

Space groups

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Definition 1 A *crystal pattern* is a set of points in \mathbb{R}^n such that the translations leaving it invariant form a (vector) lattice in \mathbb{R}^n .

Definition 2 A *space group* is a group of isometries of \mathbb{R}^n (i.e. of mappings of \mathbb{R}^n preserving all distances) which leaves some crystal pattern invariant.

A typical example of a 2-dimensional crystal pattern is displayed in Figure 1. Of course, the figure only displays a finite part of the pattern which is assumed to be infinite, but the continuation of the pattern should be clear from the displayed excerpt.

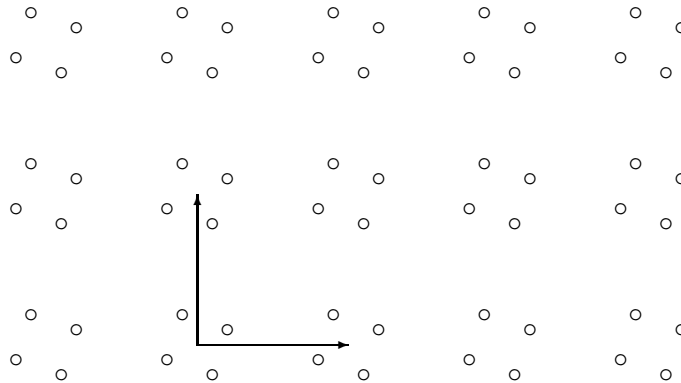


Figure 1: Crystal pattern in 2-dimensional space.

Remark: The pattern in Figure 1 was actually obtained as the orbit of some point under a space group G which in turn is just the group of isometries of this pattern. This observation already indicates that space groups can be investigated without explicit retreat to a crystal pattern, since a crystal pattern for which a space group is its group of isometries can always be constructed as the orbit of a (suitably chosen) point.

It is fairly obvious that the space group of the crystal pattern in Figure 1 contains translations along the indicated vectors and that it also contains fourfold rotations around the centers of each block of 4 points.

It is the purpose of this and the following sessions, to find an appropriate description of space groups which on the one hand reflects the geometric properties of the group elements and on the other hand allows to classify space groups under various aspects. Although the application to 2- and 3-dimensional crystal patterns is the most interesting, it costs almost no extra effort to develop the concepts for arbitrary dimensions n . We will therefore formulate most statements for general dimension n , but will illustrate them in particular for the cases $n = 2$ and $n = 3$.

1 Space group elements

Before we have a closer look at the elements of space groups, we briefly review some concepts from linear algebra.

1.1 Linear mappings

Definition 3 A linear mapping g on the n -dimensional space \mathbb{R}^n is a map that respects the sum and the scalar multiplication of vectors in \mathbb{R}^n , i.e. for which:

(i) $g(v + w) = g(v) + g(w)$ for all $v, w \in \mathbb{R}^n$;

(ii) $g(\alpha \cdot v) = \alpha \cdot g(v)$ for all $v \in \mathbb{R}^n, \alpha \in \mathbb{R}$.

Note: Since a linear mapping g respects linear combinations, it is completely determined by the images $g(v_1), \dots, g(v_n)$ on a basis (v_1, \dots, v_n) :

$$g(\alpha_1 \cdot v_1 + \alpha_2 \cdot v_2 + \dots + \alpha_n \cdot v_n) = \alpha_1 \cdot g(v_1) + \alpha_2 \cdot g(v_2) + \dots + \alpha_n \cdot g(v_n)$$

Moreover, once the images of the basis vectors are known, the image of an arbitrary linear combination $w = \alpha_1 \cdot v_1 + \alpha_2 \cdot v_2 + \dots + \alpha_n \cdot v_n$ only depends on its *coordinates* with respect to the basis.

Definition 4 Let (v_1, \dots, v_n) be a basis of \mathbb{R}^n and let $w = \alpha_1 \cdot v_1 + \alpha_2 \cdot v_2 + \dots + \alpha_n \cdot v_n$ be an arbitrary vector of \mathbb{R}^n , written as a linear combination of the basis vectors.

Then the α_i are called the *coordinates* of w with respect to the basis (v_1, \dots, v_n) and

the vector $\begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{pmatrix}$ is called the *coordinate vector* of w with respect to this basis.

Example: Choose $\left(\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \end{pmatrix} \right)$ as basis of \mathbb{R}^2 . Then the coordinate vector of $\begin{pmatrix} x \\ y \end{pmatrix}$ is $\begin{pmatrix} x - y \\ y \end{pmatrix}$, since

$$\begin{pmatrix} x \\ y \end{pmatrix} = (x - y) \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} + y \cdot \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} x - y \\ 0 \end{pmatrix} + \begin{pmatrix} y \\ y \end{pmatrix}$$

Note: If we choose the *standard basis*

$$\left(e_1 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, e_2 = \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}, \dots, e_n = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix} \right)$$

for \mathbb{R}^n , then each column vector coincides with its coordinate vector.

For every basis, the coordinate vectors of the basis are the vectors of the standard basis, since $v_i = 0 \cdot v_1 + \dots + 0 \cdot v_{i-1} + 1 \cdot v_i + \dots + 0 \cdot v_n$. Therefore it is useful to work with coordinate vectors, since that turns every basis into the standard basis.

Since linear mappings are determined by their images on basis vectors, it is very convenient to describe them by *matrices* which provide the coordinate vectors of the images of the basis vectors.

Definition 5 Let (v_1, \dots, v_n) be a basis of \mathbb{R}^n and let g be a linear mapping of \mathbb{R}^n . Then g can be described by the $n \times n$ matrix

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}$$

which has as its j -th column the coordinate vector of the image $g(v_j)$ of the j -th basis vector, i.e.

$$g(v_j) = a_{1j}v_1 + a_{2j}v_2 + \dots + a_{nj}v_n$$

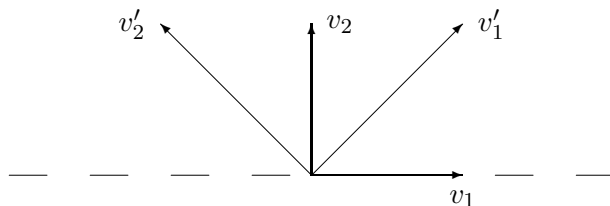
If $w = \alpha_1 \cdot v_1 + \alpha_2 \cdot v_2 + \dots + \alpha_n \cdot v_n$ is an arbitrary vector of \mathbb{R}^n , then the coordinate vector of its image under g is given by the product of the matrix A with the coordinate vector of w :

$$A \cdot \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{pmatrix} = \begin{pmatrix} \beta_1 \\ \vdots \\ \beta_n \end{pmatrix}$$

denotes that $g(w) = \beta_1 \cdot v_1 + \beta_2 \cdot v_2 + \dots + \beta_n \cdot v_n$.

Examples:

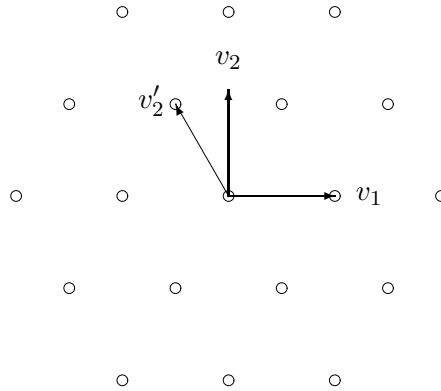
- (1) The following figure shows two bases of \mathbb{R}^2 , the first is the standard basis $\left(v_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, v_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}\right)$ the second is $\left(v'_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, v'_2 = \begin{pmatrix} -1 \\ 1 \end{pmatrix}\right)$.



We consider the linear mapping g which is the reflection in the dashed line (the x -axis). Since $v_1 \mapsto v_1, v_2 \mapsto -v_2$, with respect to the standard basis g has the matrix $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

On the other hand, we have $v'_1 \mapsto -v'_2, v'_2 \mapsto -v'_1$, hence with respect to the alternative basis, g has the matrix $\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$.

(2) The hexagonal lattice has a threefold rotation g as symmetry operation.



With respect to the standard basis (v_1, v_2) , this rotation has the matrix

$$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}.$$

However, if a symmetry adapted basis $\left(v_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, v'_2 = \begin{pmatrix} -\frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix}\right)$ is chosen, the matrix of g becomes much simpler, since $g(v_1) = v'_2$ and $g(v'_2) = -v_1 - v'_2$. The matrix of g with respect to this basis is thus

$$\begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}.$$

In the context of symmetry operations, we have to make sure that a transformation can be reversed, i.e. that it has an inverse transformation such that the composition of the two mappings is the identity operation.

Definition 6 A linear mapping g is called *invertible* if there is a linear mapping g^{-1} such that $gg^{-1} = g^{-1}g = id$, where id denotes the identity mapping leaving every vector unchanged, i.e. $id(v) = v$ for all vectors $v \in \mathbb{R}^n$.

Lemma 7 A linear mapping g is invertible if and only if the images $g(v_1), \dots, g(v_n)$ of a basis (v_1, \dots, v_n) of \mathbb{R}^n form again a basis of \mathbb{R}^n , i.e. are linearly independent.

Definition 8 The set of invertible linear mappings on \mathbb{R}^n forms a group. The group of corresponding $n \times n$ matrices is denoted by $GL_n(\mathbb{R})$ (for *general linear group*).

1.2 Affine mappings

The following argument shows that elements from space groups have to be mappings of a special kind, namely *affine mappings*:

Let o be the (chosen) origin of \mathbb{R}^n and let s be an isometry in a space group, then we denote by t the translation by the vector $s(o) - o$. Since a translation is an isometry, the mapping $s - t$ is also an isometry and by construction it fixes the origin o .

It is an elementary (but not so well-known) fact that an isometry fixing the origin actually has to be an invertible *linear* mapping g , hence the isometry s is what is called an *affine mapping*: the sum of an invertible linear mapping and a translation.

Lemma 9 Each element of a space group is the sum of an invertible linear mapping and a translation, i.e. an affine mapping.

Since the elements of space groups are affine mappings, we will now investigate in some more detail the properties of groups of affine mappings.

Definition 10 The *affine group* \mathcal{A}_n of degree n is the group of all mappings $\{g \mid t\}$ (in *Seitz* notation) consisting of a *linear part* $g \in GL_n(\mathbb{R})$ (i.e. an invertible $n \times n$ matrix) and a *translation part* $t \in \mathbb{R}^n$.

The elements of \mathcal{A}_n act as

$$\{g \mid t\}(v) := g \cdot v + t$$

on the vectors v of the vector space \mathbb{R}^n .

Note that the linear part of an element $\{g \mid t\}$ has to be an *invertible* matrix, since otherwise the element would not have an inverse.

