4. Geometry of space: lattices and space groups

We have discussed the orthogonal group $O(n)$ and the special orthogonal group $SO(n)$ for $n = 2, 3$, which are groups of rigid motions (transformations) leaving the origin fixed. The group $SO(n)$, the rotations, consists of transformations in $O(n)$ which preserve orientation. Given a coordinate system these transformations can be written in terms of vectors and square matrices called orthogonal matrices.

We now discuss a larger groups of rigid motions which contain translations as well as orthogonal transformations. These are the group of euclidean motions $E(n)$, and the group of orientation preserving euclidean motions $E^+(n)$. We describe these groups for $n = 2$ and $n = 3$.

4.1. The Euclidean Group.

The simplest example of a rigid motion that does not leave any point fixed is a translation. A translation is a motion of the form

$$X \rightarrow X + X_0.$$ 

Translations preserve orientation so they are in $E^+(n)$.

All transformations in $E(n)$ are of the form

$$X \rightarrow AX + X_0$$

where $A$ is an orthogonal matrix. This can be thought of as a composition of two motions

(i) an orthogonal transformation, $A$, leaving the origin fixed, followed by

(ii) a translation moving the origin to $X_0$.

All transformations in $E^+(n)$ are of the form (2) where $A$ is in $SO(3)$.

Orthogonal transformations are defined as rigid motions leaving a point fixed. We can write orthogonal transformations with any fixed point $X_0$ in terms of ones leaving the origin fixed.

If $A$ leaves the origin fixed then

$$X \rightarrow A(X - X_0) + X_0$$

leaves $X_0$ fixed.

4.2. Euclidean group in dimension 2.

4.2.1. Orientation preserving transformations. Orientation preserving Euclidean transformations in dimension 2 are easy to describe. The translations have no fixed points but every other transformation does.

Every orientation preserving rigid motion in dimension 2 which is not a translation is rotation about some fixed point.

We can use complex numbers to show this and to find the fixed point. Write the transformation (2) in the form

$$z \rightarrow e^{i\theta}z + z_0$$

which is a rotation an angle of theta about the origin followed by translation by $z_0$. Assume $e^{i\theta} \neq 1$. It is easy to solve for a fixed point. Suppose $f$ is a fixed point, then by definition,

$$f = e^{i\theta}f + z_0.$$
and solving get
\[ f = \frac{z_0}{1 - e^{i\theta}}. \]
Now the transformation (4) can be written as
\[ z \rightarrow e^{i\theta}(z - f) + f \]
which is a rotation of an angle \( \theta \) about the fixed point \( f \).

4.2.2. Orientation reversing transformations. A orientation reversing euclidean transformation leaving a line fixed is called a reflection or mirror symmetry. The fixed line is called the mirror axis.

A more general type of orientation reversing transformation in dimension 2 is a glide reflection, reflection in a line followed by translation in the direction of the line (the glide axis). For example, \( z \rightarrow \bar{z} + x_0 \), where \( x_0 \) is a real number is a glide reflection in the real axis.

**Figure 1.** Illustration of a glide reflection of the letter R. The dotted line is the axis of the glide reflection.

A reflection is a special type of glide reflection where the translation vector is zero.

It can be shown that Euclidean motions in dimension 2 which are not the identity can be classified into three kinds:
- translation
- rotation
- glide reflection.

4.3. Euclidean group in dimension 3. As in dimension 2 there are translation, rotations and glide reflections. In dimension 3, there is a new type of transformation which is rotation about an axis followed by translation in a direction parallel to the axis. This is called a screw transformation, and the axis of the rotation, the fixed line, is called the screw axis. For example, all screw translations with the z axis as screw axis are of the form
\[
\begin{bmatrix}
\cos \theta & -\sin \theta & 0 \\
\sin \theta & \cos \theta & 0 \\
0 & 0 & 1
\end{bmatrix}
\begin{bmatrix}
x \\ y \\ z
\end{bmatrix}
+ \begin{bmatrix}
0 \\ 0 \\ z_0
\end{bmatrix}.
\]

The following is true but we will not prove it:

*Every orientation preserving motion in dimension 3 which is not a translation is a screw transformation about some axis.*

The proof similar to the fixed point calculation in dimension 2. It is not as easy to find the axis of an orientation preserving motion in dimension 3 as it is to find the fixed point in dimension 2. The axis can be found using Chasles’ formula, which can be derived from the fixed point formula given in the previous section. This will be discussed in a later section.
In dimension 3, glide reflection is reflection in a plane (the glide plane) followed by translation by a vector in the same plane. For example, all glide reflections with glide plane the $yz$ plane, are of the form

\[
\begin{pmatrix}
-1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
x \\
y \\
z
\end{pmatrix} + \begin{pmatrix}
0 \\
y_0 \\
z_0
\end{pmatrix}.
\]

