Crystallography and Symmetry Groups

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Introduction

Crystals are assemblages of very small basic units of matter repeated periodically in 3 dimensions. The connection with group theory is that each pattern can be characterized by its symmetry group. It turns out that there are only 230 of these so-called crystallographic space groups amongst which are 22, which crystallographers prefer to regard as distinct, but which, from an abstract point of view, form 11 pairs of isomorphic groups. Thus the space groups fall into 219 isomorphism classes. The enumeration of these space groups is built upon the 14 lattices determined by Bravais. Since the enumeration is quite complicated, we here look at some of the corresponding ideas involved in the analogous 2-dimensional problem where 17 groups, no two of which are isomorphic, arise.

First recall that an isometry of the plane $\mathbb{R}^2$ is a distance- preserving mapping of R onto itself. Amongst such isometries are translations, rotations, reflections (in lines) and glide reflections. The latter being the result of an ordinary reflection in some line l followed by a translation parallel to l. Figure 1 adequately describes these movements.

Isometries of the Plane

Definition 1.4. An isometry of the plane is a distance preserving function $f : \mathbb{R}^2 \longrightarrow \mathbb{R}^2$

Here distance preserving means that for points P and Q with position vectors $\mathbf{p}$ and $\mathbf{q}$,

$|f(P)f(Q)| = |PQ|$ i.e. $|f(\mathbf{p})f(\mathbf{q})| = |pq|$

Proposition 1.5. *Let $f : \mathbb{R}^2 \longrightarrow \mathbb{R}^2$ be an isometry which fixes the origin, then F preserves scalar products and angles between vectors.*

Proof. : Let $\mathbf{u}, \mathbf{v}$ be vectors and let U, V be the points with these as position vectors. Let $f(U)$ and $f(V)$ have position vectors $\mathbf{u}' = \overrightarrow{OF(U)}$ and $\mathbf{v}' = \overrightarrow{OF(V)}$. For every pair of points, P and Q we have:

$|f(P)f(Q)| = |PQ|$, so $|\mathbf{u}' - v'|^2 = |f(U)f(V)|^2 = |UV|^2 = |u - v|^2$. Hence $|u'|^2 + |v'|^2 - 2u'.v' = |u|^2 + |v|^2 - 2u.v$.

Since $|u'| = |Of(U)| = |f(O)f(U)| = |OU| = |\mathbf{u}|$ and $|v'| = |Of(V)| = |f(O)f(V)| = |OV| = |\mathbf{v}|$

We obtain $\mathbf{u}'.\mathbf{v}' = \mathbf{u}.\mathbf{v}$, which shows that the scalar product of two position vectors is unchanged by an isometry, which fixes the origin. Similarly, angles are preserved since the angle between the vectors $\mathbf{u}'$ and $\mathbf{v}'$ is $\arccos \frac{\mathbf{u}'.\mathbf{v}'}{|\mathbf{u}'||\mathbf{u}'|} = \arccos \frac{\mathbf{u}.\mathbf{v}}{|u||u|}$.

□

Wallpaper Patterns

The 2-dimensional repeating patterns we consider are commonly called *wallpaper patterns.* By definition these are patterns in which it is possible to find a basic pattern unit repeated periodically but not ' continuously' in each of two non-parallel directions

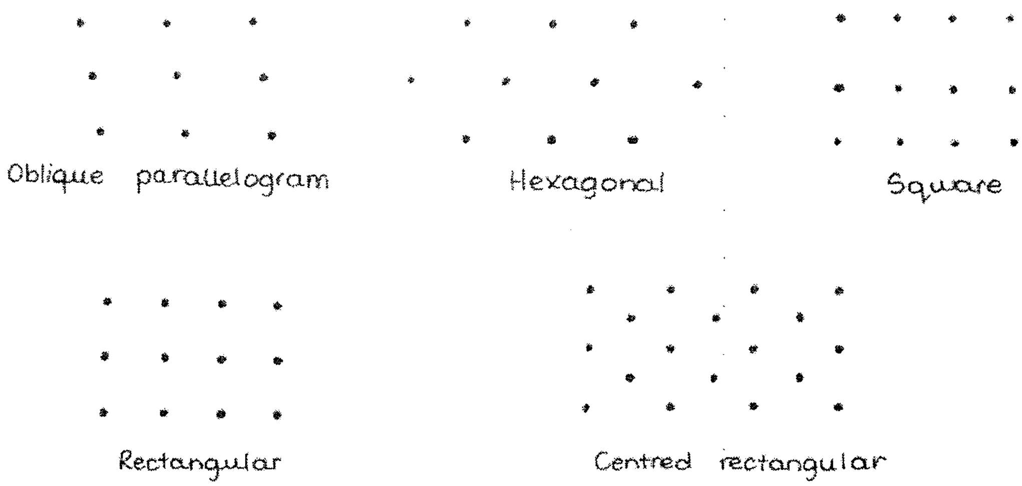
Wallpaper patterns correspond to plane symmetry groups, generated by two linearly independent translations.