Examples:

- (1) In dimension 2, a reflection in the line $x = y$ is given by

$$\{g \mid t\} = \left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \mid \begin{pmatrix} 0 \\ 0 \end{pmatrix} \right\}$$

which acts as

$$\left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \mid \begin{pmatrix} 0 \\ 0 \end{pmatrix} \right\} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} y \\ x \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} y \\ x \end{pmatrix}.$$

- (2) A glide reflection with shift $\frac{1}{2}$ along the x -axis is given by

$$\{g \mid t\} = \left\{ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \mid \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix} \right\}$$

and acts as

$$\left\{ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \mid \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix} \right\} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x \\ -y \end{pmatrix} + \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix} = \begin{pmatrix} x + \frac{1}{2} \\ -y \end{pmatrix}.$$

- (3) In 3-dimensional space, a fourfold screw rotation with a shift of $\frac{1}{4}$ around the z -axis is given by

$$\{g \mid t\} = \left\{ \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \mid \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix} \right\}$$

and acts as

$$\left\{ \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \mid \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix} \right\} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -y \\ x \\ z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix} = \begin{pmatrix} -y \\ x \\ z + \frac{1}{4} \end{pmatrix}.$$

Since we are only interested in isometries, we only have to deal with the subgroup of the affine group \mathcal{A}_n which consists of the elements preserving all distances. Clearly, translations keep all distances and a linear mapping is an isometry if and only if its matrix g is an *orthogonal matrix* (with respect to the standard basis), i.e. $g^{tr} \cdot g = id$.

Definition 11 The group $\mathcal{E}_n := \{\{g \mid t\} \in \mathcal{A}_n \mid g^{tr} = g^{-1}\}$ of affine mappings with orthogonal linear part is called the *Euclidean group*.

In particular, every space group is a subgroup of the Euclidean group. Before we focus on space groups, we state some important facts about the affine group, which will be used in the discussion of space groups.

1.3 Basic properties of the affine group

It is a fruitful exercise to compute the product of two affine mappings explicitly. For that, we apply the product of the two elements $\{g \mid t\}$ and $\{h \mid u\}$ to an arbitrary vector v :

$$\begin{aligned} (\{g \mid t\} \cdot \{h \mid u\})(v) &= \{g \mid t\}(h \cdot v + u) = g \cdot (h \cdot v + u) + t = gh \cdot v + g \cdot u + t \\ &= \{gh \mid g \cdot u + t\}(v). \end{aligned}$$

Lemma 12 The product of two affine mappings $\{g \mid t\}$ and $\{h \mid u\}$ is given by

$$\{g \mid t\} \cdot \{h \mid u\} = \{gh \mid g \cdot u + t\}.$$

The short computation above thus shows, that the linear parts of two affine mappings are simply multiplied, but that the translation part is not just the sum of the two translation parts, but that the translation part u of the second element is *twisted* by the action of the linear part g of the first element.

By Lemma 12 it is also easy to derive the inverse of an element, since for $\{h \mid u\}$ being the inverse of $\{g \mid t\}$ we require $h = g^{-1}$ and $g \cdot u = -t$, thus $u = -g^{-1} \cdot t$.

Lemma 13 The inverse of the affine mapping $\{g \mid t\}$ is given by

$$\{g \mid t\}^{-1} = \{g^{-1} \mid -g^{-1} \cdot t\}.$$

An important way of investigating subgroups of the affine group hinges on the fact that the linear parts are just multiplied. This means that forgetting about the translation part results in a homomorphism from the affine group to the matrix group $GL_n(\mathbb{R})$.

Theorem 14 Let Π be the mapping $\Pi : \mathcal{A}_n \rightarrow GL_n(\mathbb{R}) : \{g \mid t\} \mapsto g$ which forgets about the translation part of an affine mapping.

- (i) The mapping Π is a group homomorphism from \mathcal{A}_n onto $GL_n(\mathbb{R})$ with kernel $\mathcal{T} := \{\{id \mid t\} \mid t \in \mathbb{R}^n\}$ and image $GL_n(\mathbb{R})$.
- (ii) \mathcal{A}_n contains a subgroup isomorphic to the image $GL_n(\mathbb{R})$ of Π , namely the group $\mathcal{G} = \{\{g \mid 0\} \mid g \in GL_n(\mathbb{R})\}$ of elements with trivial translation part.

- (iii) Every element $\{g \mid t\}$ can be written as $\{g \mid t\} = \{id \mid t\} \cdot \{g \mid 0\}$, thus $\mathcal{A}_n = \mathcal{T} \cdot \mathcal{G}$. Since on the other hand the intersection $\mathcal{T} \cap \mathcal{G}$ consists only of the identity element $\{id \mid 0\}$, the affine group \mathcal{A}_n is the semidirect product $\mathcal{T} \rtimes GL_n(\mathbb{R})$ of \mathcal{T} and $GL_n(\mathbb{R})$.

The homomorphism Π can be applied to every subgroup $G \leq \mathcal{A}_n$ of the affine group, it has the group of linear parts as image and the normal subgroup of translations in G as its kernel. The homomorphism Π therefore allows to split a space group G into two parts.

Definition 15 Let G be a space group and let Π be the homomorphism defined in Theorem 14.

- (i) The translation subgroup $T := \{\{id \mid t\} \in G\}$ is the kernel of the restriction of Π to G .
- (ii) The group $P := \Pi(G)$ of linear parts in G is called the *point group* of G . It is isomorphic to the factor group G/T .

Note: In general, a subgroup $G \leq \mathcal{A}_n$ is not the semidirect product of its translation subgroup and its point group. For space groups, only the *symmorphic* groups are semidirect products, whereas groups containing e.g. glide reflections with a glide not contained in their translation subgroup do not contain their point group as a subgroup.

Exercise 1.

Prove that two affine mappings $\{g \mid t\}$ and $\{h \mid u\}$ commute (i.e. $\{g \mid t\} \cdot \{h \mid u\} = \{h \mid u\} \cdot \{g \mid t\}$) if and only if

- (i) the linear parts g and h commute;
- (ii) the translation parts fulfill $(g - id) \cdot u = (h - id) \cdot t$.

Conclude that an arbitrary affine mapping $\{g \mid t\}$ commutes with a translation $\{id \mid u\}$ if and only if u is fixed under the action of g .

1.4 Matrix notation

A very convenient way of representing affine mappings are the so-called *augmented matrices*.

Definition 16 The *augmented matrix* of an affine mapping $\{g \mid t\}$ with linear part $g \in GL_n(\mathbb{R})$ and translation part $t \in \mathbb{R}^n$ is the $(n + 1) \times (n + 1)$ matrix

$$\left(\begin{array}{c|c} g & t \\ \hline 0 \dots 0 & 1 \end{array} \right).$$

In order to apply such an augmented matrix to a vector $v \in \mathbb{R}^n$, the vector is also augmented by an additional component of value 1. The usual left-multiplication of a vector by a matrix now gives

$$\left(\begin{array}{c|c} g & t \\ \hline 0 & 1 \end{array} \right) \cdot \left(\begin{array}{c} v \\ 1 \end{array} \right) = \left(\begin{array}{c} g \cdot v + t \\ 1 \end{array} \right)$$

and ignoring the additional component yields the desired result.

We also check that the product of the augmented matrices coincides with the product of affine mappings as given in Lemma 12. By usual matrix multiplication we get:

$$\left(\begin{array}{c|c} g & t \\ \hline 0 & 1 \end{array} \right) \cdot \left(\begin{array}{c|c} h & u \\ \hline 0 & 1 \end{array} \right) = \left(\begin{array}{c|c} gh & g \cdot u + t \\ \hline 0 & 1 \end{array} \right),$$

thus the linear part of the product is gh and the translation part is $g \cdot u + t$ as required.

Note: In view of the representation of affine mappings by augmented matrices, the homomorphism Π becomes very natural, it just picks the upper left $n \times n$ submatrix of an $(n + 1) \times (n + 1)$ augmented matrix.

Examples

(1) $p4mm$

If we take as crystal pattern the lattice points of a common square lattice, the group of isometries of this pattern is the group generated by a rotation of order 4, the reflection in the x -axis and the two unit translations along the x - and y -axis. These four elements are given by the matrices

$$\left(\begin{array}{cc|c} 0 & -1 & 0 \\ 1 & 0 & 0 \\ \hline 0 & 0 & 1 \end{array} \right), \quad \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array} \right), \quad \left(\begin{array}{cc|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array} \right), \quad \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 1 \\ \hline 0 & 0 & 1 \end{array} \right).$$

(2) $c2mm$

If the crystal pattern consists of the lattice points of a rectangular lattice and the centers of the rectangles, the space group of this pattern is generated by two reflections in the x - and y -axis and translations to the centers of two adjacent rectangles. These generators are given by the matrices

$$\left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array} \right), \quad \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array} \right), \quad \left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array} \right), \quad \left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & 1 & -\frac{1}{2} \\ \hline 0 & 0 & 1 \end{array} \right).$$

(3) $P4_1$

In this example a 3-dimensional crystal pattern is assumed that in addition to the translations only allows a fourfold screw rotation which after 4 applications results in a unit translation along the z -axis. This space group is generated by the matrices

$$\left(\begin{array}{ccc|c} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & \frac{1}{4} \\ \hline 0 & 0 & 0 & 1 \end{array} \right), \quad \left(\begin{array}{ccc|c} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array} \right), \quad \left(\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array} \right), \quad \left(\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ \hline 0 & 0 & 0 & 1 \end{array} \right).$$

Exercise 2.

Two space group elements are given by the following transformations:

$$\mathfrak{g} : \begin{pmatrix} x \\ y \\ z \end{pmatrix} \rightarrow \begin{pmatrix} z + \frac{1}{2} \\ x + \frac{1}{2} \\ -y \end{pmatrix}, \quad \mathfrak{h} : \begin{pmatrix} x \\ y \\ z \end{pmatrix} \rightarrow \begin{pmatrix} -y \\ x + \frac{1}{2} \\ z + \frac{1}{2} \end{pmatrix}.$$

Determine the augmented matrices for \mathfrak{g} and \mathfrak{h} and compute the products $\mathfrak{g} \cdot \mathfrak{h}$ and $\mathfrak{h} \cdot \mathfrak{g}$.

2 Analysis of space groups

We have already noted that every space group is a subgroup of the Euclidean group \mathcal{E}_n and that it can be split into its translation subgroup T and its point group P via the homomorphism Π . We will now deduce some more properties of the point group P .

Since the observation of the following theorem is crucial for the analysis of space groups we include its proof (which is very short).

Theorem 17 Let G be a space group, let $P = \Pi(G)$ be its point group and denote by L the (vector) lattice

$$L = \{v \mid \{id \mid v\} \in T\}$$

of translation vectors in T . Then P acts on the lattice L , i.e. for $v \in L$ and $g \in P$ one has $g \cdot v \in L$.