4.4. **Lattices.**

The simplest type of rigid motion is a translation. A lattice is a group of translations. Each translation can be thought of as a vector, the vector $X_0$ in (1). A lattice in dimension 2 or 3 can be thought of as integer linear combinations of a set of 2 or 3 resp. vectors called basis vectors. We say the lattice is generated by the basis vectors. In dimension 2, for example, a lattice is the set of vectors of the form $mv + nw$ where $m$ and $n$ are integers and $v$ and $w$ are two vectors which are not parallel.

A lattice can be visualized as a set of points in space, the endpoints of all the translation vectors from the origin. The parallelogram formed by the basis vectors is called a unit cell. [Maple demo.]

4.5. **2D lattices.** Lattices are classified into different types depending on their symmetry properties. A symmetry of the lattice is a euclidean transformation leaving the lattice fixed. The symmetry of the lattice is often seen by looking at symmetry of the unit cell. Also in dimension 2 it helps to sketch a few of the fixed lines of glide reflections and fixed points of rotations leaving the lattice fixed. In dimension 3, screw axes can be sketched. We will see an example below.

Here is the classification in dimension 2.

![Lattices for Periodic Plane Patterns](chart.png)

**Chart 1.** The lattice units outlined are those chosen by crystallographers for purposes of classification. The "centered cell," containing 2 units, is shown in dotted outline on the rhombic lattice.

**Figure 2.** Types of 2 dimensional lattices
The 5 types of lattices are:
- parallelogram
- rectangular
- rhombic
- square
- hexagonal

Both rectangular and rhombic lattices have two perpendicular reflection axes of symmetry. What is the difference? See answer.

4.6. 3D lattices. The classification in dimension 3 is called the Bravais classification. There are 14 types and, as in dimension 2, the classification has to do with the symmetry properties of the lattice and the unit cell. The 14 types of 3D lattices are:
- triclinic P
- monoclinic P and C
- orthorhombic P, C, I and F
- tetragonal P and I
- cubic P, I and F
- trigonal P
- hexagonal P

We will not try to describe these here; they are described in books on crystallography or on the website. We will look at some examples from real protein crystals later.

4.7. Packing density. One concept often used in the study of proteins is packing density. The concept can be useful for visualizing proteins in space. It is often remarked that the packing density of proteins is high. This refers to the density of the atoms, which can be thought of as spheres, in the protein. Packing of the atoms in proteins resembles the densest lattice sphere packing in 3D, the face centered cubic lattice packing. Before looking at sphere packings in 3D, we look at simpler examples of circle packings in 2D.

4.7.1. Packing density in 2D. We look at two lattice circle packings in 2D. They are called lattice packings because the centers of the circles are on a lattice.

Consider the following question: Which of the following two 2D lattice packings is the densest, the square lattice circle packing (figure 3), or the hexagonal lattice circle packing, sometimes called the penny packing (figure 4)?

The first step to answer the question is to consider what is meant by density. The density of a circle packing is defined to be the percent of space covered by the circles.

To compute the density of the hexagonal and the square 2D lattice packings it is easiest to look at a segment of the packing which can be used as a repeating tile to fill the plane and find the whole packing (fig 5).

In the case of the square packing we have a square tile of area 1 and the portion covered by the circle of radius 1/2 has area $\pi/4$, so the

\[
density \text{ of square packing} = \frac{\pi}{4} \approx .78.
\]
In the case of the hexagonal packing we have an equilateral triangular tile of area $\sqrt{3}/4$ and the portion covered by the circle segments of radius $1/2$ has area $\pi/8$ so the density of hex packing is

$$\text{density of hex packing} = \frac{\pi}{2\sqrt{3}} \approx .91.$$ 

The above shows that the hexagonal packing has greater density than the square packing.

4.7.2. *Packing density in 3D.* To help understand the concept of packing density in 3D, we look at two sphere packings, one with sphere centers on the cubic lattice and one with centers on the face-centered cubic lattice.

The *cubic sphere packing* has centers of spheres on the lattice of points $(i, j, k)$ where $i, j,$ and $k$ are integers. This lattice is called the *integer lattice.* The radius of each sphere is $1/2$ so that each sphere touches 6 others. (figure 6)
Figure 5. Segments of square and hex packings that can be used as tiles to tile the plane and create the whole packing.

