaper group *p*2, which is generated by two translations and a half-turn, is not torsion-free, as the half-turn, repeated twice, is the identity. Torsion-free crystallographic groups are usually called *Bieberbach groups*.

The last four chapters consist of 'the most interesting results (in our opinion) from recent years'. Two of these – the chapter on spin structures and the chapter on Kähler structures – concern the theory of 'flat manifolds'. Curves are one-dimensional manifolds (and lines and line segments are flat), surfaces are two-dimensional manifolds (and planes are flat, as are faces of polyhedra), and so on up to higher dimensions. In algebraic topology, many flat manifolds are actually quilt-like arrays of simpler flat manifolds glued together. For example, we can regard the unit cell of a crystal as a three-dimensional manifold, and since opposing sides of this parallelepiped are identical, we could 'identify' them and have the unit cell be a finite, bounded manifold with no boundary: if a bug flew out one side, it would fly in through the opposite side. One could even take several unit cells and glue their sides so that a bug taking a round trip would return upside down (such a manifold would not be represented in three-dimensional space, but rather it would be treated as a space of its own). Some of these manifolds are quite complex, and the machinery in these two chapters is quite formidable.

The third of these four chapters is a brief foray into hyperbolic space. Hyperbolic space is one of the two major variants of Euclidean space: in Euclidean space, every triangle's angles add up to180 degrees, while in elliptic space, every triangle has more than 180 degrees. In hyperbolic space every triangle has less than 180 degrees. The fourth of these four chapters is an exploration of Bieberbach groups with the following property: if the dimension of the group is n, then its point group is isomorphic to the group of $(n-1)$-dimensional vectors of 0's and 1's where addition is coordinate-wise addition modulo 2. (For three-dimensional crystallographic groups, the point groups isomorphic to the group of two-dimensional vectors of 0's and 1's are 222, *mm*2 and 2/*m*. According to *CARAT*, there are three such three-dimensional Bieberbach groups.)

Finally, there is a chapter of open problems.

This book is advertised as a text for a graduate student in mathematics who has already learned 'elementary facts from algebra, cohomology of groups and topology'. Actually, the standard graduate core courses in these subjects are necessary, but might not be sufficient (*e.g.* the text presumes considerable familiarity with differential geometry, particularly with manifolds of constant curvature). I do not recommend this book for anyone who has not had these courses or equivalents. Excluding the appendices, open-problems section and other ancillaries, it is 162 pages of dense material, including 89 exercises of varying difficulty – somewhat over a semester's worth for a special topics course. Such a course would probably focus on the first five chapters, plus additional topics as time permits.

This is a text, not a handbook. But it is not self-contained. Some notions are not defined, or are presented as items from other sources; other definitions are incomplete. There are similar problems with proofs: some are riddled with citations presented without explanation, context or justification. The reader is presumed to be in a library, getting up to check a reference every fifteen minutes. This is unrealistic: a text should be something a student can take to a park and read for several hours.

So this is not a book that can be handed to a graduate student to study on their own unless that student is highly prepared. For researchers who are unfamiliar with the immediate literature and who want to understand and confirm the contents of the book, the leaps, typographical errors and over-reliance on citations are disconcerting. Its value would be greatly enhanced if it had appendices with background material (chapter-long appendices on cohomology, topological group theory, differential geometry *etc.*), complete definitions, concrete examples, and citations in proofs converted into sequences of lemmas. And an index of symbols.

There are few books in this area; the only other book I know of on this topic at this level is Leonard Charlap's *Bieberbach Groups and Flat Manifolds* (Charlap, 1986), which also begins with the Bieberbach theorems but otherwise covers a different set of topics. And Charlap's book is a quarter of a century old. However, there are other presentations of the Bieberbach results and Zassenhaus's approach; the most accessible I've found is Rolph Schwarzenberger's *N-Dimensional Crystallography* (Schwarzenberger, 1980). [A short introduction accessible to someone familiar with group theory and advanced calculus is H. Hiller's

Crystallography and Cohomology of Groups (Hiller, 1986).] Szczepański's book is a contemporary introduction to the theory of the existence and enumeration of the crystallographic groups.

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