Proof: Since T is a normal subgroup of G , conjugating the element $\left(\begin{array}{c|c} id & v \\ \hline 0 & 1 \end{array}\right)$ by an element $\left(\begin{array}{c|c} g^{-1} & t \\ \hline 0 & 1 \end{array}\right) \in G$ gives again an element of T . Working out this conjugation explicitly gives:

$$\begin{aligned} \left(\begin{array}{c|c} g^{-1} & t \\ \hline 0 & 1 \end{array}\right)^{-1} \left(\begin{array}{c|c} id & v \\ \hline 0 & 1 \end{array}\right) \left(\begin{array}{c|c} g^{-1} & t \\ \hline 0 & 1 \end{array}\right) &= \left(\begin{array}{c|c} g & -g \cdot t \\ \hline 0 & 1 \end{array}\right) \left(\begin{array}{c|c} g^{-1} & t+v \\ \hline 0 & 1 \end{array}\right) \\ &= \left(\begin{array}{c|c} id & g \cdot v \\ \hline 0 & 1 \end{array}\right) \in T. \end{aligned}$$

This shows that indeed $g \cdot v \in L$ and hence the point group P acts on the lattice L . \blacklozenge

Note: The distinction between the translation subgroup T of a space group and its translation lattice L may seem somewhat artificial, since by the mapping $\{id \mid t\} \rightarrow t$ the two groups are clearly isomorphic. However, since we multiply space group elements, but add lattice vectors, it is good practice to keep the two notions apart.

By now we have worked out that the point group P of G is a group of isometries and that it acts on the lattice L of translations in G . This means that P is a subgroup of the automorphism group

$$Aut(L) := \{g \in GL_n(\mathbb{R}) \mid g^{tr} = g^{-1}, g(L) = L\}$$

of L . From this fact we now can prove that P is a finite group.

Theorem 18 The point group P of a space group G is finite.

Proof: We fix some lattice basis (v_1, \dots, v_n) of L and assume that v_n is the longest of these basis vectors (they may of course all have the same length). Since L is a lattice, it is in particular discrete, hence it contains only finitely many vectors of length at most $\|v_n\|$. Since an automorphism of L preserves lengths, it can only permute vectors of the same length. But for a finite set of m elements there are at most $m!$ permutations, and since every element of P is determined by its action on the lattice basis, there are only finitely many possibilities for the elements of P . \blacklozenge

2.1 Transformation of a space group to a lattice basis

The observation that the point group P acts on the translation lattice L gives rise to a change of perspective:

New point of view: Instead of writing all vectors and matrices (and hence the augmented matrices) with respect to the standard basis of \mathbb{R}^n (as we did so far) it is convenient to transform the elements of a space group to a lattice basis of its translation lattice.

Lemma 19 Let G be a space group written with respect to some basis B of \mathbb{R}^n (e.g. the standard basis). Let X be the matrix of a basis transformation to a new basis B' of \mathbb{R}^n , i.e. the columns of X are the coordinate vectors of the vectors in B' with respect to the basis B .

Then writing out the conjugation by X :

$$\left(\begin{array}{c|c} X^{-1} & 0 \\ \hline 0 & 1 \end{array} \right) \left(\begin{array}{c|c} g & t \\ \hline 0 & 1 \end{array} \right) \left(\begin{array}{c|c} X & 0 \\ \hline 0 & 1 \end{array} \right) = \left(\begin{array}{c|c} X^{-1}gX & X^{-1} \cdot t \\ \hline 0 & 1 \end{array} \right)$$

shows that with respect to the new basis B' the element $\{g \mid t\}$ of G is transformed to the element

$$\{g' \mid t'\} = \{X^{-1}gX \mid X^{-1} \cdot t\}.$$

In particular, if (v_1, \dots, v_n) is a lattice basis of the translation lattice of G and X is the transformation matrix to this lattice basis, then the translation $\{id \mid v_i\}$ is transformed to

$$\{id \mid X^{-1} \cdot v_i\} = \{id \mid e_i\}$$

where e_i is the i -th unit vector having 1 in its i -th coordinate and 0 else.

Writing a space group with respect to a lattice basis (v_1, \dots, v_n) of its translation lattice L has the following consequences:

- All vectors $v \in \mathbb{R}^n$ are given as *coordinate vectors* with respect to the basis (v_1, \dots, v_n) , i.e. the coordinate vector $\begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$ denotes the vector $v = x_1v_1 + \dots + x_nv_n$.
- In particular, the translation lattice L becomes $L = \mathbb{Z}^n$, since the lattice vectors are precisely the integral linear combinations of a lattice basis.
- The translation subgroup T of G becomes $T = \{\{id \mid t\} \mid t \in \mathbb{Z}^n\}$.
- The point group P becomes a subgroup of $GL_n(\mathbb{Z})$, since the images of the vectors in the lattice basis are again lattice vectors and thus integral linear combinations of the lattice basis.

The price we pay for this transformation to a lattice basis is that the point group no longer consists of orthogonal matrices for which $g^{tr} = g^{-1}$ holds, but that they fix the *metric tensor* of the lattice basis.

Definition 20 For a basis $B = (v_1, \dots, v_n)$ the *metric tensor* of B is the matrix $F \in \mathbb{R}^{n \times n}$ of dot products of the basis vectors, i.e. $F_{ij} = v_i \circ v_j$.

If X is the matrix with v_i as i -th column, then the metric tensor is given by $F = X^{tr} \cdot X$.

Theorem 21 If a space group G is written with respect to a basis (v_1, \dots, v_n) , then the metric tensor F of this basis is invariant under transformations from the point group P of G , i.e.

$$g^{tr} F g = F \text{ for each } g \in P.$$

In particular, if G is written with respect to a lattice basis of its translation lattice, the point group elements fix the metric tensor of the lattice basis.

Proof: Let $g \in P$ be an element from the point group of G written with respect to the basis (v_1, \dots, v_n) and denote by g' the same element written with respect to the *standard basis*. Let X be the matrix of the basis transformation from the standard basis to the new basis, i.e. the matrix with v_i as i -th column. Then the rules for basis transformations state that $g = X^{-1} g' X$ and $g' = X g X^{-1}$.

For the orthogonal matrix g' we know that $g'^{tr} g' = id$ and replacing g' by $X g X^{-1}$ gives

$$g^{tr} g' = id \Rightarrow X^{-tr} g^{tr} X^{tr} X g X^{-1} = id \Rightarrow g^{tr} X^{tr} X g = X^{tr} X.$$

The metric tensor $F = X^{tr} X$ of the basis (v_1, \dots, v_n) is thus preserved by g . ◆

By a slight variation of the above proof one deduces how a metric tensor is transformed under a basis transformation.

Corollary 22 If F is the metric tensor of a basis $B = (v_1, \dots, v_n)$ and X is the basis transformation to a new basis (v'_1, \dots, v'_n) , then the metric tensor of B' is given by

$$F' = X^{tr} F X.$$

In particular, if the metric tensor F is invariant under a point group P and P is transformed to a new basis by the basis transformation X , i.e. to $P' = \{X^{-1} \cdot g \cdot X \mid g \in P\}$, then P' fixes the metric tensor $X^{tr} F X$.

Exercise 3.

Prove the above corollary, i.e. show that if $g^{tr} F g = F$ for all $g \in P$ and $P' = \{X^{-1} \cdot g \cdot X \mid g \in P\}$, then $g'^{tr} X^{tr} F X g' = X^{tr} F X$ for all $g' \in P'$.

Note: It is often the case that a space group is neither given with respect to the standard basis of \mathbb{R}^n nor with respect to a lattice basis of its translation lattice, but with respect to another convenient basis. This is for example the case for the group $c2mm$ in the examples above. The matrices there are given with respect to the (obvious) basis

$\left(\begin{pmatrix} a \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ b \end{pmatrix} \right)$, $a \neq b$ of a rectangular lattice.

In this case the point group fixes the metric tensor $\begin{pmatrix} a^2 & 0 \\ 0 & b^2 \end{pmatrix}$.

Example: In the examples above we gave the space group $c2mm$ of the centered rectangular lattice with respect to a basis of the rectangular lattice. This resulted in

translations with nonintegral coordinates. If we transform this group to the lattice basis $\left(\left(\frac{a}{2}\right), \left(\frac{a}{2}, -\frac{b}{2}\right)\right)$, the generators given above are transformed to

$$\left(\begin{array}{cc|c} 0 & 1 & 0 \\ 1 & 0 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} 0 & -1 & 0 \\ -1 & 0 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 1 \\ \hline 0 & 0 & 1 \end{array}\right).$$

Written with respect to the lattice basis, the point group fixes the metric tensor

$$\frac{1}{4} \begin{pmatrix} a^2 + b^2 & a^2 - b^2 \\ a^2 - b^2 & a^2 + b^2 \end{pmatrix}.$$

Important note: *The transformation to a lattice basis is not a standard point of view taken in crystallography. Here, one often distinguishes between primitive lattices, where the conventional cell spanned by the basis vectors contains just one lattice point and centered lattices, where it contains more than one lattice point. In a centered lattice, not all translations have integral coordinates and the translation lattice thus is actually larger than the lattice generated by the chosen basis.*

The reason for this distinction between primitive and centered lattices is that it is often convenient to work with special kinds of bases which are regarded as particularly nice and simple. In dimensions 2 and 3 it is indeed the case that for families of lattices which are contained in each other (like the cubic lattice and its centerings), one of these lattices has a particularly nice basis (such as the standard basis for the cubic lattice). Moreover, in these dimensions the primitive lattice and its centerings almost always have isomorphic automorphism groups (the only exception being the hexagonal lattice and the rhombohedral lattice as a centering of it).

However, the same is no longer true in higher dimensions. There it is often impossible to distinguish one of the lattices in a family as primitive lattice, since none of the lattices may have a basis with particular nice geometric properties.

Moreover, the automorphism groups of the lattices in one family may differ substantially, and not always the most simple one has the largest symmetry group. Two examples may illustrate this:

- In dimension 4, the standard lattice \mathbb{Z}^4 generated by the standard basis has a symmetry group of order 384. It has a sublattice of index 2 which has a symmetry group of order 1152, i.e. larger by a factor of 3. (This sublattice is the so-called root lattice of type F_4 and has the corners of the regular polytope called the 24-cell as vectors of minimal length.)
- In dimension 8 the situation is even more intriguing: The root lattice of type E_8 might be regarded as a centering of the 8-dimensional checkerboard lattice D_8 , which in turn is the sublattice of all vectors with even coordinate sum in the standard lattice \mathbb{Z}^8 . Both the standard lattice and the checkerboard lattice have a symmetry group of order 10321920, whereas the E_8 lattice has a much larger symmetry group of order 696729600.

Finally, for the interplay between the translation subgroup and the point group of a space group, it is extremely convenient to use the property that the translations are integral vectors, and we therefore will always assume that a space group is written with respect to a lattice basis.

From the perspective of classical crystallography, this may look like we are only dealing with primitive on not with centered lattices, but in our approach simply all lattices are regarded as primitive, since there is no reasonable general concept that allows to distinguish between primitive and centered lattices.

