Master Thesis

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The space groups with point group A_5

A study of the irreducible representations of space groups and their conjugacy classes.

M.C. Escher, Reptiles 1943 Lithograph

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Abstract

This master thesis is a study of space groups with a point group isomorphic to the image of an irreducible $\mathbb{Q}$-representation of the alternating group of degree 5. From these space groups the irreducible representations over $\mathbb{C}$ are described. These are the representations given by the periodic boundary condition for real crystals. Also the conjugacy classes of these groups are calculated. The theory that is used to calculate this data is described in a general setting so that it can also be used for other space groups.

This master thesis consists of two parts. In the first part the theory of space groups, especially representations over $\mathbb{C}$ and conjugacy classes, is described. In the second part the theory is applied to the space groups with a point group that is an irreducible $\mathbb{Q}$-representation. After an introducing chapter the basic algorithms for space groups are studied. In the third chapter the induction and restriction theory of representations of general groups is described and then applied to space groups. In the fourth section of this chapter a generalization of the well know fact that the order of the group is equal to the sum of the squared dimensions of its irreducible representations is proven. To get a set of mutually non-isomorphic representations fundamental domains and sets of orbit representatives are studied in the fourth chapter. In the fifth chapter a method is given to determine a set of representatives for the conjugacy classes. In the second part of the master thesis the group theoretic data of A_5 is given in chapter six. The seventh chapter is a manual for the data given in the appendix of the space groups. Since the data of the actual results of the calculation on the space groups are to much to set in the thesis they are given in an appendix.

1 Introduction

The mean object of study of this master thesis are space groups. Space groups are the automorphism groups of certain sets in $\mathbb{R}^n$. The automorphisms are affine maps, a linear map composed with a translation. Before a definition of a space group can be given, the affine maps are studied and lattices in $\mathbb{R}^n$ are defined.

Definition 1. *An* affine map *is a map* $\phi : \mathbb{R}^n \to \mathbb{R}^n$ *such that there is a linear map* g_ϕ *and a vector* $t_\phi \in \mathbb{R}^n$ *such that for all* $v \in \mathbb{R}^n$, $\phi(v) = g_\phi(v) + t_\phi$.
An affine map ϕ *will by denoted by* $\{g_\phi \mid t_\phi\}$.
The group $\mathcal{A}_n := \{\phi : \mathbb{R}^n \to \mathbb{R}^n \mid \phi$ *is a bijective affine map*$\}$ *is called the* affine group *of degree* n.

Remark that the composition of two affine maps: $\{g \mid t_g\} \circ \{h \mid t_h\}$ is equal to the affine map $\{gh \mid t_g + gt_h\}$.

Lemma 1. *Define* $GL_n := GL_n(\mathbb{R})$. *Define* $\Pi : \mathcal{A}_n \to GL_n$ *by* $\Pi(\{g \mid t_g\}) = g$.
Then Π *is a surjective group homomorphism.*
The kernel of Π *is equal to* $T_n := \{\{id \mid t\} : t \in \mathbb{R}^n\}$, *the set of translations. The complement of* T_n *is* $\{\{g \mid 0\} \mid g \in GL_n\}$
So the group $\mathcal{A}_n$ *is a semidirect product of* T_n *and* GL_n.

Definition 2. *Let* $T < T_n$, *then* $L(T) := \{t \in \mathbb{R}^n : \{id \mid t\} \in T\}$ *is called the* set of translation vectors *of* T.

Definition 3. *The group* $E_n := \{\{g \mid t\} \in \mathcal{A}_n \mid g^{tr}g = id\}$ *is called the* Euclidean group *of degree* n.
The Euclidean group is the group of isometrices on $\mathbb{R}^n$.

Definition 4. *A subgroup* $L < \mathbb{R}^n$ *is called a* lattice *if there is an* $\mathbb{R}$*-basis* $B = (b_1, \dots, b_n)$ *such that* $L = \{\sum_{i=1}^n a_i b_i : a_i \in \mathbb{Z}\}$. *The basis* B *is in that case called a* lattice basis.

Example. Let e_1, e_2 be the standard basis of $\mathbb{R}^2$.
Then $\{a\sqrt{2}e_1 + be_2 : a, b \in \mathbb{Z}\}$ is a lattice.
But $\{a\sqrt{2}e_1 + be_1 : a, b \in \mathbb{Z}\}$ is not a lattice, since the set lies dense in the one dimensional $\mathbb{R}$-vector space generated by e_1.
Also $\{(2a + 3b)e_1 + (3b + c)e_2 : a, b, c \in \mathbb{Z}\}$ is a lattice, since the set is equal to $\{Ae_1 + Be_2 : A, B \in \mathbb{Z}\}$.

Definition 5. *Let* $L < \mathbb{R}^n$ *be a lattice, then the symmetry group of* L, $Aut(L)$ *is* $\{g \in O_n \mid gL = L\}$.

Example. Let e_1, e_2 be the standard basis on $\mathbb{R}^2$, let $L := \langle e_1, e_2 \rangle$ as lattice.
An element of $Aut(L)$ preserves the distance in $\mathbb{R}^2$, since it is in O_n. So if $\phi \in Aut(L)$, then $||\phi(e_i)|| = 1$ for $i = 1, 2$. The elements of L with absolute value 1 are: $e_1, -e_1, e_2, -e_2$. Since ϕ must be invertible, the vector space generated by $\phi(e_1)$ must be different from the vector space generated by $\phi(e_2)$. Thus if for example $\phi(e_1) = e_1$, then $\phi(e_2) \in \{e_2, -e_2\}$. So the only possibilities for ϕ are the following:

$$\phi(e_1) = (-1)^j e_k, \phi(e_2) = (-1)^l e_{k+1}$$

with $j, k, l \in \{1, 2\}$ and $e_3 := e_1$.
These element form a group of maps isomorphic to D_4.
So $Aut(L) = \left\langle \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\rangle$, with the linear maps written as matrices on the basis e_1, e_2.

Definition 6. *Let* $R < E_n$, $T := R \cap T_n$ *be the translation subgroup of* R *and* $L := L(T)$.
Then R *is called a* space group *if* L *is a lattice.*
The group $G := \Pi(R)$ *is called the* point group *of* R.

Example. The group $R := \langle \left\{ \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \mid 0 \right\}, \left\{ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \mid 0 \right\}, \left\{ id \mid \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\} \left\{ id \mid \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right\} \rangle$ is a space group. This is a space group which is a semidirect product of its translation subgroup and its point group. Such a space group is called a **symmorphic space group**. There are also non-symmorphic space groups, see for example:

$$S := \langle \left\{ \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \mid \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix} \right\}, \left\{ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \mid \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix} \right\}, \left\{ id \mid \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\} \left\{ id \mid \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right\} \rangle.$$

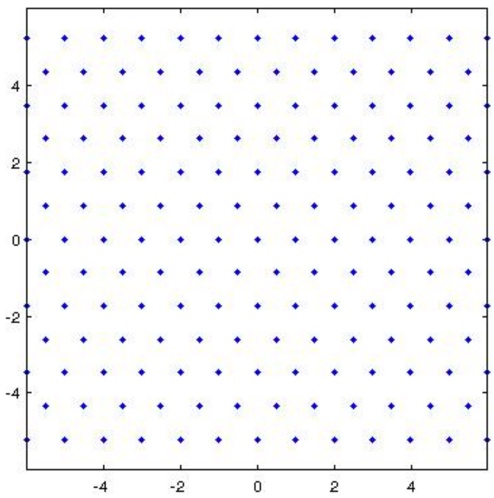
Since the second generator is a glide reflection, there is no pre-image $\{g \mid t_g\}$ of $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, such that $\{g \mid t_g\}^2 = \{id \mid 0\}$. Thus S is not a symmorphic group.

Theorem 1. *Let R be a space group with translation lattice L and point group G. Then $G \leq Aut(L)$, so G is isomorphic to a finite subgroup of $GL_n(\mathbb{Z})$.*

Example. Let R be a space group with point group G generated by $r := \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} \\ \frac{\sqrt{3}}{2} & \frac{\sqrt{3}}{2} \end{pmatrix}$ and $t := \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$, and $T < R$ the translation subgroup such that $L(T) := \langle b_1 := \begin{pmatrix} 1 \\ 0 \end{pmatrix}, b_2 := \begin{pmatrix} \frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix} \rangle$.
The linear map r is a rotation of order 6, thus $G \cong D_6$. The lattice $L(T)$ is the so called hexagonal lattice.
Writing the matrices of r and t on the basis b_1, b_2 one gets the following matrices:

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

These are indeed in $GL_n(\mathbb{Z})$. Remark that these matrices are not orthogonal any more, but there is of course a G-invariant inproduct. Below a picture of the lattice L.



Let $R < E_n$ be a space group and G its point group. Then R has a set of coset representatives with respect to $T(R)$. In such a set, every linear part $g \in G$ occurs precisely once. Such a set r has affine maps of the form $\{g \mid t_g\}$ with $g \in G$ and $t_g \in \mathbb{R}^n$. The set $\{t_g : g \in G\}$ is called a vector system for R.

From now on the space groups are written on a basis such that $T = \mathbb{Z}^n$. By theorem 1 then $G < GL_n(\mathbb{Z})$. The inproduct wrt the lattice basis is no longer the standard inproduct, but a G-invariant inproduct. An example of a G-invariant inproduct is the following:

$$\langle v, w \rangle = v^{tr} (\sum_{g \in G} g^{tr} g) w$$

The notations throughout this master thesis:
R is the space group.
G is the point group.
GL_n are the invertible $n \times n$-matrices over $\mathbb{R}$
$G^* := \{g^{tr} | g \in G\}$ is the dual point group.
id is the identity matrix of G.
$\Pi : R \to G$ is the natural projection to the linear parts
$T = ker\ \Pi$ is the translation subgroup.
t_g is a vector system of G.
L is the lattice of the space group.

2 Smith, Wyckoff and Zassenhaus

In this section a few algorithms that are useful when studying space groups are treaded. The first algorithm calculates the Smith normal form of a matrix. This algorithm is then used to calculate the Wyckoff positions of a space group. The Wyckoff positions classify the points in $\mathbb{R}^n$ according to their stabilizers. The Smith normal form is also used in the Zassenhaus algorithm. This algorithm calculates the possible space groups with a given point group up to isomorphism. At least some comments are made about the conjugacy of two point groups in $GL_n(\mathbb{Z})$, the calculation of generators for $N_{GL_n(\mathbb{Z})}(H)$ and an algorithm to find all the point groups up to conjugacy in $GL_n(\mathbb{Z})$ that are isomorphic to a particular group.

