

MaThCryst summer school

15-20 July 2007, Havana, Cuba

Space groups

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.

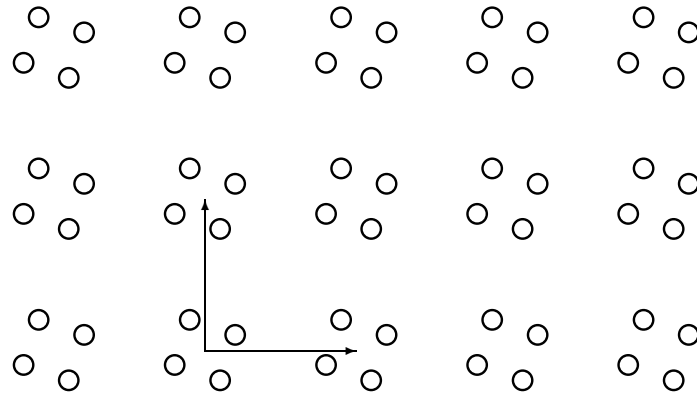


Figure 1: Crystal pattern in 2-dimensional space.

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.

Overview of today

- Space group elements
- Analysis of space groups
- Construction of space groups
- Space group classification

Space group elements

- Linear mappings
- Affine mappings
- Basic properties of the affine group
- Matrix notation

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) :

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

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 $v_i = 0 \cdot v_1 + \dots + 0 \cdot v_{i-1} + 1 \cdot v_i + \dots + 0 \cdot v_n$.

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

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

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

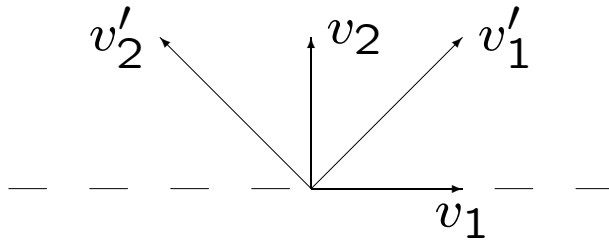
$$g(v_j) = a_{1j}v_1 + a_{2j}v_2 + \dots + a_{nj}v_n$$

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

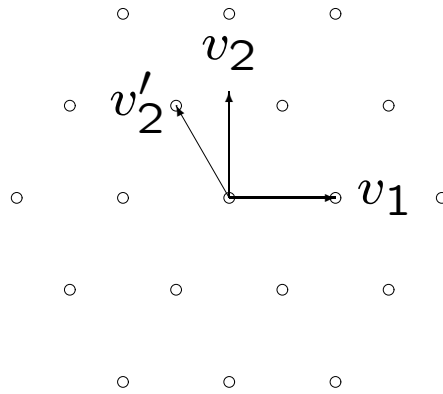
Example 1: Linear mapping g : reflection in the dashed line (the x-axis).
Two bases of \mathbb{R}^2 : The first is the standard basis $\left(v_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, v_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}\right)$,
the second is an alternative basis $\left(v'_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, v'_2 = \begin{pmatrix} -1 \\ 1 \end{pmatrix}\right)$.



W.r.t. the standard basis, g has the matrix $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

W.r.t. the alternative basis, g has the matrix $\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$.

Example 2: The hexagonal lattice has a threefold rotation g as symmetry operation.



W.r.t. the standard basis (v_1, v_2) , this rotation has the matrix $\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$.

W.r.t. the symmetry adapted basis $\left(v_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, v'_2 = \begin{pmatrix} -\frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix} \right)$, the matrix of g is much simpler, namely $\begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$.

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*).

Affine mappings

Let o be the 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 .

Fact: An isometry fixing the origin 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.

Definition 10 The *affine group* \mathcal{A}_n of degree n is the group of all mappings $\{g \mid t\}$ 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 .

Example 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

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

Example 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

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

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

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

and acts as

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

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*.

Basic properties of the affine group

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

$$\{g \mid t\} \cdot \{h \mid u\} = \{gh \mid g \cdot u + t\}, \text{ since}$$

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

Thus, the linear parts are simply multiplied, but the translation part is not just the sum of the two translation parts, but the translation part u of the second element is *twisted* by the action of the linear part g of the first element.

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

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

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 $GL_n(\mathbb{R})$.

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 .

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

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

To apply an augmented matrix to a vector $v \in \mathbb{R}^n$, the vector is also augmented by an additional component 1. The usual left-multiplication of a vector by a matrix gives the required action (by ignoring the additional component):

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

Also, the product of affine mappings is represented correctly:

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

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.

Example 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

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

Example 2: $c2_{mm}$

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

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

Example 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

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

Exercise 2.