Exercise 4.

The point group P (in the arithmetic class $\overline{3}m1P$) is generated by the matrices

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

(i) Check that P fixes the metric tensor $F = \begin{pmatrix} 2a & -a & 0 \\ -a & 2a & 0 \\ 0 & 0 & b \end{pmatrix}$. It thus acts on a hexagonal lattice.

(ii) P also acts on a rhombohedral lattice, which is obtained from the above hexagonal lattice by the basis transformation

$$X = \frac{1}{3} \begin{pmatrix} -1 & 2 & -1 \\ -2 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \text{ with inverse transformation } X^{-1} = \begin{pmatrix} 0 & -1 & 1 \\ 1 & 0 & 1 \\ -1 & 1 & 1 \end{pmatrix}$$

Transform the metric tensor F of the hexagonal lattice to the metric tensor of the rhombohedral lattice (with the columns of X as lattice basis).

(iii) Transform P to the rhombohedral lattice (thus obtaining a point group P' in the arithmetic class $\overline{3}mR$) and check that the so obtained point group fixes the metric tensor computed in (ii).

2.2 Systems of nonprimitive translations

We already remarked that in general a space group is not a semidirect product of its translation subgroup and its point group, since it does not necessarily contain a subgroup isomorphic to the point group.

Example: The smallest example for a space group that is not a semidirect product is the space group G with point group of order 2 acting on a rectangular lattice such that the nontrivial element of the point group is induced by a glide reflection g :

$$g = \left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array} \right).$$

Any product of \mathfrak{g} with a translation has a translation component along the x -axis of the form $\frac{1}{2} + k$ with $k \in \mathbb{Z}$ and $\mathfrak{g}^2 = \left(\begin{array}{cc|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array} \right)$ is itself also a translation. Hence

the space group G has besides the identity element no elements of finite order and in particular no subgroup of order 2, isomorphic to its point group.

Although the point group P may not be found as a subgroup, it still plays an important role for the description of the elements of G , since P is isomorphic to the factor group G/T .

Definition 23 For a subgroup $T \leq G$, a (*right*) *coset* of T is a set of the form

$$Tg = \{tg \mid t \in T\} \text{ for some } g \in G.$$

Two cosets are either equal or disjoint.

A set $\{g_1, \dots, g_r\}$ of elements in G is called a set of *coset representatives* or *transversal* for T in G if G is the disjoint union of the cosets Tg_1, Tg_2, \dots, Tg_r , i.e. if

$$G = Tg_1 \dot{\cup} Tg_2 \dot{\cup} \dots \dot{\cup} Tg_r.$$

In the case of space groups, one has $\{id \mid v\} \cdot \{g \mid t\} = \{g \mid t+v\}$, hence all elements in a coset of T have the same linear part. This implies that every transversal of T in G has to contain each linear part of P precisely once.

Lemma 24 Every transversal of the translation subgroup T in a space group G with point group P is of the form $\{\{g \mid t_g\} \mid g \in P\}$. It contains precisely one element for each element g in the point group P of G .

Remark: A transversal of T in G is quite useful to construct (a reasonable part of) an orbit of G on \mathbb{R}^n which in general will be a crystal pattern having G as its space group. For that, choose a point $p \in \mathbb{R}^n$ and apply all elements of the transversal to p . If not all of the so obtained points are different or if two of these points differ by a lattice vector, the point p is in *special position* and its orbit may have a space group differing from G . Otherwise, the point p is in *general position* and the full orbit of p under G is obtained by translating the $|P|$ points obtained from the transversal by lattice vectors. The space group of the orbit of a point in general position is precisely G .

Example: Figure 2 below displays the orbit of the space group $G = p2gg$ which has a transversal

$$\left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array} \right), \quad \left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & -1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array} \right), \quad \left(\begin{array}{cc|c} -1 & 0 & \frac{1}{2} \\ 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array} \right), \quad \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array} \right)$$

with respect to its translation subgroup T corresponding to a rectangular lattice.

It is convenient to plot an asymmetric symbol at the positions of the orbit points instead of a point, since this allows to recognize reflections and rotations more easily.

As point p of which the orbit is calculated, we choose the point $p = \begin{pmatrix} 0.2 \\ 0.15 \end{pmatrix}$ and we plot the symbol ϕ at each position in the appropriate orientation (the point p has the symbol \blacklozenge).

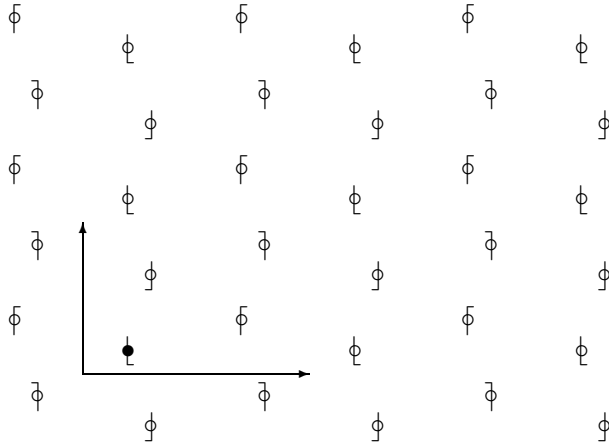


Figure 2: Orbit of a point in general position under space group $p2gg$.

Definition 25 Let $\{\{g \mid t_g\} \mid g \in P\}$ be a transversal of T in G . Then the set $\{t_g \mid g \in P\}$ of translation parts in this transversal is called a *system of nonprimitive translations* or *translation vector system* which we will abbreviate as SNoT.

Of course, the transversal and thus the SNoT is by no means unique, since each t_g may be altered by a vector from the translation lattice. This means in particular that an element t_g which lies in T can be replaced by the 0-vector.

This also explains the term 'nonprimitive translation', since one may assume that the elements of the SNoT lie inside the unit cell of the lattice, and are therefore vectors with non-integral coordinates (or 0).

From the multiplication rule of affine mappings we can deduce an important property of a SNoT.

Theorem 26 The product $\{g \mid t_g\} \cdot \{h \mid t_h\} = \{gh \mid g \cdot t_h + t_g\}$ lies in the same coset of T as the element $\{gh \mid t_{gh}\}$, therefore the elements of a SNoT conform with

$$t_{gh} = g \cdot t_h + t_g + t \text{ for some } t \in T$$

which we call the *product condition*, abbreviated as

$$t_{gh} \equiv g \cdot t_h + t_g \pmod{T}.$$

In particular, a SNoT is completely determined by its values on generators of the point group, since the value on products follows via the product condition.

If we assume that a space group is written with respect to a lattice basis, we can assume that the elements of its SNoT have coordinates $0 \leq x_i < 1$, since adjusting them by lattice vectors means to alter their coordinates by values in \mathbb{Z} . This actually makes the SNoT unique.

Definition 27 A space group G that is written with respect to a lattice basis of its translation lattice is determined by:

- the metric tensor F of the lattice basis;
- a finite group $P \leq GL_n(\mathbb{Z})$ fixing the metric tensor F ;
- a SNoT $\{t_g \mid t \in P\}$ with coordinates in the interval $[0, 1)$

The space group can then be written as:

$$G = \left\{ \left(\begin{array}{c|c} g & t_g + t \\ \hline 0 & 1 \end{array} \right) \mid g \in P, t \in \mathbb{Z}^n \right\}.$$

A space group given in this form is said to be given in *standard form*.

Exercise 5.

A space group G is generated by the elements

$$\mathfrak{g} = \left(\begin{array}{cc|c} 1 & 0 & \frac{1}{4} \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array} \right), \quad \mathfrak{h} = \left(\begin{array}{cc|c} -1 & 0 & \frac{3}{2} \\ 0 & 1 & 1 \\ \hline 0 & 0 & 1 \end{array} \right), \quad \left(\begin{array}{cc|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array} \right), \quad \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 1 \\ \hline 0 & 0 & 1 \end{array} \right).$$

The point group P of G has 4 elements, the identity element and the linear parts of \mathfrak{g} , \mathfrak{h} and $\mathfrak{g} \cdot \mathfrak{h}$.

- Determine the translation subgroup of G (which is not the standard lattice), transform G to a lattice basis of its translation lattice and write G in standard form. (Hint: \mathfrak{g}^2 and \mathfrak{h}^2 are translations.)
- The elements $\mathfrak{g} \cdot \mathfrak{h}$ and $\mathfrak{h} \cdot \mathfrak{g}$ have the same linear part. Check that their translation part only differs by a lattice vector of the translation lattice.

3 Construction of space groups

So far we have analyzed what a space group G looks like. We have seen that G contains a translation subgroup T as a normal subgroup and that the factor group by this normal subgroup is (isomorphic to) the group of linear parts of the space group, and is a finite group called the point group P . The way in which G is built from T and P is controlled by a system of nonprimitive translations.

We will now investigate the somewhat opposite problem, how for a given translation lattice L and a point group P acting on L , a space group G can be built that has translation subgroup $T \cong L$ and point group $P \cong G/T$ and what the different possibilities are.

We will always assume that we write a space group with respect to a lattice basis of its translation lattice, hence we have $L = \mathbb{Z}^n$ and $P \leq GL_n(\mathbb{Z})$.

Since we have seen that a space group is completely determined by its translation subgroup T , its point group P and a SNoT, the question boils down to finding the different possible SNoTs for a point group $P \leq GL_n(\mathbb{Z})$.

One possible solution to our question always exists, namely the trivial SNoT which has $t_g = 0$ for all $g \in P$.

Definition 28 For a given point group $P \leq GL_n(\mathbb{Z})$, the space group

$$G = \left\{ \left(\begin{array}{c|c} g & t \\ \hline 0 & 1 \end{array} \right) \mid g \in P, t \in \mathbb{Z}^n \right\}$$

with trivial SNoT is called the *symmorphic* space group with point group P . It is the semidirect product of \mathbb{Z}^n and P .

3.1 Shift of origin

Before we address the question how nontrivial SNoTs can be found, we first note a slight complication.

Example: The 1-dimensional example of the space group generated by the 'glide-reflection' $g = \left(\begin{array}{c|c} -1 & \frac{1}{2} \\ \hline 0 & 1 \end{array} \right)$ and the translation $\left(\begin{array}{c|c} 1 & 1 \\ \hline 0 & 1 \end{array} \right)$ is a space group in standard form, since $g^2 = \left(\begin{array}{c|c} 1 & 0 \\ \hline 0 & 1 \end{array} \right)$. But of course, there is nothing like a glide-reflection in 1-dimensional space, there are only two space groups, one with trivial point group and the other with a point group of order 2 and both are symmorphic.

If we check how g acts, we see that 0 is mapped to $\frac{1}{2}$ and $\frac{1}{2}$ is mapped to 0, but $\frac{1}{4}$ remains fixed. We therefore have a reflection in the point $\frac{1}{4}$ which means that our space group is indeed symmorphic, but that the origin is not chosen in a clever way.