2.1 Smith Normal Form

Notation. A diagonal matrix $D \in \mathbb{Z}^{n\times m}$ has $d_i := D_{ii}$ for $1 \leq i \leq \min(n,m)$ and $D_{ij} = 0$. So $D_{ij} := \delta_{ij} d_i$.

Definition 7. *Let $A \in \mathbb{Z}^{n\times m}$, then the* Smith normal form *of A is a diagonal matrix D with $d_i|d_{i+1}$, such that there are matrices $P \in GL_n(\mathbb{Z})$, $Q \in GL_m(\mathbb{Z})$, with $PAQ = D$.*

Lemma 2. [Sm61] *Every matrix $A \in \mathbb{Z}^{n\times m}$ has a Smith normal form.*

The algorithm for calculating the Smith normal form is as follows:
Define $d_1 := gcd(A_{ij} \,|\, 1 \leq i \leq n, 1 \leq j \leq m)$. With elementary row and column operations one can substitute A_{11} by d_1. Now one can sweep the first row and column with A_{11}. The problem has been reduced to a $(n-1) \times (m-1)$ matrix. The matrices P and Q can be calculated simultaneously by keeping track of the row and column operations on two identity matrices □

The calculation of the Smith normal form of a matrix is very useful algorithm for the study of particular space groups. It is used to calculate linear congruences modulo $\mathbb{Z}$, thus of the form $Ax \equiv b \mod \mathbb{Z}^n$.

Corollary 1. *Let L be a lattice and L' be a subgroup of L, then there is a lattice basis $b_1, \ldots b_n$ and integers $d_1, \ldots, d_n$ with $d_i|d_{i+1}$, such that*

$$L := \langle b_1, \ldots, b_n\rangle \text{ and } L' := \langle d_1 b_1, \ldots, d_n b_n\rangle.$$

The bases $b_1, \ldots b_n$ and $d_1 b_1, \ldots, d_n b_n$ are called compatible bases *for L and L'.*

Take $v_1, \ldots, v_r$ such that

$$L'' := \{\sum_{i=1}^{r} a_i v_i : a_i \in \mathbb{Z}\} < L' < \{\sum_{i=1}^{r} a_i v_i : a_i \in \mathbb{R}\}.$$

Since there are only finitely many points of L in the set $\{\sum_{i=1}^{r} a_i v_i : 0 \leq a_i \leq 1\}$, the group L'' has finite index in L'. Hence L' is finitely generated. Let A be the matrix of the generators of L'. Take P and Q such that $D := PAQ$ is the Smith normal form of A. The columns of P^{-1} are the vectors that form the basis for L and the columns of $P^{-1}D$ are the vectors that form the basis for L'. □

2.2 Wyckoff positions

Definition 8. *If R is an n-dimensional space group and $x \in \mathbb{R}^n$, then $R_x := Stab_R(x)$ is called the* site symmetry group *of x.*
The points $x, y \in \mathbb{R}^n$ belong to the same Wyckoff position *if R_x and R_y are conjugated in R.*

The goal is to calculate all Wyckoff positions of a given space group. This can be done by an algorithm described in [EGN97]. Below is a brief summary of that algorithm.

Lemma 3. *Let $S \leq R$ with $\Pi(S)$ generated by $g_1 \ldots g_s \in \Pi(R)$ and $\{g_1|t_1\}, \ldots \{g_s|t_s\} \in R$. Let $x \in \mathbb{R}^n$. Then $\Pi(S) \leq \Pi(R_x) \Leftrightarrow \forall_i\ (g_i - id)x \equiv -t_i\ (mod\ \mathbb{Z}^n)$.*

⇒: For all g_i there is a $u_i \in \mathbb{Z}^n$ such that $\{g_i|t_i + u_i\} \in S$ and $x = \{g_i|t_i+u_i\}(x) = g_i x + t_i + u_i$. So $(g_i - id)x \equiv t_i\ (mod\ \mathbb{Z})$.
⇐: It is clear that x is a fixed point for a pre-image of $\Pi(s)$ for each $s \in S$. □

The next algorithm for calculating Wyckoff positions with $\Pi(R_x)$ generated by $g_1, \ldots, g_s$ is described in [EGN97].
Join the matrices g_i vertically to a $ns \times n$ matrix A. Do the same for the vectors $-t_i$ to get a vector b. By lemma 3: $H \leq \Pi(R_x)$ iff $Ax \equiv b\,(\mathrm{mod}\ \mathbb{Z}^n)$.
Calculate $P \in GL_{ns}(\mathbb{Z})$ and $Q \in GL_n(\mathbb{Z})$ such that $D := (d_1, \ldots, d_r, 0, \ldots, 0) = PAQ$ is the Smith normal form of A. Then $Ax \equiv b \,\mathrm{mod}\ \mathbb{Z}^n \Leftrightarrow D(Q^{-1}x) \equiv Pb \,\mathrm{mod}\ \mathbb{Z}^n$. This has only a solution if $Pb_j \in \mathbb{Z}$ for $j > r$. If so, then the solutions are the set of vectors Qv, where $v_j := \begin{cases} \frac{i_j + Pb_j}{d_j} & \text{if } j \leq r \\ x_j & \text{if } j > r \end{cases}$ with $i_j \in \mathbb{Z}$ and $x_j \in \mathbb{R}$.
So far one knows that $H < \Pi(R_x)$ by lemma 3, but it is still possible that $\Pi(R_x)$ is greater than H. To check if $\Pi(R_x) = H$ calculate the orbit of $x + \mathbb{Z}^n$ in $\mathbb{R}^n/\mathbb{Z}^n$ under R. If the orbit has $[G : H]$ elements then $\Pi(R_x) = H$. The orbit gives also the other Wyckoff positions with $\Pi(R_x)$ a to H conjugated subgroup.

2.3 Zassenhaus algorithm

The space group is an extension of its point group with its translation subgroup, since $G \cong R/T$. The goal is to classify the space groups for a given point group. For each $g \in G$ there is a $t_g \in \mathbb{R}^n$ such that $\{g \mid t_g\} \in R$. The set $\{t_g : g \in G\}$ is called a vector system.

Definition 9. *Let M be a G-module. Then $\tau : G \to M$ is called a* derivation *of G with values in M if $\tau(gh) = \tau(g) + g\tau(h)$. The set $C^1(G, M)$ is the* Abelian group of derivations*, with the addition inherited from M.*
Let $m \in M$, then $\tau_m : G \to M$ is defined as follows: $\tau_m : g \mapsto (g - id)m$. Such a derivation is called an inner derivation *and the subgroup of inner derivations is noted by $B^1(G, M)$. The factor group $H^1(G, M) := C^1(G, M)/B^1(G, M)$ is the* first cohomology group *of G with values in M.*

Let R be a space group, $G < GL_n(\mathbb{Z})$ its point group and $\mathbb{Z}^n$ its translation subgroup. A vector system $\{t_g : g \in G\}$ corresponds with a derivation $\tau : G \to \mathbb{R}^n$, $g \mapsto t_g$. The inner derivations correspond to translations of the origin. Let t_g and s_g be two vector systems. If $t_g - s_g \in \mathbb{Z}^n$, then the corresponding groups are the same. So for classifying the different space groups the derivations are with values in $\mathbb{R}^n/\mathbb{Z}^n$. Thus a first step in the classification is calculating $H^1(G, \mathbb{R}^n/\mathbb{Z}^n)$.

The next algorithm gives all elements of $C^1(G, \mathbb{R}^n/\mathbb{Z}^n)$.
Give for the group G a set of generators $X_1, \ldots, X_m$ and a set of defining relations $r_1, \ldots, r_k$ (the kernel of $F(X) \mapsto G$, $X_i \mapsto X_i$ is generated by $r_1, \ldots, r_k$). Now every relation gives in G the identity, thus in R an element of the translation subgroup: $\mathbb{Z}^n$. The idea is to evaluate the relations for a vector system in indeterminates. Define x_{ij} variables for $1 \leq i \leq m$, $1 \leq j \leq n$. The vector system is $t_{X_i} := (x_{i1}, \ldots, x_{in})$. For a relation $r = \prod_{j=1}^{l} X_{i_j}$ this gives in R the product $\prod_{j=1}^{l} \left\{ X_{i_j} \mid t_{X_{i_j}} \right\} = \{id \mid C_r(x_{11}, \ldots, x_{mn})\}$, with C_r a $mn \times n$-matrix. Thus $C_r x \equiv 0\ (\mathrm{mod}\ \mathbb{Z}^n)$. The set of congruences module $\mathbb{Z}^n$ for every relation are called the **Frobenius congruences**. Set the matrices C_r below each other and call this matrix A. Thus t_{X_i} is a possible vector system iff $Ax \equiv 0\ (\mathrm{mod}\ \mathbb{Z}^n)$. The solution space of $Ax \equiv 0\ (\mathrm{mod}\ \mathbb{Z}^n)$ can then be calculated by taking the Smith normal form of A.

With a translation of the origin by $\frac{1}{|G|}\sum_{g \in G} t_g$ all the translation parts t_g are in $\frac{1}{|G|}\mathbb{Z}^n$. So $H^1(G, \mathbb{R}^n/\mathbb{Z}^n)$ is finite. The action of the inner derivations on $C^1(G, \mathbb{R}^n/Z^n)$ corresponds with the infinite part of the solution of the Frobenius congruences.

Lemma 4. *Let A be the integral matrix for the Frobenius congruences. Take P, Q such that $D := PAQ$ is the Smith normal form of A, then*

$$a_1 d_1^{-1} Q e_1 + \ldots + a_r d_r^{-1} Q e_r$$

with $0 \leq a_i < d_i$ are representatives of $H^1(G, \mathbb{R}^n/\mathbb{Z}^n)$

Theorem 2 (L.Bieberbach [Bie11])**.** *Two space groups are affine equivalent if and only if they are isomorphic.*

Let $N := N_{GL_n(\mathbb{Z})}$ be the normalizer of G in $GL_n(\mathbb{Z})$. Then R is affine equivalent with nRn^{-1} for all $n \in N$. On the point group the action of N is just conjugacy. So N acts on $H^1(G, \mathbb{R}^n/\mathbb{Z}^n)$ by $(n \cdot \tau)(g) := n\tau(n^{-1}gn)$ for $n \in N$.

Theorem 3. *The affine equivalence classes of the space groups with point group G are in bijection with the orbits of $N := N_{GL_n(\mathbb{Z})}(G)$ on $H^1(G, \mathbb{R}^n/\mathbb{Z}^n)$.*

The method described above is called the Zassenhous-algorithm [Za48].