Two space group elements are given by the following transformations:

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

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

Analysis of space groups

- Transformation of a space group to a lattice basis
- Systems of nonprimitive translations

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:

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

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 $Aut(L)$ of L , given by

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

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

Transformation of a space group to a lattice basis

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

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

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) .
- 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.

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 $g' \in P'$.

Example: In the examples above we gave the space group $c2_{mm}$ 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

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

Exercise 4.

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

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

(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 $\bar{3}_mR$) and check that the so obtained point group fixes the metric tensor computed in (ii).

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 :

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

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

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

Lemma 24 Since $\{id \mid v\} \cdot \{g \mid t\} = \{g \mid t + v\}$, all elements in a coset of T have the same linear part. Hence, every transversal of the translation subgroup T in a space group G with point group P is of the form

$$\{\{g \mid t_g\} \mid g \in P\}.$$

Remark: A transversal of T in G is very 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 $p \in \mathbb{R}^n$ in general position and apply all elements of the transversal to p . 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 \downarrow at each position in the appropriate orientation (the point p has the symbol \bullet).

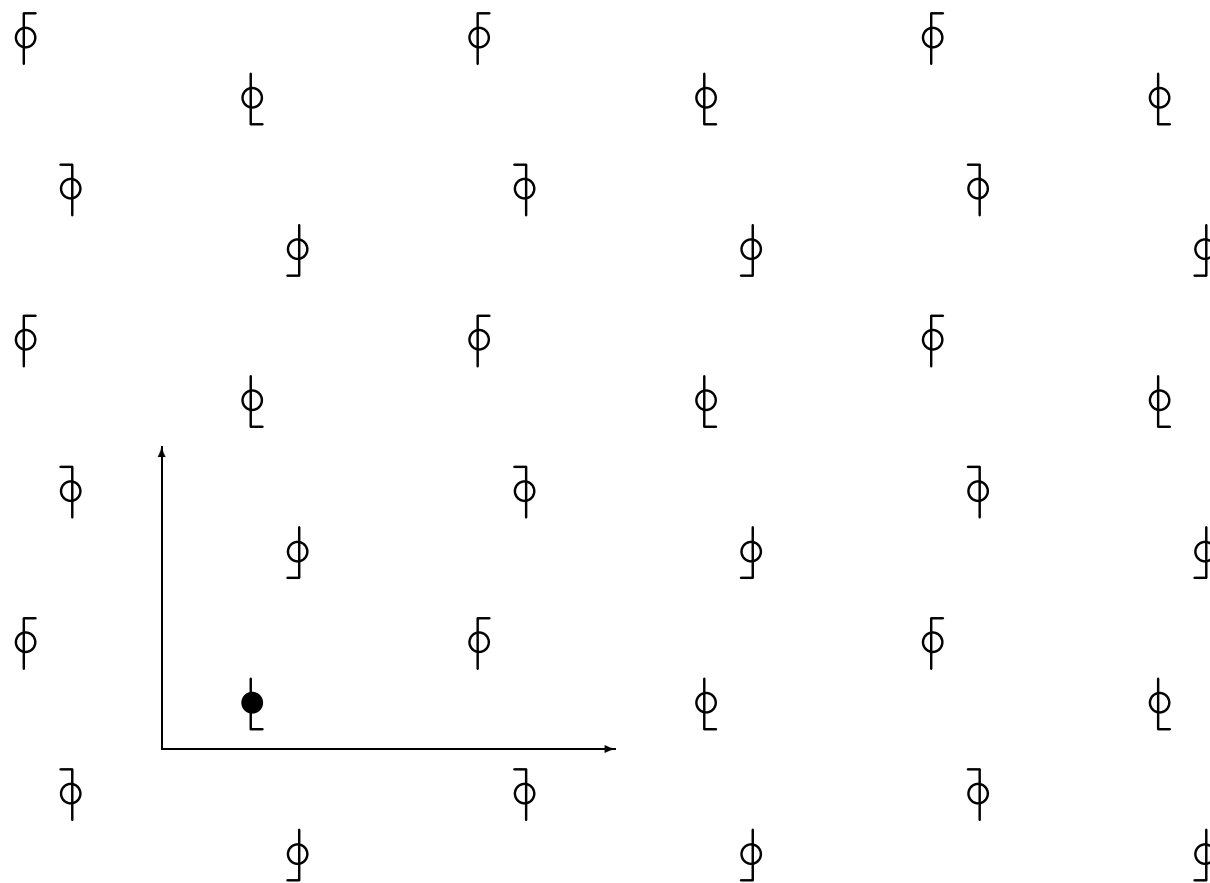


Figure 2: Orbit of a point in general position under space group $p2gg$.

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.

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

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

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 $0 \leq x_i < 1$.

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

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

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

- (i) 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: g^2 and h^2 are translations.)
- (ii) The elements $g \cdot h$ and $h \cdot g$ have the same linear part. Check that their translation part only differs by a lattice vector of the translation lattice.