What we have seen in the example above is that a shift of the origin alters the SNoT of a space group. We can actually compute quite easily how the SNoT is changed by a shift of the origin by a vector v . To compute how the matrices change, we have to

conjugate with the matrix $\left(\begin{array}{c|c} id & v \\ \hline 0 & 1 \end{array}\right)$:

$$\begin{aligned} \left(\begin{array}{c|c} id & -v \\ \hline 0 & 1 \end{array}\right) \left(\begin{array}{c|c} g & t_g \\ \hline 0 & 1 \end{array}\right) \left(\begin{array}{c|c} id & v \\ \hline 0 & 1 \end{array}\right) &= \left(\begin{array}{c|c} id & -v \\ \hline 0 & 1 \end{array}\right) \left(\begin{array}{c|c} g & g \cdot v + t_g \\ \hline 0 & 1 \end{array}\right) \\ &= \left(\begin{array}{c|c} g & g \cdot v + t_g - v \\ \hline 0 & 1 \end{array}\right) = \left(\begin{array}{c|c} g & t_g + (g - id) \cdot v \\ \hline 0 & 1 \end{array}\right). \end{aligned}$$

The translation part t_g from the SNoT is thus changed by $(g - id) \cdot v$.

Definition 29 A SNoT of the form $\{(g - id) \cdot v \mid g \in P\}$ for some vector v is called an *inner derivation*.

The strange term 'inner derivation' has its origin in differential geometry and is commonly used in cohomology theory. We only remark that a SNoT can actually be regarded as an element of a cohomology group.

Note: The inner derivations form a vector space, since for $t_g = (g - id) \cdot v$ and $t'_g = (g - id) \cdot v'$ we have $t_g + t'_g = (g - id) \cdot (v + v')$.

Theorem 30 A space group with SNoT $\{t_g \mid g \in P\}$ is symmorphic if and only if each t_g is of the form $t_g = (g - id) \cdot v$ for some fixed vector v , i.e. if the SNoT is an inner derivation.

If the SNoTs $\{t_g \mid g \in P\}$ and $\{t'_g \mid g \in P\}$ of two space groups with the same point group P differ only by an inner derivation (i.e. $t_g - t'_g = (g - id) \cdot v$ for some vector v), then the space groups are actually the same, only written with respect to different origins (differing by the vector v).

Example: Let P be the point group 2mm generated by

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

For a vector $v = \begin{pmatrix} x \\ y \end{pmatrix}$ we get $(g - id) \cdot v = \begin{pmatrix} 0 \\ -2y \end{pmatrix}$ and $(h - id) \cdot v = \begin{pmatrix} -2x \\ 0 \end{pmatrix}$ as inner derivations.

An arbitrary SNoT $\{t_g = \begin{pmatrix} a \\ b \end{pmatrix}, t_h = \begin{pmatrix} c \\ d \end{pmatrix}\}$ can thus be changed to $\{t'_g = \begin{pmatrix} a \\ 0 \end{pmatrix}, t'_h = \begin{pmatrix} 0 \\ d \end{pmatrix}\}$ by an inner derivation by choosing $v = \frac{1}{2} \begin{pmatrix} c \\ b \end{pmatrix}$.

Exercise 6.

Show that an inner derivation $\{t_g = (g - id) \cdot v \mid g \in P\}$ fulfills the product condition $t_{gh} \equiv g \cdot t_h + t_g \pmod T$ by showing that even the equality $t_{gh} = g \cdot t_h + t_g$ holds.

The following theorem (which is not hard to prove) states that by an appropriate shift of the origin, the coordinates of a SNoT become rational numbers with denominators at most the order $|P|$ of the point group. This immediately shows that there are only finitely many different space groups for a given point group and lattice, since there are only finitely many rational numbers $0 \leq \frac{p}{q} < 1$ with denominator at most $|P|$.

Theorem 31 Let $\{t_g \mid g \in P\}$ be the SNoT of a space group. If the origin is shifted by the vector

$$v = \frac{1}{|P|} \sum_{g \in P} t_g,$$

then for the SNoT $\{t'_g \mid g \in P\}$ with respect to the new origin one has $t'_g \in \frac{1}{|P|}\mathbb{Z}^n$, i.e. the denominators of the coordinates of each t'_g are divisors of $|P|$.

3.2 Frobenius congruences

We have seen that the different possible space groups built from T and P are determined by the different SNoTs modulo inner derivations. The possible SNoTs are restricted by:

- (1) the product condition $t_{gh} \equiv g \cdot t_h + t_g \pmod{\mathbb{Z}^n}$;
- (2) the translation part t of $\{id \mid t\}$ has to be an integral vector, i.e. $t \in \mathbb{Z}^n$.

The product condition reduces the determination of the SNoT to generators of the point group P . But even then the second restriction - although appearing fairly innocent - amounts in a seemingly infinite task:

Problem: If an arbitrary product in the generators of P gives the identity element of P , then the translation part of the corresponding product in the space group has to be an integral vector. In principle these are infinitely many different products which one would have to check.

Fortunately, the question of describing all products in the generators of a group which result in the identity is a classical problem in group theory and actually was one of the first problems to be addressed computationally. The idea is to use a *presentation* of the point group by *abstract generators* and *defining relators*.

Definition 32 A group $P = \langle g_1, \dots, g_s \rangle$ has the *presentation*

$$\langle x_1, \dots, x_s \mid r_1, \dots, r_t \rangle$$

with *abstract generators* x_i and *defining relators* $r_j = r_j(x_1, \dots, x_s)$ which are products in the x_i and their inverses x_i^{-1} , if the following hold:

- substituting g_i for x_i in the relators yields the identity element of P ;
- all products of the g_i giving the identity can be derived from the relators r_j by the following transformations:
 - insertion or deletion of a relator in a product;
 - conjugation with a generator x_i or its inverse x_i^{-1} ;
 - insertion or deletion of subterms of the form xx^{-1} and $x^{-1}x$.

Examples:

- (1) The cyclic group C_n of order n has the presentation $\langle x \mid x^n \rangle$.

(2) The symmetry group D_n of a regular n -gon has the presentation

$$\langle x, y \mid x^n, y^2, (xy)^2 \rangle$$

where x represents a rotation of order n and y a reflection.

The first two relators allow to reduce the powers of x and y by n and 2, respectively. The third relator can be read as $xy = yx^{-1}$ and allows to collect all powers of x to the left and all y to the right. The relators thus allow to reduce every product in x and y to one of the $2n$ products $x^i y^j$ with $0 \leq i < n$ and $0 \leq j < 2$. These $2n$ products correspond to the $2n$ elements of D_n .

(3) The symmetric group S_4 of all permutations of 4 symbols has the presentation

$$\langle x, y, z \mid x^2, y^2, z^2, (xy)^3, (yz)^3, (xz)^2 \rangle$$

where x, y, z represent the permutations $(1, 2), (2, 3), (3, 4)$, respectively. In this example it is slightly harder to check that the given relations are actually sufficient.

(4) The symmetry group O_h of the cube has generators

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

A presentation for this group with x and y representing g and h is given by

$$\langle x, y \mid x^6, y^4, (xyx)^2, (xy^{-1})^2 \rangle.$$

Remarks:

- (1) For a finite group it is always possible to find defining relators. For small groups this can usually be done by hand, but often it is more convenient to use standard tools from computer algebra packages.
- (2) The opposite problem, to identify a group given by a presentation is much harder. In general, it is even impossible to decide whether a product in a group given by abstract generators and defining relations is the identity element of the group.

The application of group presentations to the problem of determining SNoTs is based on the following observation.

Theorem 33 Let g_1, \dots, g_s be generators of a point group P and let $\langle x_1, \dots, x_s \mid r_1, \dots, r_t \rangle$ be a presentation of P .

Assume that $\mathfrak{g}_i = \left(\begin{array}{c|c} g_i & t_i \\ \hline 0 & 1 \end{array} \right)$ are augmented matrices for $1 \leq i \leq s$ such that substituting x_i by \mathfrak{g}_i in the relators of P gives translations with translation vector in \mathbb{Z}^n .

Then all products in the \mathfrak{g}_i which have the identity of P as linear part have translation parts in \mathbb{Z}^n .

This theorem is proved by checking that the transformations given in Definition 32 by which the products evaluating to the identity may be manipulated do not change the property of having a translation part in \mathbb{Z}^n .

Corollary 34 Let P be a point group with presentation as above and let \mathfrak{g}_i be augmented matrices such that the relators of P evaluate to translations with translation vectors in \mathbb{Z}^n .

Then, extending the translations t_i for the generators of P to all elements of P via the product condition $t_{gh} = g \cdot t_h + t_g$ gives a SNoT for P .

We are thus reduced to the problem of choosing translation parts for the generators of P such that evaluating the relators of P on these elements gives translations with integral coordinates. But this means just to solve a (finite) system of linear congruences modulo \mathbb{Z} , which are called the *Frobenius congruences*.

Definition 35 Let g_1, \dots, g_s be generators of a point group P and let $\langle x_1, \dots, x_s \mid r_1, \dots, r_t \rangle$ be a presentation of P .

Let $\mathfrak{g}_i = \left(\begin{array}{c|c} g_i & t_i \\ \hline 0 & 1 \end{array} \right)$ be augmented matrices for $1 \leq i \leq s$ where the coordinates of the translation vectors t_i are *indeterminates*.

Then evaluating the relators of P in the augmented matrices \mathfrak{g}_i and equating the result with $0 \pmod{\mathbb{Z}}$ gives rise to a system of linear congruences which are called the *Frobenius congruences*.

Every solution of the Frobenius congruences gives rise to a SNoT for P .

Since we already know that SNoTs differing only by an inner derivation represent the same space group with respect to a different origin, in order to determine the different space groups with point group P and translation lattice \mathbb{Z}^n , we only have to consider representatives of the solutions of the Frobenius congruences up to inner derivations.

To whom it may concern: We are by now heavily busy with cohomology theory. The solutions of the Frobenius congruences modulo inner derivations are nothing but the first cohomology group $H^1(P, \mathbb{R}^n / \mathbb{Z}^n)$ which is isomorphic to the second cohomology group $H^2(P, \mathbb{Z}^n)$.

Example: We consider the point group 2mm generated by

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

which has presentation $\langle x, y \mid x^2, y^2, (xy)^2 \rangle$.

Evaluating the relators on the augmented matrices

$$\mathfrak{g} = \left(\begin{array}{c|c} 1 & 0 & a \\ \hline 0 & -1 & b \\ \hline 0 & 0 & 1 \end{array} \right), \mathfrak{h} = \left(\begin{array}{c|c} -1 & 0 & c \\ \hline 0 & 1 & d \\ \hline 0 & 0 & 1 \end{array} \right)$$

gives the three matrices

$$\left(\begin{array}{c|c} 1 & 0 & 2a \\ \hline 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array} \right), \left(\begin{array}{c|c} 1 & 0 & 0 \\ \hline 0 & 1 & 2d \\ \hline 0 & 0 & 1 \end{array} \right), \left(\begin{array}{c|c} 1 & 0 & 0 \\ \hline 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array} \right).$$

The Frobenius congruences are thus

$$2a \equiv 0 \pmod{\mathbb{Z}} \quad \text{and} \quad 2d \equiv 0 \pmod{\mathbb{Z}}.$$

We have already seen that the inner derivations for this group allow to set $b = 0$ and $c = 0$, and it is indeed a good idea to first compute the inner derivations and eliminate as many of the indeterminates as there are linearly independent inner derivations before evaluating the relations.