2.4 Splitting a $\mathbb{Q}$-class in $\mathbb{Z}$-classes

For a given point group the Zassenhaus-algorithm gives the different space groups. To classify the space groups one can set the groups with isomorphic point groups in one class. The point group of the space group can then be seen as a $\mathbb{Z}$-representation of the abstract group. For fields with character 0 the representation theory has standard methods to find all the representations of a certain abstract group. This gives a good reason to classify the $\mathbb{Z}$-representations by their $\mathbb{Q}$-representation.

Definition 10. *Let $G, H < GL_n(\mathbb{Z})$. The group G is in the same* $\mathbb{Z}$-class *as H if they are conjugated in $GL_n(\mathbb{Z})$. If G and H are conjugated in $GL_n(\mathbb{Q})$, then they are in the same* $\mathbb{Q}$-class. *If G and H are in the same $\mathbb{Z}$- resp. $\mathbb{Q}$-class, then they are called $\mathbb{Z}$- resp.* $\mathbb{Q}$-equivalent.

Whether two groups are $\mathbb{Q}$-equivalent can be calculated by standard methods. The difficulty is to split the $\mathbb{Q}$-class in $\mathbb{Z}$-classes.

Lemma 5. *Every $\mathbb{Q}$-representation of G can be written with matrices over $\mathbb{Z}$.*

Let M be an irreducible $\mathbb{Q}$ representation and $v \in M$. Now $\{gv : g \in G\}$ is complete since M is irreducible. Take a basis for the $\mathbb{Z}$-lattice generated by the gv's. Writing the matrices with respect to this basis gives a representation over $\mathbb{Z}$. □

The question whether two finite linear groups are in the same $\mathbb{Q}$-class or $\mathbb{Z}$-class can be made equivalent to a couple of homogeneous polynomials f_i being not all 0 resp. having solutions $f_i = \pm 1$ in $\mathbb{Z}$.
If two groups are is the same $\mathbb{Z}$- or $\mathbb{Q}$-class they are certainly isomorphic. Let $\phi : G \to H$ be a group isomorphism. Let g_i be a set of generators of G. Then G is in the same $\mathbb{Z}$- respectively $\mathbb{Q}$-class as H, if there is a matrix M in $GL_n(\mathbb{Z})$ respectively $GL_n(\mathbb{Q})$ with $Mg_i = \phi(g_i)M$. This gives a set of linear equations that can be solved with the Smith normal form. For M being in $GL_n(\mathbb{Z})$, the determinant of M must be ± 1. Let $\langle b_1, \ldots, b_m \rangle$ be a basis for the matrices $M \in GL_n(\mathbb{Z})$ such that $Mg_i = \phi(g_i)M$. A matrix written on this basis has then as determinant a homogeneous polynomial of degree n in m variables. Let $f(x_1, \ldots, x_m) := \det(x_1 b_1 + \ldots + x_m b_m)$. So there is a matrix $M \in GL_n(\mathbb{Z})$ respectively in $GL_n(\mathbb{Q})$ so that $Mg_i = \phi(g_i)M$ if $f(x_1, \ldots, x_m) = \pm 1$ has integral solutions respectively f is non-zero. The isomorphisms that must be studied correspond with representatives of $Out(G) := Aut(G)/Inn(G)$. If for all these isomorphisms there is no solution, then H and G are not in the same $\mathbb{Z}$- or $\mathbb{Q}$-class. For deciding if two groups are in the same $\mathbb{Q}$-class this works very well, since it is only deciding if a polynomial is 0. Unfortunately for $\mathbb{Z}$-equivalence it is a Diophantine equation, which can be very difficult to solve: i.e. finding all solutions or show that there are none. In the case that the groups are as $\mathbb{Q}$-representations absolutely irreducible the polynomial has one variable. So then it can be easily seen if there are solutions in $\mathbb{Z}$. This is the case for the 4- and 5-dimensional representations of A_5.

Example. Let $G := \left\langle \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\rangle$ and $H := \left\langle \begin{pmatrix} -1 & 1 \\ 0 & 1 \end{pmatrix} \right\rangle$, both are isomorphic to C_2. The solution space of matrices M such that $M \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} -1 & 1 \\ 0 & 1 \end{pmatrix} M$ is of dimension 2 and has basis $b_1 := \begin{pmatrix} 1 & 0 \\ 2 & 0 \end{pmatrix}$ and $b_2 := \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$. So the determinant of a matrix in the solution space is $|xb_1 + yb_2| = -2xy$. So G and H are is the same $\mathbb{Q}$-class. Since $2| - 2xy$ for all $x, y \in \mathbb{Z}$, there is no matrix in $GL_2(\mathbb{Z})$ that conjugate G in H. So G and H are in different $\mathbb{Z}$-classes.

The general algorithm for checking if two point groups are conjugated in $GL_n(\mathbb{Z})$ is described in [OPS98] and the calculation of the normalizer in [Opg01]. Both algorithms are implemented in CARAT [OPS98] and MAGMA [BCP97]. These algorithms are to complicated too describe here. In [OPS98] also an algorithm is described that for a given $\mathbb{Q}$-class calculates its $\mathbb{Z}$-classes.

Theorem 4. *[EGN97] Let G be a finite group and L a G-lattice. If $M \leq L$ is a maximal G-invariant sublattice, then $[L : M] = p^a$ and $L/M = C_p \times \cdots \times C_p$. Also L/M is an irreducible $\mathbb{F}_pG$-module.*

To show that $[L : M] = p^a$ at first will be shown that $[L : M]$ is finite. Let $e_1, \ldots, e_n$ and $d_1e_1, \ldots, d_re_r$ be compatible bases for L and M. If $r \neq n$, then $M < d_1e_1, \ldots, d_re_r, 2e_n < L$. Since M is maximal, $r = n$. If $d|d_i$, then $M < \langle d_1e_1, \ldots, d_{i-1}e_{i-1}, de_i, \ldots, de_n\rangle < L$. Thus $[L : M] = p^a$ and $L/M = C_p \times \cdots \times C_p$. Assume that V is a submodule of L/M and $V \neq L/M$. Then the pre-image N of V in L is a G-invariant sublattice. Thus $N = M$, because $M < N$ and M maximal. So $V = 0$. Concluding that L/M is an irreducible $\mathbb{F}_pG$-module. □

Theorem 5. *If $p \not| \, |G|$, then the space groups of the G invariant lattices M with $[L : M] = p^a$ are isomorphic to the space group R.*

Now one can calculate step by step the maximal G-invariant lattices. In each step one calculates which of the found point groups are $\mathbb{Z}$-equivalent.

Example. Let $r_3 = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$ and $t = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. Thus $D_3 \cong \langle r_3, t\rangle$. Since the representation is 2-dimensional the non-trivial submodules are of dimension 1 and therefore common eigenvectors of t and r_3. The eigenvectors of t are $\begin{pmatrix} a \\ a \end{pmatrix}$ and $\begin{pmatrix} a \\ -a \end{pmatrix}$. Now $r_3 \begin{pmatrix} a \\ a \end{pmatrix} = \begin{pmatrix} -a \\ 0 \end{pmatrix}$ and $r_3 \begin{pmatrix} a \\ -a \end{pmatrix} = \begin{pmatrix} a \\ 2a \end{pmatrix}$. So the only case that there is a non-trivial submodule is when $-a = 2a$, thus when $p := 3$.
Thus a D_3-invariant sublattice L' is spanned by $\begin{pmatrix} 3 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 3 \end{pmatrix}, \begin{pmatrix} 1 \\ 2 \end{pmatrix}$. This has basis $\begin{pmatrix} 1 \\ 2 \end{pmatrix}, \begin{pmatrix} 0 \\ 3 \end{pmatrix}$ and on that basis r_3 acts like $s_3 := \begin{pmatrix} -2 & -3 \\ 1 & 1 \end{pmatrix}$ and t acts like $u := \begin{pmatrix} 2 & 3 \\ -1 & -2 \end{pmatrix}$. Since $Out(D_3) \cong 1$, it is enough to calculate a basis for the set of matrices that conjugate r_3 and t respectively to s_3 and u. So let $M := \begin{pmatrix} a & b \\ c & d \end{pmatrix}$, then

$$\begin{pmatrix} b & -a-b \\ d & -c-d \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}\begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix} = \begin{pmatrix} -2 & -3 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} -2a-3c & -2b-3d \\ a+c & b+d \end{pmatrix}$$
$$\begin{pmatrix} b & a \\ d & c \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 2 & 3 \\ -1 & -2 \end{pmatrix}\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} 2a+3c & 2b+3d \\ -a-2c & -b-2d \end{pmatrix}$$

One sees that $-2a - 3c = b = 2a + 3c$, so $b = 0$ and $2a = 3c$. Then $a = 3d$ and $c = -2d$. Thus the solution space has basis $b_1 := \begin{pmatrix} 3 & 0 \\ -2 & 1 \end{pmatrix}$. Since b_1 has determinant 3, the two groups are not in the same $\mathbb{Z}$-class.
Now the maximal modules of $s_3 := \begin{pmatrix} -2 & -3 \\ 1 & 1 \end{pmatrix}, u := \begin{pmatrix} 2 & 3 \\ -1 & -2 \end{pmatrix}$ must be calculated. The eigenvectors of u are $\begin{pmatrix} -3a \\ a \end{pmatrix}$ and $\begin{pmatrix} a \\ -a \end{pmatrix}$. Now $s_3 \begin{pmatrix} -3a \\ a \end{pmatrix} = \begin{pmatrix} 3a \\ -2a \end{pmatrix}$ and $s_3 \begin{pmatrix} a \\ -a \end{pmatrix} = \begin{pmatrix} a \\ 0 \end{pmatrix}$. So only if $p = 3$ the representation is reducible. The D_3-invariant sublattice is spanned by $\begin{pmatrix} 3 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 3 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. This has as basis $\begin{pmatrix} 3 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. On this basis s_3 acts like $\begin{pmatrix} -2 & -1 \\ 3 & 1 \end{pmatrix}$ and T acts like $\begin{pmatrix} 2 & 1 \\ -3 & -2 \end{pmatrix}$. One sees that $\begin{pmatrix} 1 & 0 \\ -2 & 1 \end{pmatrix}$ conjugates the group generated by r_3, t to the group generated by those two matrices.
So D_3 splits in two $\mathbb{Z}$-classes: $\langle r_3, t\rangle$ and $\langle s_3, u\rangle$.