The Crystallographic Restriction

Imagine you wish to tile your bathroom with only one type of tiles with the shape of a regular polygon. While this is easily possible with hexagons triangles and squares, you run into trouble with pentagons,say.

This is due to crystallographic restriction. Since the vertex angles of regular polygons are each equal to $\frac{(2n-4) \text{ right angles}}{n}$, a periodic tiling is possible only if these are integral fractions of 360^o degrees. This requires that $\frac{2n}{n-2}$ is a positive integer.

Let G be a plane symmetry group. Each rotation of G necessarily has order 1, 2, 3, 4 or 6. There are only 5 basic types of lattice, which can underlie a plane symmetry group. Lattices possessing reflectional symmetry in a line must be made up of rectangles or rhombuses. Also if a lattice has glide-reflection symmetry it is necessarily of centered rectangular type. Thus there are only 5 kinds of lattices, which these are the 2-dimensional analogues of the 14 Bravais lattices.

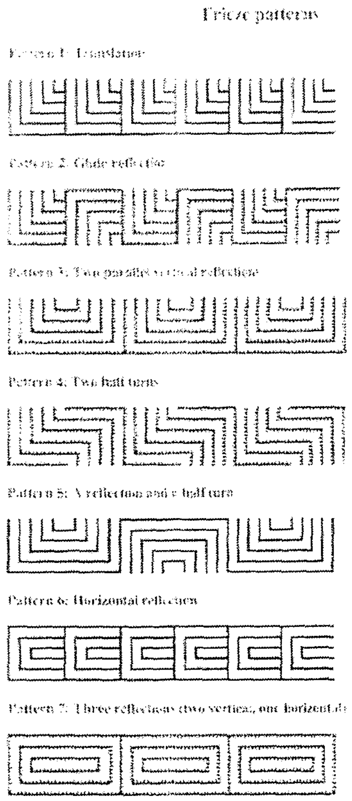


Definition 1.6. : A **2**-dimensional crystallographic point group K is a group of isometries of $\mathbb{R}$, which fixes a point P and maps a 2-dimensional lattice containing P into itself.

In any such group there can be neither translations nor glide reflections. Consequently either all the elements of K are rotations or one half of them are rotations and the other half reflections. It follows that K is isomorphic to one of the cyclic (rotational) groups C_n or one of the dihedral groups (with two orthogonal axes of rotational symmetry), D_n where $n = 1, 2, 3, 4$ or 6. Each plane group G determines a crystallographic point group as a homomorphic image.

Frieze Patterns

These are 2-dimensional repeating patterns whose symmetry groups are discrete and infinite but also leave a line in $\mathbb{R}^2$ fixed. In such groups the subgroup of translations must be isomorphic to the infinite cyclic group. There are seven distinct frieze patterns; their symmetry groups fall into four isomorphism classes.



New Models for Quasicrystals

In 1984 a group of experimentalists has discovered diffraction patterns for electrons diffracted at the atoms of an alloy composed of an Aluminium and Manganese.

The striking features are:

1. A rotational symmetry around a 10-fold axis, called 'Forbidden Symmetry' in crystallography because it cannot occur in crystals
2. Non-translational symmetry: it is not possible to construct the whole pattern by gluing together identical copies of one shape (called the 'Unit Cell' in crystallography)
3. Long-range order: One observes a well-ordered pattern, which may be extended over the entire space according to a well-defined prescription.

These observations imply that, the new object cannot be described mathematically by the laws of usual crystallography and is called Quasicrystal.

Mathematical Models for Quasicrystals

There are new mathematical models (affine extensions of noncrystallographic Coexeter groups) for quasicrystals, which use a projection from a higher dimensional periodic lattice to construct a periodic point set of lower dimensions. The vertex of particular tilings of the plane e.g. the Penrose tiling is an example of aperiodic point sets compatible with 10-fold symmetry.