Thus, modulo the inner derivations we have the possible solutions $a \in \{0, \frac{1}{2}\}$ and $d \in \{0, \frac{1}{2}\}$ which give rise to the following four SNoTs:

- (1) $t_g = t_h = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$: this is the symmorphic space group.
- (2) $t_g = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}$, $t_h = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$: the space group has a glide reflection along the x -axis and an ordinary reflection along the y -axis.
- (3) $t_g = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$, $t_h = \begin{pmatrix} 0 \\ \frac{1}{2} \end{pmatrix}$: the space group has an ordinary reflection along the x -axis and a glide reflection along the y -axis.
- (4) $t_g = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}$, $t_h = \begin{pmatrix} 0 \\ \frac{1}{2} \end{pmatrix}$: the space group has glide reflections along the x - and y -axis.

Exercise 7.

Compute the inner derivations and the solutions of the Frobenius congruences modulo the inner derivations for the following point groups P :

- (1) P is generated by

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

and has presentation $\langle x, y \mid x^2, y^2, (xy)^2 \rangle$.

- (2) P is generated by

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

and has presentation $\langle x, y \mid x^4, y^2, (xy)^2 \rangle$.

Example: In order to show that the concept of finding SNoTs via Frobenius congruences carries over to higher dimensions, we consider a 4-dimensional example.

The symmetry group of a regular octagon is the dihedral group of order 16, which is generated by the matrices

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

and has presentation $\langle x, y \mid x^8, y^2, (xy)^2 \rangle$. Note that representing the group by 2×2 matrices is possible, but involves irrational numbers like $\sqrt{2}$ and thus results in a non-crystallographic group.

We first determine the inner derivations. Since $g - id$ is an invertible matrix, letting v run over \mathbb{R}^4 results in $(g - id) \cdot v$ running over all vectors of \mathbb{R}^4 . Thus the translation part of g can be chosen as the 0-vector and only the translation part of h has to be considered in indeterminates.

The first relator is now superfluous. Evaluating the other two relators on the matrices

$$\mathfrak{g} = \left(\begin{array}{cccc|c} 0 & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 1 \end{array} \right), \quad \mathfrak{h} = \left(\begin{array}{cccc|c} 0 & 0 & 0 & 1 & a \\ 0 & 0 & 1 & 0 & b \\ 0 & 1 & 0 & 0 & c \\ 1 & 0 & 0 & 0 & d \\ \hline 0 & 0 & 0 & 0 & 1 \end{array} \right)$$

gives the two matrices

$$\mathfrak{h}^2 = \left(\begin{array}{cccc|c} 1 & 0 & 0 & 0 & a+d \\ 0 & 1 & 0 & 0 & b+c \\ 0 & 0 & 1 & 0 & b+c \\ 0 & 0 & 0 & 1 & a+d \\ \hline 0 & 0 & 0 & 0 & 1 \end{array} \right), \quad (\mathfrak{g}\mathfrak{h})^2 = \left(\begin{array}{cccc|c} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & a+c \\ 0 & 0 & 1 & 0 & 2b \\ 0 & 0 & 0 & 1 & a+c \\ \hline 0 & 0 & 0 & 0 & 1 \end{array} \right)$$

The Frobenius congruences are thus:

$$a + d \equiv 0 \pmod{\mathbb{Z}}, \quad b + c \equiv 0 \pmod{\mathbb{Z}}, \quad a + c \equiv 0 \pmod{\mathbb{Z}}, \quad 2b \equiv 0 \pmod{\mathbb{Z}}$$

We either have $b = 0$ which implies $c = 0, a = 0, d = 0$ or $b = \frac{1}{2}$ which implies $c = \frac{1}{2}, a = \frac{1}{2}, d = \frac{1}{2}$.

The only nontrivial SNoT is thus given by

$$t_g = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad t_h = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}.$$

3.3 Normalizer action

There is still one issue we have to consider in order to arrive at truly different space groups. So far, we have regarded the point group P as the set of linear parts of the space group G . However, these elements can be permuted by an automorphism of the point group. Since we are dealing with space groups, we can only apply such automorphisms which respect that the space group has translation lattice \mathbb{Z}^n . In particular, an automorphism has to map the standard basis of \mathbb{Z}^n to another lattice basis of \mathbb{Z}^n and therefore must be given by conjugation with an element of $GL_n(\mathbb{Z})$.

Definition 36 For a point group $P \leq GL_n(\mathbb{Z})$ the group

$$N := N_{GL_n(\mathbb{Z})}(P) := \{a \in GL_n(\mathbb{Z}) \mid a^{-1}ga \in P \text{ for all } g \in P\}$$

is called the *integral normalizer* of P .

It is the group of automorphisms of P which additionally map the lattice \mathbb{Z}^n to itself.

Remark: It can in general be a fairly difficult task to determine the integral normalizer of a point group P . However, in low dimensions the point groups are well-known groups and also their automorphisms can be computed easily. It then remains to check whether an abstract automorphism is induced by conjugation with an integral matrix.

Examples:

(1) The group $P = \{id, -id\}$ has $N = GL_n(\mathbb{Z})$ as its integral normalizer, since $\pm id$ commutes with any matrix. This shows that the integral normalizer is not necessarily a finite group. However, since the finite group P has only finitely many different automorphisms, there are only finitely many different conjugation actions on P . The subgroup of N which fixes P elementwise, i.e. for which $a^{-1}ga = g$ holds for all $g \in P$ is called the *integral centralizer* of P . It is a subgroup of finite index in the integral normalizer.

(2) The point group P generated by the matrices

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

has an integral normalizer which is generated by g, h and the additional element

$$a = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

which interchanges the two basis vectors.

Note that the group P has an abstract automorphism φ of order 3 which cyclically interchanges the elements g, h and gh . But since gh has trace -2 , whereas g and h have trace 0, an automorphism which is given by matrix conjugation has to fix gh and can only interchange g and h , since the trace is invariant under matrix conjugation.

(3) The full symmetry group P of the square lattice generated by the matrices

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

has an abstract automorphism which interchanges the two types of reflections (reflections in x - and y -axis vs. diagonal reflections). This automorphism is induced by conjugation with the matrix

$$a = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

which is an element of $GL_n(\mathbb{Q})$ but not of $GL_n(\mathbb{Z})$ and thus is not contained in the integral normalizer of P . The integral normalizer $N_{GL_2(\mathbb{Z})}(P)$ is thus just P itself.

Lemma 37 Assume that $a \in N_{GL_n(\mathbb{Z})}(P)$ and that $\{g \mid t_g\} \in G$. The action of a on $\{g \mid t_g\}$ is given by

$$\left(\begin{array}{c|c} a^{-1} & 0 \\ \hline 0 & 1 \end{array} \right) \cdot \left(\begin{array}{c|c} g & t_g \\ \hline 0 & 1 \end{array} \right) \cdot \left(\begin{array}{c|c} a & 0 \\ \hline 0 & 1 \end{array} \right) = \left(\begin{array}{c|c} a^{-1}ga & a^{-1} \cdot t_g \\ \hline 0 & 1 \end{array} \right).$$

In particular, if $g' \in P$ such that $g = a^{-1}g'a$, then conjugation by a maps $\{g \mid t_g\}$ to $\{g' \mid a^{-1} \cdot t_{g'}\}$.

The element t_g of a SNoT is thus changed by the action of a , namely according to

$$t_g \mapsto a^{-1} \cdot t_{aga^{-1}}.$$

We have just seen that transforming a space group with an element from the integral normalizer will in general change the SNoT. However, conjugation by a matrix certainly is an isomorphism of groups, and hence the space group which is obtained via the action of the integral normalizer should not be regarded as a new space group.

Important note: The integral normalizer reveals an *inherent ambiguity* in the geometric situation. In example (2) above we have seen that the integral normalizer of the group P generated by

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

contains the transformation which interchanges the two basis vectors. This means that after interchanging the basis vectors, the group P remains the same. But this means, that the two basis vectors are *geometrically indistinguishable*. The crucial point is that g and h are reflections in two perpendicular lines, but none of these lines can be distinguished geometrically as belonging to the first basis vector.

Example: We have already computed that there are four SNoTs modulo inner derivations for the point group $P = 2\text{mm}$ generated by

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

$$(1) t_g = t_h = \begin{pmatrix} 0 \\ 0 \end{pmatrix};$$

$$(2) t_g = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}, t_h = \begin{pmatrix} 0 \\ 0 \end{pmatrix};$$

$$(3) t_g = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, t_h = \begin{pmatrix} 0 \\ \frac{1}{2} \end{pmatrix};$$

$$(4) t_g = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}, t_h = \begin{pmatrix} 0 \\ \frac{1}{2} \end{pmatrix}.$$

Since the normalizer element

$$a = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

interchanges g and h , its action on the SNoTs can be seen immediately.

Applying a to the SNoTs (1) and (4) does not change them, but for the SNoT (2) with $t_g = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}, t_h = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ we get

$$t_g \mapsto a^{-1} \cdot t_{aga^{-1}} = a \cdot t_h = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad t_h \mapsto a^{-1} \cdot t_{aha^{-1}} = a \cdot t_g = \begin{pmatrix} 0 \\ \frac{1}{2} \end{pmatrix}$$

and this is precisely the SNoT (3).

The two SNoTs (2) and (3) are thus interchanged by the integral normalizer and give rise to the same space group.

Discussion: It is worthwhile to discuss this example in full detail: The point group $2mm$ is the symmetry group of a rectangular lattice. It fixes a metric tensor of the form

$$F = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}, \quad a, b > 0, a \neq b.$$

However, from the point group it can not be concluded whether $a < b$ or $a > b$, i.e. whether the first or the second basis vector is the short one. If we thus have a space group with a reflection along one of the axes and a glide reflection along the other one, we can not tell whether the glide is along the short or the long side. Thus, the two space groups with a glide for the first and for the second basis vectors are regarded as equivalent.

Note: The algorithm consisting of:

- finding the inner derivations;
- setting up and solving the Frobenius congruences;
- finding orbit representatives for the action of the integral normalizer modulo the inner derivations

was described by H. Zassenhaus in 1948 and is therefore often called the *Zassenhaus algorithm*.

Exercise 8.

A certain point group P (known as $m\bar{3}$) is generated by

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

and has presentation $\langle x, y \mid x^6, y^2, (xy)^3, (x^3y)^2 \rangle$.