Example. Look at the group generated by $g := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. For $p = 2$, g acts like the identity on $\mathbb{F}_2^2$. So the maximal G-invariant lattices are $\langle \begin{pmatrix} 2 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 2 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}\rangle$, $\langle \begin{pmatrix} 2 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 2 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \end{pmatrix}\rangle$, $\langle \begin{pmatrix} 2 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 2 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \end{pmatrix}\rangle$.
For the first two lattices the action of g is the same as on L. On the last one, one takes the basis $\begin{pmatrix} 2 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and g acts on this basis like $h := \begin{pmatrix} 1 & 1 \\ 0 & -1 \end{pmatrix}$. Now h and g are not $\mathbb{Z}$-conjugated, since h acts non-trivially on $\mathbb{Z}^2/2\mathbb{Z}^2$ and g acts trivially on $\mathbb{Z}^2/2\mathbb{Z}^2$. The maximal G-invariant lattices of $\langle h\rangle$ is:

$\langle \begin{pmatrix} 2 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 2 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \end{pmatrix} \rangle$. With the basis $\langle \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 2 \end{pmatrix} \rangle$, h acts on the lattice as $k := \begin{pmatrix} 1 & 2 \\ 0 & 1 \end{pmatrix}$. Now k is equal to g conjugated with $\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$.

3 Induction and Restriction of Representations

The following is a brief summary of the theory of induced and restricted representations. This theory is used to induce the linear representations of T for the irreducible representations of R.

Definition 11. *Let $G = \langle g_1, \dots, g_n \rangle$ and $M_1, \dots, M_n \in GL_m(\mathbb{C})$, then $(M_1, \dots, M_n)$ is a* representation *if $g_i \mapsto M_i$ is a group homomorphism. A representation Δ will be denoted with $(\Delta(g_1), \dots, \Delta(g_n))$.*

Example. For $D_3 = \langle r, t \rangle$ and Δ the representation $\Delta(r^i t^j) = (-1)^j$ of D_3, Δ is given by $(1, -1)$.

Theorem 6. *Let Δ be a representation of H, $g_1, \dots, g_m$ a transversal of H in G, then Δ^G is defined by*

$$\Delta^G(g) := \begin{pmatrix} \dot{\Delta}(g_1^{-1} g g_1) & \dots & \dot{\Delta}(g_1^{-1} g g_m) \\ \vdots & & \vdots \\ \dot{\Delta}(g_m^{-1} g g_1) & \dots & \dot{\Delta}(g_n^{-1} g g_m) \end{pmatrix}$$

where $\dot{\Delta}(h) := \Delta(h)$ if $h \in H$ and 0 otherwise.
This gives a representation of G and is called the induced representation *of Δ.*

The matrices of the induced representation are often given by a permutation $\rho \in S_m$ and a sequence L of m matrix blocks of size $\deg \Delta$. Let $\rho(i)$ be the unique j such that $g_j^{-1} g g_i \in H$ and $L_i := \Delta(g_{\rho(i)}^{-1} h g_i)$. Then $\Delta^G(g) = (P \otimes I)D$, where $P(e_i) = e_{\rho(i)}$, I is the $n \times n$ identity matrix and $D = \bigoplus_i L_i$. Often the permutation ρ will be given by the sequence $[\rho(1), \dots, \rho(m)]$ and the sequence of matrix blocks by $B(A_1, \cdots A_n)$, so that the induced representation is notated in the form $[k_1, \cdots, k_n], B(A_1, \cdots, A_n)$

Example. $D_3 = \langle r, t \rangle$ has subgroup $C_3 := \langle r \rangle$ with transversal r, t. Let $\Delta(r) := \zeta_3$. Then

$$\Delta^{D_3}(r) = \begin{pmatrix} \zeta_3 & 0 \\ 0 & \zeta_3^2 \end{pmatrix}, \Delta^{D_3}(t) = \begin{pmatrix} 0 & \zeta_3^2 \\ \zeta_3 & 0 \end{pmatrix}$$

With the permutation notations these become $[1, 2]$,$B(\zeta_3, \zeta_3^2)$ and $[2, 1]$,$B(\zeta_3, \zeta_3^2)$. The corresponding matrices P,D are then:

$$\text{for } r : \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} \zeta_3 & 0 \\ 0 & \zeta_3^2 \end{pmatrix}, \text{ for } t : \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} \zeta_3 & 0 \\ 0 & \zeta_3^2 \end{pmatrix}$$

Example. Assume $H \triangleleft G$ and $G/H = \langle gH \rangle$ a cyclic group of order n. Let Δ be a representation of H. Now $id, g, \dots, g^{n-1}$ is a transversal for H in G. If $h \in H$, then

$$\Delta^G(h) = [1, \dots, n], B(\Delta(h), \Delta(g^{-1} h g), \dots, \Delta(g^{1-n} h g^{n-1})).$$

Also $\Delta^G(g) = [2, \dots, n, 1], B(1, \dots, 1, \Delta(g^n))$. For $n = 3$ this is then:

$$\Delta^G(h) = \begin{pmatrix} \Delta(h) & 0 & 0 \\ 0 & \Delta(g^{-1} h g) & 0 \\ 0 & 0 & \Delta(g^{-2} h g^2) \end{pmatrix}, \Delta^G(g) = \begin{pmatrix} 0 & 0 & \Delta(g^3) \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

Theorem 7 (Frobenius reciprocity)**.** *Let $H \leq G$ be a subgroup, χ and ϕ representations of G respectively H, then $(\chi, \phi^G)_G = (\chi|_H, \phi)_H$.*

Definition 12. *Let $H \triangleleft G$ and ϕ a character of H, then ϕ^g is the character defined by $\phi^g(h) := \phi(g^{-1} h g)$. The group $I_G(\phi) := \{g \in G \mid \phi^g = \phi\}$ is called the* inertia group *of ϕ in G.*

Theorem 8 (Clifford's theorem)**.** *Let $H \triangleleft G$, χ an irreducible character of G and ϕ an irreducible constituent of $\chi|_H$. Let $T := I_G(\phi)$ be the inertia group of ϕ in G. Then $\chi|_H = e(\sum_{i=1}^m \phi_i)$ where $m = [G : T]$ and $\phi_i = \phi^{g_i}$ for a transversal $g_1, \dots, g_m$ of T in G. Moreover define $A := \{\psi$ irreducible character of $T \mid (\psi_H, \phi) \neq 0\}$ and $B := \{\chi$ irreducible character of $G \mid (\chi_H, \phi) \neq 0\}$, then $\psi \mapsto \psi^G$ is a bijection of A onto B.*

Theorem 9 (Mackey)**.** *Let $H \triangleleft G$, with $G/H = \langle gH \rangle$, and Δ an n-dimensional irreducible representation of H which is G-invariant. Then there is a $T \in GL_n$ such that $\Delta^g = T \Delta T^{-1}$. The irreducible representations of G that extend Δ are $g \mapsto \zeta_n^i c T$ for a $c \in \mathbb{C}$.*

Since $\Delta^g \equiv \Delta$ there is a $T \in GL_n$ such that $\Delta^g = T\Delta T^{-1}$. Because $g^n \in H$ one has $\Delta(g^{-n})T^n \in End_{KH}(W)$. By Schur's lemma there is a $c \in \mathbb{C}$ such that $\Delta(g^{-n})T^n = c^n$. This is the asked constant in the theorem.
Let χ_i be the representation with $g \mapsto \zeta_n^i cT$. Then $\chi_i \equiv \chi_j$ if and only if $i = j$, since by Schur's lemma $End_{KH}(\Delta) = \mathbb{C}$. □

The only problem is now to find a matrix T. One way of solving this problem is the following: let $h_1, \ldots, h_s$ be generators of H. Then a matrix T has the property $\Delta^g = T\Delta T^{-1}$ iff $\Delta^g(h_i) = T\Delta(h_i)T^{-1}$ for $1 \leq i \leq s$. The second statement is equivalent with $\Delta^g(h_i)T = T\Delta(h_i)$. This gives a set of linear equations for the entries of T. By parameterizing the solutions of the linear equations one can choose an invertible matrix in the solution space.

Example. The representations of A_4 can be calculated with the use of Mackey's theorem. Define $c := (12)(45)$, $b := (14)(25)$ and $e := (124)$. The normal subgroup $V_4 = \langle c, b\rangle$ has the following irreducible representations: $((-1)^i, (-1)^j)$ (e.g. $c \mapsto (-1)^i, b \mapsto (-1)^j$ for $i, j \in \{1, 2\}$). For the orbits of the irreducible representations first the action of the conjugation by e on V_4 will be calculated: $e^{-1}ce = bc$ and $e^{-1}be = c$. Thus $(1, 1)$ is fixed by e and $(1, -1) \mapsto (-1, 1) \mapsto (-1, -1)$. Thus the irreducible representations of A_4 are:

$$(1, 1, \zeta_3^i), (\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix})$$

3.1 Induction of representations on $\mathbb{Z}^n$

Since the space group R is infinite it is more difficult to calculate the representations of R than in the finite case. The finite representations can be calculated. These representations factor through $m\mathbb{Z}^n$ for a certain $m \in \mathbb{N}$. The periodic boundary condition for real crystals gives representations of the group R/mT for a large $m \in \mathbb{N}$. Since $\mathbb{Z}^n \triangleleft R$ and the representations of $\mathbb{Z}^n$ are well known, there the induction of the representations starts.
Let Γ be a finite representations of $\mathbb{Z}^n$ and $I(\Gamma)$ be its inertia group. The problem is now to find all irreducible representations of $I(\Gamma)$ which restricted to $\mathbb{Z}^n$ have Γ as constituent. Let Δ be such an irreducible representation. Let δ, γ be the characters of Δ respectively Γ, then by Clifford's theorem $\delta|_H = e\gamma$. Thus $\Delta(t) = \Gamma(t)id$, for all $t \in \mathbb{Z}^n$. So the irreducible representations of $I(\Gamma)$ that restricted to T have Γ as constituent, let T act as diagonal matrices.

By theorem 9 the induction over a cyclic factor group is solved. This gives reason to look at the composition series of the inertia group. For solvable inertia groups the representations can be calculated through the composition series by applying at each level theorem 9. For non-solvable inertia groups the composition series ends at a perfect group. Thus the question is reduced to finding representations for that perfect group. Now one looks at maximal subgroups of the perfect group and tries to split the induced irreducible modules of the maximal subgroups.

3.2 Representations and Wyckoff positions

To find all the irreducible representations of a space group one looks at all the irreducible representations of $\mathbb{Z}^n$. Since there are infinitely many irreducible representations of $\mathbb{Z}^n$, the method described above can not be applied separately to each irreducible representation. Because the point group is finite the possible inertia groups are also finite. Thus instead of calculating for each linear character its inertia group one calculates for a group which linear characters have that group as inertia group.

Definition 13. *Let* $k \in (\mathbb{R}^n)^* := \{\phi : \mathbb{R}^n \to \mathbb{R} \mid \phi \text{ a linear map }\}$*, define* $\Gamma_k(t) := exp(2\pi i k(t))$.
The dual lattice *of a lattice* L *is* $L^* := \{k \in (\mathbb{R}^n)^* \mid \forall_{t\in L}\, k(t) \in \mathbb{Z}\}$.
Assume $G \subset GL_n(\mathbb{R})$*, then the* dual group *of* G *is* $G^* := \{(g^{-1})^{tr} : g \in G\}$.