Figure 6. The cubic lattice packing.

The *face centered cubic* (fcc) packing has centers at each point on the lattice generated by the three vectors $(0,1,1)$, $(1,0,1)$, and $(1,1,0)$ (Figure 7). This lattice
is called the fcc lattice. It is also described as the set of points in the integer lattice whose coordinates sum to an even integer. Points in the fcc lattice are a distance $\sqrt{2}$ from 12 neighboring points, so we take spheres whose radius is $\sqrt{2}/2$. Each sphere touches 12 others.

Here is a [Maple demo] of the two packings.

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**Figure 7.** The face centered cubic lattice packing. From this perspective, the projection of the centers forms a hexagonal lattice.

Which of these two sphere packings has the greatest density? To answer this question, find tiles which can be used to create the packing, and compute the density of the spheres in one of the tiles.

For the integer lattice, space can be divided into cubes of side 1 and volume 1, each containing one sphere of radius $1/2$ and volume $\pi/6$. So

\[
\text{the density of the integer lattice sphere packing is } \pi/6 \approx .52.
\]

(Recall that the volume of a sphere of radius $r$ is $4\pi r^3/3$.)

For the f.c.c. lattice, each sphere has volume $2\pi/(3\sqrt{2})$. Now space can be tiled with cubes of side 2 and volume 8 each containing 1 sphere and 12 quarter spheres (see figure 8). Thus

\[
\text{the density of the f.c.c. lattice sphere packing is } \pi/(3\sqrt{2}) \approx .74.
\]

So the fcc lattice packing is denser than the cubic lattice packing. In fact, it is the densest sphere packing in three dimensions.

4.8. **Space groups.** A lattice is the origin together with its image under a group of translations given by lattice vectors. A lattice remains unchanged if you translate it in the directions of the lattice vectors.

When you begin with a pattern instead of a point and take repeated images of it under euclidean motions which are not simply translations, you get more complex patterns. These patterns in 2 dimensions are a good introduction to the study of space groups and crystallography. In two dimensions they are called wallpaper patterns.
Figure 8. Cross section of the face centered cubic lattice packing showing a cube with one sphere in the center and quarters of 12 others touching it. The 12 spheres have centers \((0, \pm 1, \pm 1), (\pm 1, 0, \pm 1), (\pm 1, \pm 1, 0)\) and radius \(\sqrt{2}/2\). This cube can be used as a tile to create the entire packing.

4.8.1. 2D space groups. There are 17 possible wallpaper patterns. Here is a picture of 17 different 2D patterns corresponding to the wallpaper groups from a paper by Doris Schattschneider. See also the website on wallpaper groups.

Note that each pattern is constructed by applying a few euclidean motions (the generators) repeatedly to just one part of the pattern. To construct your own patterns, have fun with [Java Kali] which will construct a wallpaper pattern from your own small pattern.

Each group is associated with a lattice symmetry type from the list. Each group has both a crystallographic name and a Conway name (see table). The Conway naming system was invented by the mathematician J. H. Conway in a paper.

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Table 1. The 14 2D space groups given in crystallographic and Conway notation. Also indicated is the lattice type associated with each group.
4.8.2. 3D space groups. Patterns corresponding to space groups in 3D are much harder to picture. There are 230 of them each associated with a 3D lattice symmetry type. Information on them can be found in crystallography tables. Here is an online table of crystallographic groups.

We look at just one of these to see how euclidean transformations are used to describe it. We consider the space group P2₁2₁2₁ commonly seen in protein crystals, for example in a protein kinase, pdb number [1AQ1]. It is generated by three screw rotations

\[
\begin{align*}
(x, y, z) &\rightarrow (1/2 + x, \ 1/2 - y, \ -z) \\
(x, y, z) &\rightarrow (-x, \ 1/2 + y, \ 1/2 - z) \\
(x, y, z) &\rightarrow (1/2 - x, \ -y, \ 1/2 + z)
\end{align*}
\]

(5)

This 3D space group is related to the 2D space group pgg. If you project a pattern in this 3D space group onto a coordinate plane, you get a pgg wallpaper pattern.

Figure 9 shows molecules crystallized in the space group P2₁2₁2₁. Can you find equations for the axes of the screw rotations given in (5) and find them on the figure above?
Answer to question in caption to figure 2: The fixed lines for symmetries of the rhombic lattice all contain lattice points. There are fixed lines for symmetries of the rectangular lattice which contain no lattice points. Also for the rectangular lattice there are four fixed points of order two rotation symmetries in a unit cell. For the rhombic lattice there are two.