Construction of space groups

- Shift of origin
- Frobenius congruences
- Normalizer action

We will now investigate 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.

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 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 .

Shift of origin

Complication: 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 $g^2 = \left(\begin{array}{c|c} 1 & 0 \\ \hline 0 & 1 \end{array} \right)$.

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.

To compute how a shift of origin by v alters the SNoT, 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*.

Theorem 30 A space group with SNoT $\{t_g \mid g \in P\}$ is symmmorphic 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 2_{mm} 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 derivation.

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.

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 $|P|$.

As a consequence, 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 $|P|$.

Frobenius congruences

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. $t \in \mathbb{Z}^n$.

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.

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 $x^{-1}x$.

Example 1: The cyclic group C_n of order n has the presentation $\langle x \mid x^n \rangle$.

Example 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.

Example 3: 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

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

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 .

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 .

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 $g_i = \left(\begin{array}{c|c} g_i & t_i \\ \hline 0 & 1 \end{array} \right)$ 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 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 2_{mm} 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

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

gives the following three matrices:

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

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 $c = 0$.

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 $\langle x, y \mid x^8, y^2, (xy)^2 \rangle$.

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

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

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

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

Normalizer action

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.

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.

Example 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.

Example 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 can not be realized by matrix conjugation.

Example 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

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

Transforming a space group with an element from the integral normalizer will in general change the SNoT, but results in an isomorphic space group which is not regarded as a new 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

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

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: The group 2_{mm} is the point 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 .

Space group classification

- Space group types
- Arithmetic classes
- Bravais flocks
- Geometric classes
- Lattice systems
- Crystal systems
- Crystal families

Space group types

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.

Arithmetic classes

Starting from the space groups, it is natural to collect those space groups together which only differ by their SNoTs.

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.

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.

Vertically: Starting with a Bravais group P , we can join the arithmetic class of P with the arithmetic classes of its subgroups. However, 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.

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 .

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

Bravais flocks

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 .

Example 1: Let $P = 2mm$ 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

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

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

hence $c = 0$ and a and b are arbitrary. 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.

Example 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.

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.

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).