Since $g - id$ is invertible, $(g - id) \cdot v$ runs over all vectors in \mathbb{R}^3 , hence by a shift of origin the translation part of g may be assumed to be 0.

The integral normalizer of P contains the matrix $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$ which interchanges the

second and third basis vector.

Determine the solutions of the Frobenius congruences for P (assuming that $t_g = 0$) and check which of the resulting SNoTs lie in one orbit under the integral normalizer of P .

4 Space group classification

In this section we will consider various aspects under which space groups may be grouped together. We will start with the finest notion of equivalence, which are the *space group types* and will end with the coarsest, the notion of *crystal family*.

4.1 Space group types

By the approach via translation lattices and point groups which are glued together to a space group via a SNoT, we can (in principle) determine all space groups up to isomorphism, provided the possible lattices and point groups are known.

By a famous theorem of Bieberbach (1911) isomorphism of space groups is the same as affine equivalence.

Theorem 38 Two space groups in n -dimensional space are isomorphic if and only if they are conjugate by an affine mapping from \mathcal{A}_n .

In crystallography, usually a slightly different notion of equivalence than affine equivalence is used. Since crystals occur in physical space and physical space can only be transformed by orientation preserving mappings, space groups are only regarded as equivalent if they are conjugate by an *orientation preserving* affine mapping, i.e. by an affine mapping that has linear part with positive determinant.

Definition 39 Two space groups are said to belong to the same *space group type* if they are conjugate under an orientation preserving affine mapping.

Thus, although space groups generated by a fourfold right-handed screw and by a fourfold left-handed screw are clearly isomorphic, they do not belong to the same space group type.

Definition 40 Two space groups G and G' are said to form an *enantiomorphic pair* if they are conjugate under an affine mapping, but not under an orientation preserving affine mapping.

If G is the group of isometries of some crystal pattern, then its enantiomorphic counterpart G' is the group of isometries of the mirror image of this crystal pattern.

The number of space group types is thus the number of isomorphism classes plus the number of enantiomorphic pairs. For dimensions up to 6, these numbers are displayed in Table 1.

dimension	1	2	3	4	5	6
isomorphism classes	2	17	219	4783	222018	28927922
enantiomorphic pairs	0	0	11	111	79	7052
space group types	2	17	230	4894	222097	28934974

Table 1: Number of space group types in dimensions up to 6.

4.2 Arithmetic classes

Starting from the space groups, it is natural to collect those space groups together which only differ by their SNoTs. Assuming that the space groups are given in standard form, i.e. with respect to a lattice basis of their translation subgroups, this means that two groups are regarded as equivalent if they only differ by the choice of the lattice basis.

Definition 41 Two space groups lie in the same *arithmetic class* if their point groups P and P' are conjugate by an integral basis transformation, i.e. if $P' = \{X^{-1}gX \mid g \in P\}$ for some $X \in GL_n(\mathbb{Z})$.

We will also say that two point groups $P, P' \leq GL_n(\mathbb{Z})$ lie in the same arithmetic class if they are conjugate by a matrix in $GL_n(\mathbb{Z})$.

Point groups in the same arithmetic class act on the same lattice and differ only by the choice of the lattice basis.

The numbers of arithmetic classes of space groups are given in Table 2.

dimension	1	2	3	4	5	6
arithmetic classes	2	13	73	710	6079	85311

Table 2: Number of arithmetic classes in dimensions up to 6.

We have seen that the point group P of a space group G is a subgroup of the full automorphism group $Aut(L)$ of the translation lattice L of G . But $Aut(L)$ is a finite subgroup of $GL_n(\mathbb{Z})$, hence it is a point group itself, namely of the symmorphic space group with point group $Aut(L)$ and translation lattice L .

This shows that some of the arithmetic classes are distinguished, because their groups are full automorphism groups of their lattices, while others are proper subgroups.

Definition 42 A point group P acting on a lattice L is called a *Bravais group* if it is the full automorphism group of L .

The arithmetic class containing P is then called a *Bravais class*.

Since the groups in one Bravais class act on the same lattice, but groups from different Bravais classes act on different lattices, the Bravais classes correspond to the different *Bravais types of lattices* or *lattice types* for short.

There are now two obvious directions in which arithmetic classes can be merged into larger classes. The word 'direction' can be taken literally, if groups are considered to be positioned in a plane, where groups of the same order are on the same horizontal level and subgroups thus lie below their supergroups.

Vertically: Starting with a Bravais group P , we can join the arithmetic class of P with the arithmetic classes of its subgroups. However, since P acts on a particular lattice, we will only consider those subgroups of P which do not act on a *more general* lattice, i.e. on a lattice which has a smaller Bravais group than P .

This direction of joining arithmetic classes leads to the notion of *Bravais flocks*.

Horizontally: Suppose that P is a point group acting on some lattice L . We assume as always that P is written with respect to a lattice basis of L , thus $P \leq GL_n(\mathbb{Z})$. But P also acts on other lattices than L , obvious examples are scalings like $2L$, $3L$, or $\frac{1}{2}L$. The interesting cases are those lattices L' which lie between L and one of its scalings, these are the *centerings* of L .

In general, the action of P on L' gives rise to a point group P' which does not lie in the same arithmetic class as P , but is isomorphic with P' and it is worthwhile to join the arithmetic classes of P and P' .

This direction of joining arithmetic classes leads to the notion of *geometric classes*.

4.3 Bravais flocks

We have already seen that a lattice can be characterized by its metric tensor containing the dot products of a lattice basis. If a point group P acts on a lattice L , it fixes the metric tensor of L . However, a point group in general fixes not only a single metric tensor (or multiples thereof), but it actually fixes all metric tensors from a vector space.

Definition 43 Let $P \leq GL_n(\mathbb{Z})$ be a finite integral matrix group. Then

$$\mathcal{F}(P) := \{F \in \mathbb{R}^{n \times n} \mid F = F^{tr}, g^{tr} F g = F \text{ for all } g \in P\}$$

is called the *space of metric tensors* of P .

The dimension of $\mathcal{F}(P)$ is called the *number of parameters* for the metric tensors of P .

If P is generated by the matrices g_1, \dots, g_r , the space $\mathcal{F}(P)$ of metric tensors can be computed as the space of solutions of a system of linear equations in the entries of F , namely

$$g_i^{tr} F g_i - F = 0, \quad 1 \leq i \leq r.$$

Examples:

(1) Let $P = 2\text{mm}$ be the group generated by

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

and let $F = \begin{pmatrix} a & c \\ c & b \end{pmatrix}$. Then

$$\begin{aligned} g^{tr} F g - F &= \begin{pmatrix} a & -c \\ -c & b \end{pmatrix} - \begin{pmatrix} a & c \\ c & b \end{pmatrix} = \begin{pmatrix} 0 & -2c \\ -2c & 0 \end{pmatrix}, \\ h^{tr} F h - F &= \begin{pmatrix} a & -c \\ -c & b \end{pmatrix} - \begin{pmatrix} a & c \\ c & b \end{pmatrix} = \begin{pmatrix} 0 & -2c \\ -2c & 0 \end{pmatrix}, \end{aligned}$$

hence $c = 0$ and a and b are arbitrary, thus the number of parameters is 2 and

$$\mathcal{F}(P) = \left\{ \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} \mid a, b \in \mathbb{R} \right\}.$$

This space of metric tensors characterizes the rectangular lattice.

(2) Let $P = 4$ be the group generated by $g = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ and let $F = \begin{pmatrix} a & c \\ c & b \end{pmatrix}$.
Then

$$g^{tr} F g - F = \begin{pmatrix} b & -c \\ -c & a \end{pmatrix} - \begin{pmatrix} a & c \\ c & b \end{pmatrix} = \begin{pmatrix} b-a & -2c \\ -2c & b-a \end{pmatrix},$$

hence $c = 0$ and $a = b$ is arbitrary, thus the number of parameters is 1 and

$$\mathcal{F}(P) = \left\{ \begin{pmatrix} a & 0 \\ 0 & a \end{pmatrix} \mid a \in \mathbb{R} \right\}.$$

This space of metric tensors characterizes the square lattice.

The space of metric tensors is useful to decide whether a subgroup of a Bravais group acts on a more general lattice than the Bravais group. For example, the group 4 from example (2) above has the same space of metric tensors as the Bravais group 4mm of the square lattice. However, the subgroup 2 of 4 (generated by g^2) has a space of metric tensors of dimension 3. It acts on the oblique lattice, which is more general than the square lattice.

Definition 44 Let P be a Bravais group. Then the *Bravais flock* of P consists of the arithmetic classes of subgroups of P , which have the same space of metric tensors as P .

The Bravais flocks collect together those arithmetic classes which genuinely act on the same lattice. They are thus in correspondence with the lattice types and Bravais classes, since each Bravais flock contains exactly one Bravais class. The numbers of Bravais flocks, and thus also of Bravais classes and lattice types are given in Table 3.

dimension	1	2	3	4	5	6
lattice types	1	5	14	64	189	841

Table 3: Number of lattice types in dimensions up to 6.

4.4 Geometric classes

Let P be a point group acting on a lattice L and written with respect to a lattice basis of L . Assume that P also acts on a lattice L' which is different from L and let X be the transformation matrix from the lattice basis of L to a lattice basis of L' . Written with respect to that basis of L' the action of P is given by

$$P' = \{X^{-1}gX \mid g \in P\}.$$

Since $L \neq L'$, we have that $X \notin GL_n(\mathbb{Z})$, but clearly $X \in GL_n(\mathbb{R})$.

Definition 45 Two space groups lie in the same *geometric class* if their point groups P and P' are conjugate by a real basis transformation, i.e. if $P' = \{X^{-1}gX \mid g \in P\}$ for some $X \in GL_n(\mathbb{R})$.

We will also say that two point groups $P, P' \leq GL_n(\mathbb{Z})$ lie in the same geometric class if they are conjugate by a matrix in $GL_n(\mathbb{R})$.

Point groups in the same geometric class are the actions of a matrix group on different lattices.

Historically, the geometric classes in dimension 3 were determined much earlier than the space groups, because they can be obtained from the face normals of crystal faces and thus describe the morphological symmetry of macroscopic crystals.

The numbers of geometric classes of space groups are given in Table 4.

dimension	1	2	3	4	5	6
geometric classes	2	10	32	227	955	7104

Table 4: Number of geometric classes in dimensions up to 6.

Note: It is common to speak of the geometric classes as the *types of point groups*. This emphasizes the point of view to regard a point group as the group of linear parts of a space group, written with respect to an *arbitrary basis* of \mathbb{R}^n (not necessarily a lattice basis).