Lemma 6. *The linear representation* Γ_k *is fixed by* $\{g \mid t_g\}$ *iff* $k - (g^{-1})^{tr}k \in T^*$.

Let $\{g \mid t_g\} \in R$, then:

$$\Gamma_k^{\{g \mid t_g\}}(t) = \Gamma_k(\{g^{-1} \mid -g^{-1}t_g\}\{I \mid t\}\{g \mid t_g\}) = \Gamma_k(\{I \mid g^{-1}(t)\}) = \Gamma_{(g^{-1})^{tr}(k)}(\{I \mid t\})$$

Now $\Gamma_k|_T = \Gamma_{k'}|_T \Leftrightarrow k - k' \in T^*$. Thus $\Gamma_k^{\{g \mid t_g\}}|_T = \Gamma_k|_T$ iff $k - (g^{-1})^{tr}k \in T^*$ □

Theorem 10. *Let $H < G$, then the linear representation of T that have H as inertia group are the linear representations of T that have H^* as stabilizer.*
Assume that k and k' have the same stabilizer in $R^* := G^* \ltimes T$, then

$$\Psi : \{\phi : \phi \text{ representation of } H \mid \phi|_T = \bigoplus \Gamma_k\} \to \{\phi : \phi \text{ representation of } H \mid \phi|_T = \bigoplus \Gamma_{k'}\}$$

defined by $\Psi(\phi)(\{h \mid t_h\}) := exp(2\pi i(k'-k)(t_h))\phi(\{h \mid t_h\})$ is a bijective function.
So the irreducible representations of the inertia group extended from Γ_k differ only by a factor from the irreducible representation extended from $\Gamma_{k'}$.

Let $h^* \in H^*$, then $k = \{h^* \mid t\}\, k = h^*k + t$ and $k' = \{h^* \mid t\}\, k' = h^*k' + t$, thus $\{h^* \mid 0\}\,(k'-k) = k'-k$. Now $\Psi(\phi)$ is a representation of the inertia group:

$$\begin{aligned}
\Psi(\phi)(\{h \mid t_h\})\Psi(\phi)(\{g \mid t_g\}) &= exp(2\pi i(k'-k)(t_g + t_h))\phi(\{h \mid t_h\})\phi(\{g \mid t_g\}) \\
&= exp(2\pi i(k'-k)(t_g + t_h))\phi(\{hg \mid t_h + ht_g\}) \\
&= exp(2\pi i(k'-k)(t_g - ht_g))\Psi(\phi)(\{hg \mid t_h + gt_g\})
\end{aligned}$$

Since $h^{tr}(k'-k) = k'-k$, one has $\Psi(\phi(\{h \mid t_h\}))\Psi(\phi)(\{g \mid t_g\}) = \Psi(\phi)(\{hg \mid t_h + gt_g\}$.
Now $\Psi(\phi)(\{id \mid t\}) = exp(2\pi i(k'-k)(t))\phi(\{id \mid t\}) = exp(2\pi ik'(t))$.
So $\Psi(\phi)$ is a representation that restricted to T has $\Gamma_{k'}$ as constituent.
The inverse of Ψ is just Ψ', defined by $\Psi'(\phi)(\{h \mid t_h\}) := exp(2\pi i(k-k')(t_h))\phi(\{h \mid t_h\})$. □

So the linear representations of T that are in the same Wyckoff position of R^* have up to a factor the same extensions of the irreducible representations to the inertia group.
Thus an algorithm to find all the irreducible representations of R is the following:
Calculate the Wyckoff positions of $R^* := G^* \ltimes T$. For each Wyckoff position calculate for one point k in the Wyckoff position the extensions of the irreducible representations to the inertia group. For the other points in the Wyckoff position that have the same stabilizer as k set the factor for it. Now the to the group R induced irreducible representations are the desired irreducible representations of R.

Example. The representations of the space groups with point group generated by $c := \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$, $b := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ are studied. The point group is isomorphic to V_4.
There are three non-isomorphic space groups with the following generators:

$$\begin{aligned}
R_1 &:= \{c \mid 0\}, \{b \mid 0\} \\
R_2 &:= \left\{c \mid (\frac{1}{2}, 0)\right\}, \left\{b \mid (\frac{1}{2}, 0)\right\} \\
R_3 &:= \left\{c \mid (\frac{1}{2}, \frac{1}{2})\right\}, \left\{b \mid (\frac{1}{2}, \frac{1}{2})\right\}
\end{aligned}$$

Let C and B denote the representatives of c respectively b in the space group. Thus in the space group R_2, $C = \left\{c \mid (\frac{1}{2}, 0)\right\}, B = \left\{b \mid (\frac{1}{2}, 0)\right\}$.
The subgroups of the point group are the cyclic groups generated by c,b and bc.
It turns out that the dual group of the point group is the same as the point group since c and b are orthogonal matrices. The Wyckoff positions of the dual point group are:
For c there are two: $(0, x), (\frac{1}{2}, x)$.
For b there are two: $(x, 0), (x, \frac{1}{2})$.
For bc there are none.
For V_4 there are four: $(0,0), (0, \frac{1}{2}), (\frac{1}{2}, 0), (\frac{1}{2}, \frac{1}{2})$.
For each of these Wyckoff positions the representations must be extended to the inertia group. That is the group generated by the stabilizer and the translations subgroup.
For R_1, the symmorphic case: c: $C \mapsto \pm 1$, b: $B \mapsto \pm 1$ and V_4: $(\pm 1, \pm 1)$.
For R_2: c: now $C^2 = \{id \mid 0\}$, thus $C \mapsto \pm 1$, b: $B^2 = \{id \mid (1, 0)\}$, thus $B \mapsto \pm exp(\pi i x)$. For V_4 it is a little more complicated. The strategy is to use the induction theory for the cyclic case. The composition series that is chosen is $\langle c \rangle \triangleleft \langle c, b \rangle$. For all four positions the extensions up to c is $C \mapsto \pm 1$. To calculate the action of B on these representations look at the conjugation of C: $B^{-1}CB = \{id \mid (-1, 0)\}\, C$. Thus if

Δ is an extension to C then $\Delta^B(C) = \Delta(\{id \mid (-1,0)\})\Delta(C)$. So $\Delta^B \equiv \Delta$ iff $\Delta(\{id \mid (-1,0)\}) = 1$. The representations $(0,0)$ and $(0,\frac{1}{2})$ have $\{id \mid (-1,0)\}$ in their kernel. Thus for these representations the induced representations are respectively $(\pm 1, \pm 1)$ and $(\pm 1, i)$. In the case that $\Delta(\{id \mid (-1,0)\}) \neq 1$ the representation can just be induced. Thus for $(\frac{1}{2},0)$ there is one representation: $(\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix})$.
For $(\frac{1}{2},\frac{1}{2})$ there is one representation: $(\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix})$.
For R_3 now $C^2 = \{id \mid (0,1)\}$ thus $C \mapsto \pm exp(\pi i x)$, b: $B^2 = \{id \mid (1,0)\}$, $B \mapsto \pm exp(\pi i x)$. Again for V_4 the action of B on the representations up to C must be calculated. Now $B^{-1}CB = \{id \mid (-1,-1)\}\, C$. In this case the representations $(0,0)$ and $(\frac{1}{2},\frac{1}{2})$ are fixed thus have respectively $(\pm 1, \pm 1)$ and $(\pm i, \pm i)$ as irreducible representations. For $(0,\frac{1}{2})$ and $(\frac{1}{2},0)$ the representations just must be induced so they are respectively $(\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix})$ and $(\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix})$.
The data is listed in the tables below. The first table gives for subgroups the translation vector for the generators by space group and for these groups the relations calculated in the space group with the chosen representatives. The second table gives the representations of the inertia group for the linear representations.

$group$	R_1	R_2	R_3	rel	R_1	R_2	R_3
c	0	$(\frac{1}{2},0)$	$(\frac{1}{2},\frac{1}{2})$	c^2	0	0	$(0,1)$
b	0	$(\frac{1}{2},0)$	$(\frac{1}{2},\frac{1}{2})$	b^2	0	$(1,0)$	$(1,0)$
c,b				$b^{-1}cb = c$	0	$(-1,0)$	$(-1,-1)$

$group$	$Wyckoff$	R_1	R_2	R_3
c	$(0,x)$	± 1	± 1	$\pm exp(\pi i x)$
	$(\frac{1}{2},x)$	± 1	± 1	$\pm exp(\pi i x)$
b	$(x,0)$	± 1	$\pm exp(\pi i x)$	$\pm exp(\pi i x)$
	$(x,\frac{1}{2})$	± 1	$\pm exp(\pi i x)$	$\pm exp(\pi i x)$
c,b	$(0,0)$	$\pm 1, \pm 1$	$\pm 1, \pm 1$	$\pm 1, \pm 1$
	$(\frac{1}{2},0)$	$\pm 1, \pm 1$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$
	$(0,\frac{1}{2})$	$\pm 1, \pm 1$	$\pm 1, \pm i$	$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
	$(\frac{1}{2},\frac{1}{2})$	$\pm 1, \pm 1$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\pm i, \pm i$

3.3 Induction to a space group

After extending the irreducible representations of T to the inertia group, these extended representations must be induced to the space group to get all the irreducible representations of the space group. Before the induction can be started a transversal must be chosen.