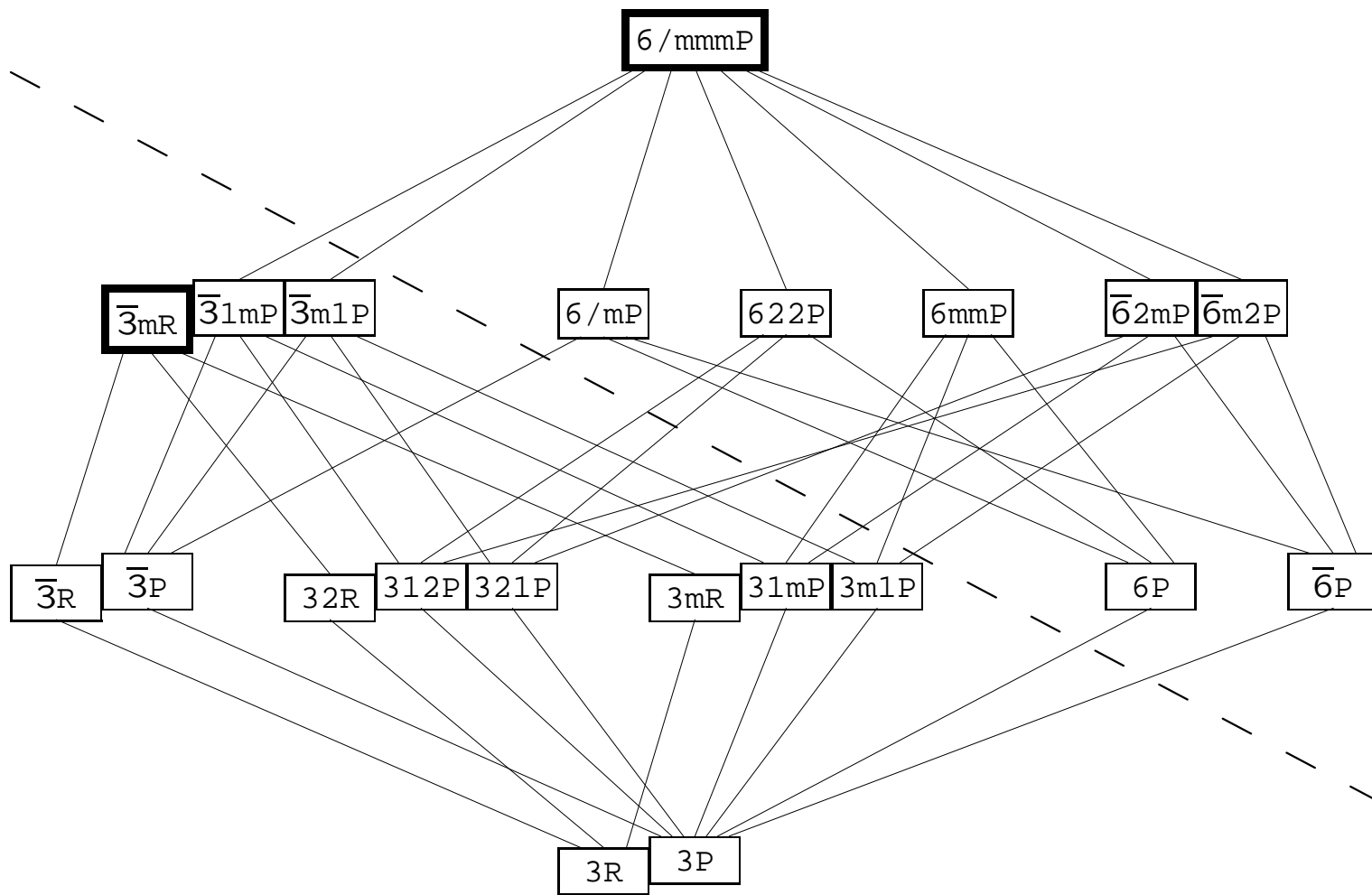


Figure 3: Subgroup diagram of the arithmetic classes in the hexagonal crystal family: boxes directly joined together belong to the same geometric class.

Lattice systems

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.

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.

Crystal systems

For the geometric class of a point group P , the arithmetic classes contained in it determine on which lattices P acts.

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, i.e. if they act on the same lattices.

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.

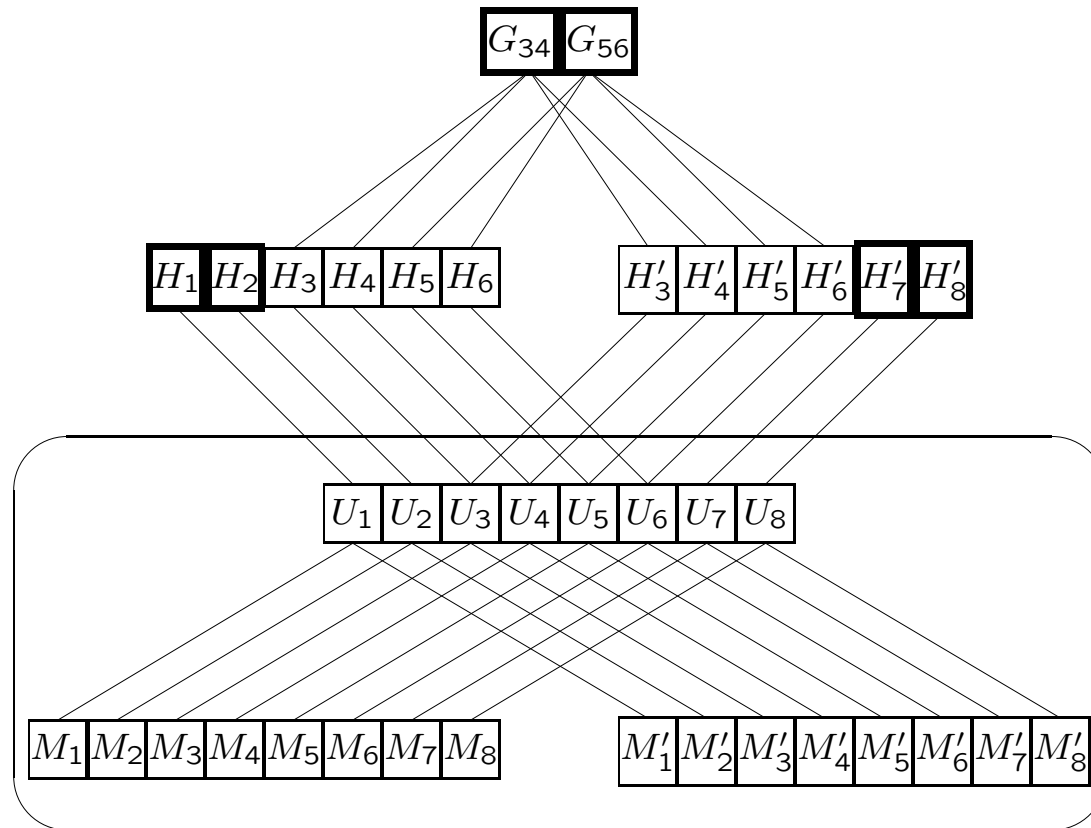


Figure 4: Crystal system without a holohedry in 5-dimensional space.

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).

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.

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.

We finish this part 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

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