Starting with the space group types, we therefore get the classification into arithmetic classes if we keep the information about the point groups **and** lattices and forget about the SNoTs, and we get the classification into geometric classes if we also forget about the lattices, thus keeping only the point group information:

$$\text{space group types} \xrightarrow{\text{forget SNoT}} \text{arithmetic classes} \xrightarrow{\text{forget lattice}} \text{geometric classes}$$

Diagram of arithmetic classes

In Figure 3 the subgroup diagram of arithmetic classes in the hexagonal crystal family (we will explain this term below) in dimension 3 is displayed.

This diagram illustrates the different possibilities of moving between arithmetic classes discussed so far:

- the boxes represent the arithmetic classes;
- the thick boxes represent the Bravais classes;
- if boxes are joined by a line, the lower group is a maximal subgroup of the higher group;
- the Bravais flock of a Bravais class consists of those boxes which can be joined by a chain to the box of the Bravais class (note that in this diagram all groups have spaces of metric tensors of dimension 2);
- boxes which are directly joined together lie in the same geometric class and are thus actions of the same group on different lattices;
- for the sake of clearness, some boxes are slightly lowered (the boxes with symbols ending on \mathbb{R}) in order to emphasize that the action is on a *different* lattice.

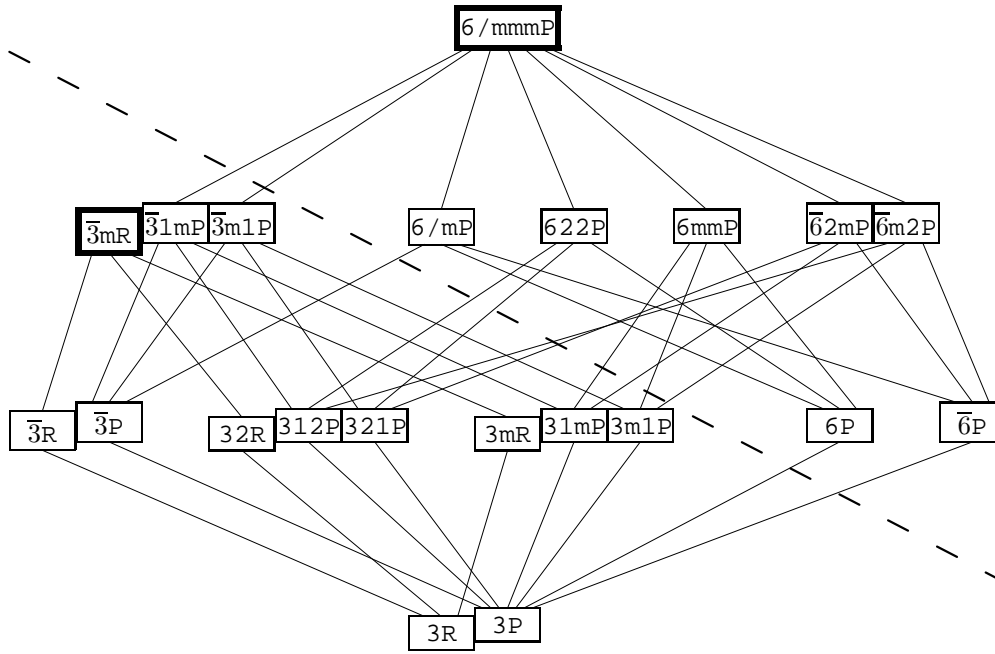


Figure 3: Arithmetic classes in the hexagonal crystal family.

In particular, we can read off that the 21 arithmetic classes fall into 12 geometric classes and 2 Bravais flocks, the Bravais flock of Bravais class $6/mmmP$ contains all arithmetic classes with symbols ending on P and contains the groups genuinely acting on a hexagonal lattice, the Bravais flock of Bravais class $3mR$ contains all classes with symbols ending on R and contains the groups acting on a rhombohedral lattice.

4.5 Lattice systems

The idea by which arithmetic classes are joined into geometric classes can analogously be applied to Bravais classes and Bravais flocks. If two Bravais groups for different lattices are conjugate by a basis transformation $X \in GL_n(\mathbb{R})$, the corresponding Bravais flocks may be joined into a larger class.

Definition 46 Two Bravais flocks are said to belong to the same *lattice system* if their Bravais classes belong to the same geometric class.

Analogously, we will say that two lattice types belong to the same lattice system if their Bravais groups belong to the same geometric class.

On the one hand every lattice system contains a Bravais class, on the other hand all the Bravais classes in a lattice system lie in the same geometric class, hence there are as many lattice systems as there are geometric classes containing Bravais classes.

Definition 47 A geometric class is called a *holohedry* if at least one of the arithmetic classes contained in it is a Bravais class.

Every holohedry belongs to precisely one lattice system and every lattice system contains precisely one holohedry.

Note: In the hexagonal crystal family displayed in Figure 3 every lattice system consists just of a single Bravais flock, since both holohedries contain only one Bravais class. This is not a typical situation, usually a holohedry contains more than one Bravais class the Bravais flocks of which are then joined into a lattice system.

The numbers of lattice systems are given in Table 5.

dimension	1	2	3	4	5	6
lattice systems	1	4	7	33	57	220

Table 5: Number of lattice systems in dimensions up to 6.

4.6 Crystal systems

For the geometric class of a point group P , the arithmetic classes contained in it determine on which lattices P acts. A further possibility to classify point groups therefore is given by joining those geometric classes which act on the same set of lattices.

Definition 48 Two geometric classes belong to the same *crystal system* if the arithmetic classes contained in them belong to the same set of Bravais flocks.

Example: In the hexagonal crystal family displayed in Figure 3, the dashed line separates the two crystal systems. The geometric classes below the dashed line act both on the hexagonal and on the rhombohedral lattice, this crystal system is called the *trigonal crystal system*. The geometric classes above the dashed line only act on the hexagonal lattice and belong to the *hexagonal crystal system*.

A crystal system can contain at most one holohedry, and in the example above it does so. Indeed, all crystal systems in dimensions up to 4 contain a holohedry, but for higher dimensions this is no longer true.

Figure 4 displays a part of the arithmetic classes in a crystal family in 5-dimensional space. There are six Bravais classes, indicated by the bold boxes and only the geometric classes in the oval frame act on all the six different lattices, whereas the holohedries only act on four or two of the different lattices.

The numbers of lattice systems are given in Table 6.

dimension	1	2	3	4	5	6
crystal systems	1	4	7	33	59	251

Table 6: Number of crystal systems in dimensions up to 6.

Note that in dimension 6 there are already 31 crystal systems that do not contain a holohedry (251 crystal classes vs. 220 holohedries).

4.7 Crystal families

The coarsest classification level for space groups (and point groups) collects all arithmetic classes together which can be reached by moving inside Bravais flocks and inside geometric classes.

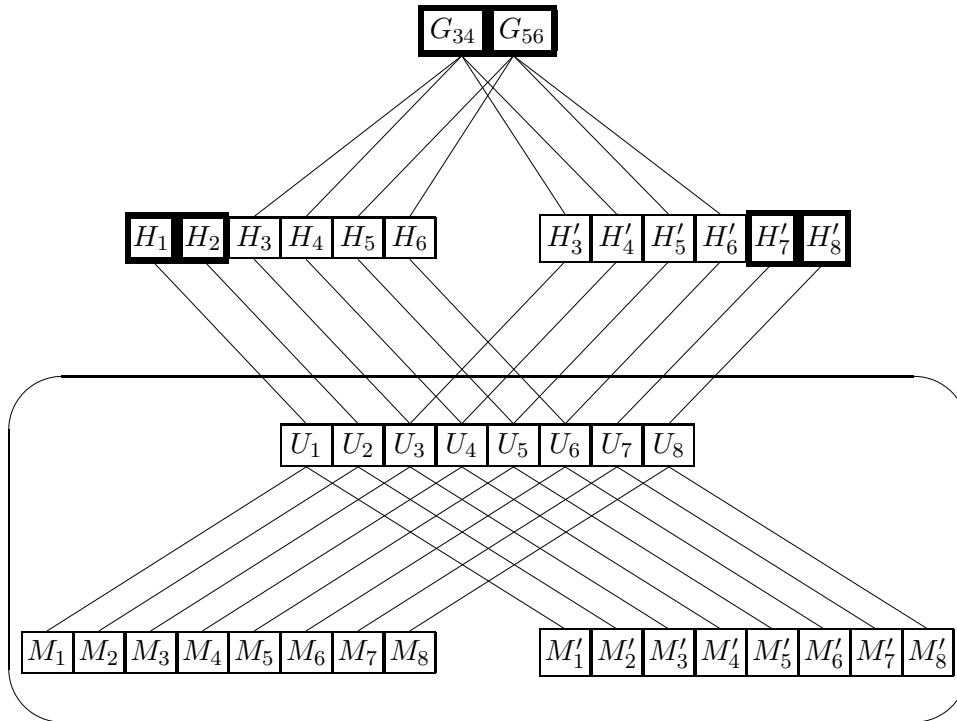


Figure 4: Crystal system without a holohedry in 5-dimensional space.

Definition 49 The *crystal family* of a space group G is the smallest set of arithmetic classes containing G which contains full Bravais flocks and full geometric classes.

Thus, if we graph all arithmetic classes of dimension n in the way shown in Figures 3 and 4, the crystal families are the connected components if we regard boxes joined by lines or directly joined as being linked.

The numbers of crystal families are given in Table 7.

dimension	1	2	3	4	5	6
crystal families	1	4	6	23	32	91

Table 7: Number of crystal families in dimensions up to 6.

Up to dimension 3 it seems exceptional that a crystal family splits into different crystal systems, since the only instance of this phenomenon is the splitting of the hexagonal crystal family into the trigonal and the hexagonal crystal systems. However, in higher dimensions it becomes rare that a crystal family consists of a single crystal system, hence this is actually the exceptional case and the splitting into several crystal systems is the rule.

Summary

We finish this section by collecting together the numbers of classes on the different classification levels for dimensions up to 6 in Table 8.

dimension	1	2	3	4	5	6
crystal families	1	4	6	23	32	91
lattice systems	1	4	7	33	57	220
crystal systems	1	4	7	33	59	251
lattice types	1	5	14	64	189	841
geometric classes	2	10	32	227	955	7104
arithmetic classes	2	13	73	710	6079	85311
space group types	2	17	230	4894	222079	28934974

Table 8: Number of classes on different classification levels in dimensions up to 6.

Some useful literature

- T. Hahn (ed.), *International Tables for Crystallography, Vol. A, 5th ed.*, Springer, Dordrecht, 2005.
- H. Zassenhaus, *Über einen Algorithmus zur Bestimmung der Raumgruppen*, Comm. Math. Helv. 21, pp. 117-141, 1948.
- T. Janssen, *Crystallographic Groups*, North-Holland, Amsterdam, 1973.
- J. Opgenorth, W. Plesken, T. Schulz, *Crystallographic Algorithms and Tables*, Acta Cryst. A54, pp. 517-531, 1998.
- B. Souvignier, *Enantiomorphism of crystallographic groups in higher dimensions with results in dimensions up to 6*, Acta Cryst. A59, pp. 210-220, 2003.