Definition 14. *Let $g_1, \ldots g_n \in G$ and $s_1, \ldots, s_n \in \mathbb{N}$. If for every element of $g \in G$ there are unique $0 \le m_i < s_i$ such that $g = g_1^{m_1} \cdots g_n^{m_n}$, then the sequence $g_1, \ldots, g_n$ together with the sequence $s_1, \ldots s_n$ is called a* presentation sequence *of G.*
A presentation sequence of G gives rise to an enumeration of the elements of G:

$$E : G \to \{1, \ldots, |G|\},\ g_1^{m_1} \cdots g_n^{m_n} \mapsto 1 + m_n + m_{n-1}s_n + m_{n-2}s_n s_{n-1} + \ldots + m_1(s_n \cdots s_2)$$

The multiplication action of g on G can then be seen as a permutation of order $|G|$ defined by $\rho_g : m \mapsto E(g(E^{-1}(m)))$. If $H := \langle g_k, \ldots, g_n \rangle$ is a group of order $s_k \cdots s_n$, then $g_1^{m_1}, \ldots, g_{k-1}^{m_{k-1}}$ is a transversal of H in G. Analogously to above the cosets can then be enumerated by

$$E_H : G/H \to \{1, \ldots, [G : H]\},$$

$$g_1^{m_1} \cdots g_{k-1}^{m_{k-1}} H \mapsto 1 + m_{k-1} + m_{k-2}s_{k-1} + m_{k-3}s_{k-1}s_{k-2} + \ldots + m_1(s_{k-1} \cdots s_2)$$

The multiplication of g on the cosets can then be seen as a permutation defined by $\rho_g^H : m \mapsto E_H(g(E_H^{-1}(m)))$. Define $T_H : \{1, \ldots [G : H]\} \to \{g_1^{m_1} \cdots g_{k-1}^{m_{k-1}} \mid 0 \le m_i < s_i\}$ to be the inverse of the following function

$$g_1^{m_1} \cdots g_{k-1}^{m_{k-1}} \mapsto 1 + m_{k-1} + m_{k-2}s_{k-1} + m_{k-3}s_{k-1}s_{k-2} + \ldots + m_1(s_{k-1} \cdots s_2)$$

T_H gives for every coset $E_H^{-1}(i)$ a representative $T_H(i)$. Thus the image of T_H is a sequence of coset representatives.
If $H = \langle id \rangle$ then one writes T instead of T_H. Remark that $T = E^{-1}$.

Example. Let $D_5 = \langle r := (12345), t := (25)(34) \rangle$ and $H := \langle t \rangle$. Then r, t with $5, 2$ is a presentation sequence of D_5.
Thus $E(r^m t^n) = 1 + n + 2m$ for $n \in \{0, 1\}$ and $m \in \{0, 1, 2, 3, 4\}$.
The action of r on D^5 is $r^m t^n \mapsto r^{m+1}t^n$. So $\rho_r = (13579)(246810)$.
The multiplication of r on the cosets of H gives then: $\rho_r^H := (12345)$. The coset representatives are $T_H(i) = r^i$.

Lemma 7. *Let $g_1, \ldots, g_n$ with $s_1, \ldots, s_n$ be a presentation sequence of G, $H = \langle g_k, \ldots, g_n \rangle$ and $|H| = s_k \cdots s_n$. Let $I = \langle g_l, \ldots, g_n \rangle$ and $|I| = s_l \cdots s_n$ such that $H < I$.*
Let $g \in G$ and define $N := [I : H] = s_l \cdots s_{k-1}$, then for $t \ge 0$:

$$\{\rho_g^H(j) : j \in \{1 + (t-1)N, \ldots, tN\}\} = \{\rho_g^I(t)N - j : j \in \{0, \ldots, N-1\}\}$$

Thus if one has already calculated ρ_g^H, then ρ_g^I can be extracted from ρ_g^H in a numerical way.

Let $gT_H(1 + (t-1)N) = g_1^{m_1} \cdots g_n^{m_n}$ with $0 \le m_i < s_i$.
Since $N = s_l \cdots s_{k-1}$, the element $T_H(1+(t-1)N) = g_1^{n_1} \cdots g_n^{n_n} = g_1^{n_1} \cdots g_{l-1}^{n_{l-1}}$, ie for $i \ge l$ the numbers $n_i = 0$. Since $g_l, \ldots, g_{k-1} \in I$, the coset $T_H(tN)I = T_H(j)I$ for $j \in \{1 + (t-1)N, \ldots, tN\}$. Thus the representatives of the cosets $gT_H(j)H$ for $j \in \{1+(t-1)N, \ldots, tN\}$ have in their canonical expression all the same first part $g_1^{m_1} \cdots g_{l-1}^{m_{l-1}}$, ie for $j \in \{1+(t-1)N, \ldots, tN\}$ if $0 \le n_i < s_i$ and $gT_H(j) = g_1^{n_1} \cdots g_n^{n_n}$, then for $1 \le i \le l-1$ the number $n_i = m_i$. Thus $\rho_g^H(j) \in \{\rho_g^I(t)N - j : j \in \{0, \ldots, N-1\}\}$. Because ρ_g^H is injective the two sets have the same order. So they are equal to each other. □

Example. The group $D_4 = \langle r, t \mid r^4, t^2, t^{-1}rt = r^{-1} \rangle$ has presentation sequence r, r^2, t with $2, 2, 2$. For the calculation of ρ_r the values $T(i)$ and $rT(i)$ are evaluated:

i	1	2	3	4	5	6	7	8
$T(i)$	id	t	r^2	r^2t	r	rt	rr^2	rr^2t
$rT(i)$	r	rt	rr^2	rr^2t	r^2	r^2t	id	t
$\rho_r(i)$	5	6	7	8	3	4	1	2

Define $C_2 := \langle t \rangle$, then one has the following table for the calculation of $\rho_r^{C_2}$:

i	1	2	3	4
$T_{C_2}(i)$	id	r^2	r	rr^2
$rT_{C_2}(i)$	r	rr^2	r^2	id
$\rho_r^{C_2}(i)$	3	4	2	1

One sees that this table is up to the last row exactly the columns of the first table headed by the odd numbers. One gets $\rho_r^{C_2}(i)$ by dividing the even number of the $\rho_r(2i-1)$ and $\rho_r(2i)$ by 2. eg $\rho_r(1) = 5$ and $\rho_r(2) = 6$, thus $\rho_r^{C_2}(1) = \frac{6}{2} = 3$.

Lemma 8. *Let $g_1, \ldots, g_n$ and $s_1, \ldots s_n$ be a presentation sequence of G.*
Let $H < G$ such that $N := |H| = s_k \cdots s_n$ and $1 \le i \le \frac{|G|}{|H|}$.
If one takes $0 \le m_j < s_j$ such that $gT(1 + (i-1)N) = g_1^{m_1} \cdots g_{k-1}^{m_{k-1}} g_k^{m_k} \cdots g_n^{m_n}$, then

$$T_H(\rho_g^H(i))^{-1} g T_H(i) = g_k^{m_k} \cdots g_n^{m_n}.$$

Thus if one induces a representation ϕ of H to G, then the i-th matrix block is equal to $\phi(g_k^{m_k} \cdots g_n^{s_n})$.

Let Λ be a linear representation, S its inertia group in R and $\Pi(S) = G$. Let Γ be an extension of Λ to S. Let $g_1, \ldots, g_n$ and $s_1, \ldots, s_n$ be a presentation sequence of $G := \Pi(R)$, such that $H = \langle g_k, \ldots, g_n \rangle$ and $|H| = s_k \cdots s_n$. Now one wants to calculate Γ^R.
Since the to S extended linear representations of the same Wyckoff position differ by a constant, it is handy to evaluate Γ^R for one linear representation in the Wyckoff position and then calculate the factors for the different matrix blocks.
As transversal one takes: $\{g_1 \mid t_{g_1}\}^{m_1} \cdots \{g_{k-1} \mid t_{g_{k-1}}\}^{m_{k-1}}$ with the same enumeration as on the cosets of H, thus $\Pi(T_S(i)) = T_H(i)$. This choice of enumeration gives the same permutation matrix for S as for H.
To look how the induction of the representation Γ relates to a representation that differs only by a factor from Γ the following situation is studied:
Let $\Gamma : S \to GL_k$ be a representation and $\lambda_0, \ldots, \lambda_{n-k} \in \mathbb{C}$. Define $\Delta : \{g_k, \ldots, g_n\} \to GL_k$ to be the function such that $\Gamma(\{g_{k+i} \mid t_{g_{k+i}}\}) = \lambda_i \Delta(g_{k+i})$ for $0 \le i \le n-k$.

So $\Gamma(T_S(\rho(i))^{-1} \{g \mid t_g\} T_S(i))$ must be calculated for the matrix block. Take $m_1, \ldots, m_n$ such that $0 \le m_i < s_i$ and

$$gT_H(i) = g_1^{m_1} \cdots g_{k-1}^{m_{k-1}} g_k^{m_k} \cdots g_n^{m_n}$$

This gives in the space group:

$$T_S(\rho(i))^{-1} \{g \mid t_g\} T_S(i) = (\{g_1 \mid t_{g_1}\}^{m_1} \cdots \{g_{k-1} \mid t_{g_{k-1}}\}^{m_{k-1}})^{-1} \{g \mid t_g\} T_S(i) \in S$$

So

$$\begin{aligned}
&\Gamma(T_S(\rho(i))^{-1} \{g \mid t_g\} T_S(i)) = \Gamma(\,(\{g_1 \mid t_{g_1}\}^{m_1} \cdots \{g_{k-1} \mid t_{g_{k-1}}\}^{m_{k-1}})^{-1} \{g \mid t_g\} T_S(i)\,) \\
&= \Gamma(\{g_k \mid t_{g_k}\}^{m_k} \cdots \{g_n \mid t_{g_n}\}^{m_n}) \\
&\qquad \cdot \Gamma((\{g_1 \mid t_{g_1}\}^{m_1} \cdots \{g_{k-1} \mid t_{g_{k-1}}\}^{m_{k-1}} \{g_k \mid t_{g_k}\}^{m_k} \cdots \{g_n \mid t_{g_n}\}^{m_n})^{-1} \{g \mid t_g\} T_S(i)) \\
&= \lambda_0^{m_k} \cdots \lambda_{n-k}^{m_n} \Lambda \left[(\{g_1 \mid t_{g_1}\}^{m_1} \cdots \{g_{k-1} \mid t_{g_{k-1}}\}^{m_{k-1}} \{g_k \mid t_{g_k}\}^{m_k} \cdots \{g_n \mid t_{g_n}\}^{m_n})^{-1} \{g \mid t_g\} T_S(i) \right] \\
&\qquad \cdot \Delta(g_k)^{m_k} \cdots \Delta(g_n)^{m_n}
\end{aligned}$$

Thus if one has a list of matrices $\Delta(g_k)^{m_k} \cdots \Delta(g_n)^{m_k}$ then one only has to multiply the matrix block with the constant

$$\lambda_0^{m_k} \cdots \lambda_{n-k}^{m_n} \Lambda \left[(\{g_1 \mid t_{g_1}\}^{m_1} \cdots \{g_{k-1} \mid t_{g_{k-1}}\}^{m_{k-1}} \{g_k \mid t_{g_k}\}^{m_k} \cdots \{g_n \mid t_{g_n}\}^{m_n})^{-1} \{g \mid t_g\} T_S(i) \right]$$

to get the matrix block $\Gamma(T_S(\rho(i))^{-1} \{g \mid t_g\} T_S(i))$.

The function Δ determines an irreducible projective representation of H. So one only has to calculate the matrices $\Delta(g_k)^{m_k} \cdots \Delta(g_n)^{m_k}$ for the non-isomorphic irreducible projective representations of H. The constants

$$\lambda_0^{m_k} \cdots \lambda_{n-k}^{m_n} \Lambda \left[(\{g_1 \mid t_{g_1}\}^{m_1} \cdots \{g_n \mid t_{g_n}\}^{m_n})^{-1} \{g \mid t_g\} T_S(i) \right]$$

are calculated for every Wyckoff position and space group in the general coordinates of the Wyckoff position.

Note that the induction of irreducible representations in the symmorphic case is on the point group the same as the induction of the regular irreducible representations of a subgroup.
On the translation subgroup the induced representation is a matrix with on the diagonal matrix blocks that are diagonal with the orbit of Λ under G^*. So

$$t \mapsto [1, \cdots, [G:H]]B(e^{2\pi ik\cdot t}, \cdots, e^{2\pi i(T_H([G:H])^{-1})^{tr}k\cdot t})$$

Example. In this example we study irreducible representations of the space groups with point group generated by $r := \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ and $t := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. This point group is D_4. The space groups with point group D_4 up to isomorphism are:

$$R_1 := \{r \mid 0\}, \{t \mid 0\}$$
$$R_2 := \{r \mid 0\}, \left\{t \mid (\frac{1}{2}, \frac{1}{2})\right\}$$

The Wyckoff positions for $R^* = R_1$ are:
for t: $(x, 0)$ and $(x, \frac{1}{2})$
for rt: (x, x)
for r^2 none
for t, r^2: $(\frac{1}{2}, 0)$
for r none
for D_4: $(0, 0)$, $(\frac{1}{2}, \frac{1}{2})$
The representations for R_1, the symmorphic case. The groups generated by t and rt are isomorphic to C_2, thus these have -1 and 1 as irreducible representations. The group generated by t, r^2 is isomorphic to V_4, thus has $(\pm 1, \pm 1)$ as irreducible representations. For the irreducible representations of D_4 use the composition series $\langle r\rangle \lhd D_4$. Now r is of order 4, thus the group generated by r has the irreducible representations $\phi_k(r) := i^k$ for $k \in \{0, 1, 2, 3\}$. For the action of t on the representations first the action of t on r: now $trt^{-1} = r^{-1}$. Thus $\phi_k^t(r) = i^{-k}$. If k is 0 or 2 then $\phi_k^t = \phi_k$. So in that case the representations must be extended. That gives respectively $(1,1)$,$(1,-1)$ and $(-1,1)$,$(-1,-1)$. The representations i and $-i$ must be induced. That gives then $\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$.
For the space group R_2: define $Q := \{r \mid 0\}$ and $S := \left\{t \mid (\frac{1}{2}, \frac{1}{2})\right\}$
The representation for t: since $S^2 = \{id \mid (1, 0)\}$ the representations are $S \mapsto exp(\pi ix)$
for rt: take $Q \cdot S = \left\{rt \mid (-\frac{1}{2}, \frac{1}{2}\right\}$ as representative. Now $(Q \cdot S)^2 = \{id \mid 0\}$. Thus the representations are $QS \mapsto \pm 1$.
for t, r^2: the representative for r^2 is Q^2. The representations up to S are $\pm i$. Now $Q^{-2}SQ^2 = \{id \mid (-1, -1)\} S$. So $\Delta^{Q^2}(S) = -\Delta(S)$. Thus the representations are swapped by R^2. So there is one representation: $\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$.
For D_4: the representations extended to Q are ζ_4^j. Now $S^{-1}QS = \{id \mid (-1, 0)\} Q^{-1}$. Thus $\Delta^S(Q) = \Delta(\{id \mid (-1, 0)\})\Delta(Q^{-1})$. So for $(0, 0)$: $\Delta^S(Q) = \Delta(Q^{-1})$. Thus one has four one dimensional representations: $\pm 1, \pm 1$ and one two dimensional $\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. And for $(\frac{1}{2}, \frac{1}{2})$ one has four one dimensional representations: $\pm i, \pm i$ and one two dimensional $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$. The summary of above is in the tables below. The first table gives for elements of D_4 representatives. The translation part of the last element of the sequence in the first column is given in the next two columns by space group. So t, r^2 0 means that $\left\{r^2 \mid 0\right\}$ is an element of the space group. In the last two columns the relations are calculated for the representatives in Q. For the relations $r^{-2}tr^2 = t$ and $t^{-1}rt = r^{-1}$ the vectors u respectively v are given such that $Q^{-2}SQ^2 = \{id \mid u\} S$ and $S^{-1}QS = \{id \mid v\} Q^{-1}$. For each group up to conjugacy that is an inertia group, the Wyckoff positions are calculated. The linear representation in the column headed Wyckoff is extended to the irreducible representations given in the columns headed R_1 and R_2. In the column of R_i are the extended irreducible representations to the inertia group in R_i of the linear representation in the column headed Wyckoff. Again $\pm c$, with $c \in \{1, i\}$ indicates that the generator can be mapped both to c as to $-c$ to get the different extended irreducible

representation.

group	R_1	R_2	*rel*	R_1	R_2
t	0	$(\frac{1}{2}, \frac{1}{2})$	t^2	0	$(1, 0)$
rt	0	$(-\frac{1}{2}, \frac{1}{2})$	$(rt)^2$	0	0
t, r^2	0	0	$r^{-2}tr^2 = t, r^2$	0	$(-1, -1), 0$
r, t	0	0	$t^{-1}rt = r^{-1}, r^4$	$0, 0$	$(-1, 0), 0$

group	*Wyckoff*	R_1	R_2
t	$(x, 0)$	± 1	$\exp(\pi i x)$
	$(x, \frac{1}{2})$	± 1	$\exp(\pi i x)$
rt	(x, x)	± 1	± 1
t, r^2	$(\frac{1}{2}, 0)$	$\pm 1, \pm 1$	$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
r, t	$(0, 0)$	$\pm 1, \pm 1$	$\pm 1, \pm 1$
		$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
	$(\frac{1}{2}, \frac{1}{2})$	$\pm 1, \pm 1$	$\pm i, \pm i$
		$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$

Define $e : \mathbb{C} \to \mathbb{C}$ by $e(z) := exp(2\pi i z)$ for all $z \in \mathbb{C}$.
For the induction to the whole space group of the representations of $C_2 := \langle t \rangle$ and $V_4 := \langle t, r^2 \rangle$ we take the presentation sequence r, r^2, t with $2, 2, 2$. For r we have then the following table

i	1	2	3	4	5	6	7	8
$T(i)$	id	t	r^2	r^2t	r	rt	rr^2	rr^2t
$rT(i)$	r	rt	rr^2	rr^2t	r^2	r^2t	id	t
$\rho_r(i)$	5	6	7	8	3	4	1	2

Thus $\rho_r^{C_2} = [3, 4, 2, 1]$ and $\rho_r^{V_4} = [2, 1]$
For t we have then the following table

i	1	2	3	4	5	6	7	8
$T(i)$	id	t	r^2	r^2t	r	rt	rr^2	rr^2t
$tT(i)$	t	id	r^2t	r^2	rr^2t	rr^2	rt	r
$\rho_r(i)$	2	1	4	3	8	7	6	5

Thus $\rho_t^{C_2} = [1, 2, 4, 3]$ and $\rho_t^{V_4} = [1, 2]$.
First the induction to the symmorphic space group R_1 is calculated for the representation of C_2 and V_4.
The representations $\phi_i : t \mapsto (-1)^i$.
For the values of $(t_1, t_2) \in T$ one must calculate the orbit of $k := (x, 0)$ and $k' := (x, \frac{1}{2})$:

g	id	r^2	r	r^3
$(g^{-1})^{tr}k$	$(x, 0)$	$(-x, 0)$	$(0, -x)$	$(0, x)$
$(g^{-1})^{tr}k'$	$(x, \frac{1}{2})$	$(-x, -\frac{1}{2})$	$(\frac{1}{2}, -x)$	$(-\frac{1}{2}, x)$

Thus $\phi_i^{D_4}(t_1, t_2) = [1, 2, 3, 4]B(e(xt_1), e(-xt_1), e(-xt_2), e(xt_2))$
Since in the table of r for all odd i the $rT(i)$ involve no t, for all i the following holds:
$T_{C_2}(\rho_r^{C_2}(i))^{-1} r T_{C_2}(i) = id$.
So $\phi_i^{D_4}(r) = \rho_r^{C_2} B(1, 1, 1, 1) = [3, 4, 2, 1]B(1, 1, 1, 1)$
In the table of t for all odd i the $tT_{C_2}(i)$ involve t, so for all i the following holds: $T_{C_2}(\rho_r^{C_2}(i))^{-1} r T_{C_2}(i) = t$.
So $\phi_i^{D_4}(t) = \rho_t^{C_2} B((-1)^i, (-1)^i, (-1)^i, (-1)^i) = [2, 1, 4, 3]B((-1)^i, (-1)^i, (-1)^i, (-1)^i)$.
The representations of V_4 are $\phi_{ij} : t \mapsto (-1)^i, r^2 \mapsto (-1)^j$.
Now $rT(1) = r$ thus the first matrix block is $\phi_{ij}(id) = 1$. Since $rT(5) = r^2$ the second matrix block is $\phi_{ij}(r^2) = (-1)^j$.
Thus $\phi_{ij}(r) = [2, 1]B(1, (-1)^j)$
Because $tT(1) = t$ the first matrix block is $\phi_{ij}(t) = (-1)^i$. Now $tT(5) = rr^2t$, thus the second matrix block is $\phi_{ij}(r^2t) = (-1)^i(-1)^j$.
Thus $\phi_{ij}(t) = [1, 2]B((-1)^i, (-1)^{j+i})$.

The induction to R_2 of the extension of the representation of k to C_2 is calculated.
The representation $\Gamma_i : S \mapsto (-1)^i e(\frac{x}{2})$ must be induced to R_2.
Now $\Gamma_i(S) = e(\frac{x}{2})\phi_i(t)$, thus the representations differ by the factor $e(\frac{x}{2})$ and the algorithm to calculate the factors can start.
Since for the odd i the $rT(i) \in \langle r \rangle$, all the factors are 1.
So $\Gamma_i^{D_4}(r) = \phi_i^{D_4}(r)$.
The factors for S are now calculated for each matrix block.
Since $tT(1) = t$, one has the factor $e(\frac{x}{2})k[T^{-1}Tid] = k[id] = e(\frac{x}{2})$.
Since $tT(3) = r^2t$, one must calculate $S^{-1}Q^{-2}SQ^2$:

$$S^{-1}Q^{-2}SQ^2 = \left\{ id \mid (-t^{-1} + t^{-1}r^2) \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} \right\} = \left\{ id \mid \begin{pmatrix} -1 \\ 0 \end{pmatrix} \right\}$$

Since $k[(-1, 0)] = -x$ and r^2t has a t the factor is $e(\frac{x}{2})e(-x) = e(-\frac{x}{2})$.
Because $tT(5) = rr^2t$, one must calculate $S^{-1}Q^{-3}SQ$:

$$S^{-1}Q^{-3}SQ = \left\{ id \mid (-t^{-1} + t^{-1}r) \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} \right\} = \left\{ id \mid \begin{pmatrix} -1 \\ 0 \end{pmatrix} \right\}$$

Since $k[(-1, 0)] = -x$ and rr^2t has a t the factor is $e(\frac{x}{2})e(-x) = e(-\frac{x}{2})$.
Now $tT(7) = rt$, thus one must calculate $S^{-1}Q^{-1}SQ^3$:

$$S^{-1}Q^{-1}SQ = \left\{ id \mid (-t^{-1} + t^{-1}r^3) \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} \right\} = \left\{ id \mid \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\}$$

Since $k[(0, 1)] = 0$ and rt has a t the factor is $e(\frac{x}{2})e(0) = e(\frac{x}{2})$.
Thus $\Gamma_i^{D_4}(t) = [2, 1, 4, 3]B((-1)^i e(\frac{x}{2}), (-1)^i e(\frac{x}{2}), (-1)^i e(-\frac{x}{2}), (-1)^i e(\frac{x}{2}))$.
For $k' = (x, \frac{1}{2})$ the image of S is the same. Thus one wants to induce $\Gamma'_i : S \to (-1)^i e(\frac{x}{2})$. The induced representation has the same image of Q as for k. For S one gets the factors $k'[(0, 0)], k'[(-1, 0)], k'[(-1, 0)]$ and $k'[(0, 1)]$. Thus

$$\begin{aligned}
{\Gamma'}_i^{D_4}(Q) &= [3, 4, 2, 1]B(1, 1, 1, 1) \\
{\Gamma'}_i^{D_4}(S) &= [2, 1, 4, 3]B((-1)^i e(\frac{x}{2}), (-1)^i e(\frac{x}{2}), (-1)^i e(-\frac{x}{2}), -(-1)^i e(\frac{x}{2}))
\end{aligned}$$

We calculate the induction of the from $(\frac{1}{2}, 0)$ extended projective representation

$$\Gamma : S \mapsto \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, Q^2 \mapsto \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

For $g \in \{r, t\}$ if $gT_{V_4}(n) = r^i(r^2)^j t^k$ then the n-th matrix block is $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}^j \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}^k$.
This gives for Q the matrix blocks $\Gamma(id), \Gamma(Q^2)$.
For S gives this the matrix blocks $\Gamma(id), \Gamma(Q^2)\Gamma(S)$. Since $(\frac{1}{2}, 0) \cdot (-1, 0) = -\frac{1}{2}$ the second matrix block has factor -1. Thus

$$\begin{aligned}
\Gamma^{D_4}(Q) &= [2, 1]B(\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}) \\
\Gamma^{D_4}(S) &= [1, 2]B(\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix})
\end{aligned}$$

3.4 The dimensions of the extended irreducible representations

The following is about a proof of the next theorem that is a generalization of the well known fact that the order of a group is equal to the sum of the squares of the dimensions of its irreducible representations. The representations are over K a splitting field of both G and $N \triangleleft G$.

Theorem 11. *Let $N \triangleleft G$ and Δ an irreducible G-invariant representation of N. Let $\Psi_1, \ldots, \Psi_r$ be the irreducible representations of G that restricted to N have Δ as irreducible constituent. Then:*

$$(\dim \Delta)^2 |G/N| = \sum_{i=1}^{r} (\dim \Psi_i)^2$$

In the case that G/N is solvable there is a short proof of the theorem.

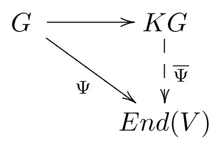
Theorem 12. *If G/N is solvable, then preceding theorem holds.*

With induction on $|G/N|$ the theorem will be proven. Let Δ be a G-invariant representation of N. Take $G' \triangleleft G$ such that $[G'/N : G/N] = p$. Let O be an orbit of irreducible representations of G' and B the set of irreducible representations of G that restricted to G' have a character of O as constituent. Now $p \sum_{\Psi \in O} (\dim \Psi)^2 = \sum_{\lambda \in B} (\dim \lambda)^2$, because
if $I_G(\phi) = G'$, then $|O| = p$, $|B| = 1$ and $\frac{\dim \lambda}{\dim \Psi} = p$.
if $I_G(\phi) = G$, then $|O| = 1$, $|B| = p$ and $\frac{\dim \lambda}{\dim \Psi} = 1$.
Let $\Psi_1, \ldots, \Psi_r$ be the irreducible representations of G' that restricted to N have Δ as constituent and $\Lambda_1, \ldots, \Lambda_k$ the irreducible representations of G that restricted to N have Δ as constituent. Since Δ is G-invariant it is also G'-invariant. So by induction $(\dim\ \Delta)^2 |G'/N| = \sum_{i=1}^{r} (\dim\ \Psi_i)$. Thus

$$(\dim \Delta)^2 |G/N| = p(\dim \Delta)^2 |G'/N| = p \sum_{i=1}^{r} (\dim \Psi_i)^2 = p \sum_{j=1}^{k} \sum_{\Psi \in O_j} (\dim \Psi)^2 = \sum_{j=1}^{k} (dim\ \Lambda_j)^2$$

□

The proof of the general case will be analogue to the proof of the fact that the sum of the squares of the dimensions of the irreducible representations is equal to the order of the group. The proof of that is split into two parts. The first part is that representations are in one to one correspondence to modules of the group ring KG. The irreducible representations correspond exactly with the simple modules. The correspondence is illustrated by the diagram below: For every representation Ψ on a vector space V, there is a unique ring homomorphism $\overline{\Psi}$ such that the diagram commutes.

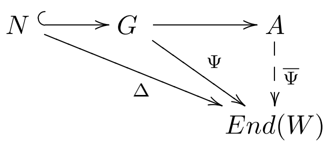


The second part is that the group ring is semisimple and hence the theory of semisimple rings can be used. In particular the following theorem is used:

Theorem 13. *If K is the splitting field of the semisimple K-algebra A, then the sum of the squares of the dimensions of the irreducible A-modules is equal to $\dim_K(A)$. If K is algebraically closed then it is a splitting field.*

In the text below $N \triangleleft G$ and V is an irreducible G-invariant KN-module with representation Δ.

So first find a ring which irreducible modules are exactly the irreducible representation of G that restricted to N have Δ as constituent. By Clifford's theorem $\Psi|_N = e\Delta$. Thus the ring must force $n \in N$ to act on the modules like $\Delta(n)$. For an appropriate algebra A the following must hold. For each KG-module W that as KN-module is isomorphic to a direct sum of V's with representation $\Psi : G \to GL(W)$, there is a unique ring homomorphism $\overline{\Psi} : A \to End(W)$ such that the diagram below commutes.



For $n, m \in N$ and $g, h \in G$ the following holds: $\Psi(ngmh) = \Delta(n)\Delta(gmg^{-1})\Psi(gh)$. Now $\Delta(n)$ generates as K-vector space the simple ring of $n \times n$-matrices $M_{n\times n}$. The action of G on Δ can be extended linearly to $M_{n\times n}$.

Lemma 9. *For $M \in M_{n\times n}$ and $g \in G$ define M^g as follows:*
For $n \in N$ take $a_n \in K$ such that $\sum_{n\in N} a_n\Delta(n) = M$. Now $M^g := \sum_{n\in N} a_n\Delta(gng^{-1})$.
This definition is independent of the choice of the a_n's. Let $M, L \in M_{n\times n}$, $k \in K$ and $g, h \in G$, then $M^{gh} = (M^h)^g$, $(ML)^g = M^gL^g$, $(M+L)^g = M^g + L^g$ and $(k\,id)^g = k\,id$.
Also if $n \in N$, then $M^n = \Delta(n)M\Delta(n)^{-1}$.

Since $G = I_G(\Delta)$, one has $\Delta \equiv \Delta^g$. Thus there is a $T \in GL_n(K)$ such that for all $n \in N$: $T\Delta(n)T^{-1} = \Delta(gng^{-1})$. So $M^g = TMT^{-1}$. The statements of the lemma follow from this. □

With the comments above in mind one comes to the following definition.

Definition 15.

$$M^{\Delta}_{n\times n}G := \{\sum_{g\in G} a_g g : g \in G, a_g \in M_{n\times n}\}$$

With the addition and multiplication defined by:

$$\sum_{g\in G} a_g g + \sum_{g\in G} b_g g = \sum_{g\in G}(a_g + b_g)g$$

$$(\sum_{g\in G} a_g g)(\sum_{g\in G} b_g g) = \sum_{g,h\in G}(a_g b_h^g)gh = \sum_{g\in G}(\sum_{h\in G} a_g b^g_{h^{-1}g} g)$$

Let $I := \langle n - \Delta(n) | n \in N\rangle$ generated as two-sided ideal in $M^{\Delta}_{n\times n}G$.

$$A^{\Delta}_G := M^{\Delta}_{n\times n}G/I.$$

So A^{Δ}_G will play the same role as KG for the special case.

Lemma 10. *$M^{\Delta}_{n\times n}G$ is an associative algebra.*

Only the associativity of the algebra will be proven. Let $a, b, c \in M_{n\times n}$ and $g_1, g_2, g_3 \in G$. Then by lemma 9:
$(ag_1bg_2)cg_3 = (ab^{g_1}g_1g_2)cg_3 = ab^{g_1}c^{g_1g_2}g_1g_2g_3 = a(bc^{g_2})^{g_1}g_1g_2g_3 = ag_1(bc^{g_2})g_2g_3 = ag_1(bg_2cg_3)$. □

With a chosen transversal of N, one sees that A^{Δ}_G is isomorphic to a kind of $M_{n\times n}(G/N)$ ring.

Lemma 11. *Let $g_1, \ldots, g_s$ be a transversal of N. Define $n_{ij} \in N$ and $\delta(i,j)$ by $g_ig_j = n_{ij}g_{\delta(i,j)}$. Then $B := \{\sum_{i=1}^s a_ig_i | a_i \in M_{n\times n}\}$ with addition and multiplication defined by:*

$$\sum_{i=1}^s a_ig_i + \sum_{i=1}^s b_ig_i = \sum_{i=1}^s(a_i + b_i)g_i$$

$$(\sum_{i=1}^s a_ig_i)(\sum_{i=1}^s b_ig_i) = \sum_{i,j}(a_ib_i^{g_i}\Delta(n_{ij}))g_{\delta(i,j)}$$

is an associative algebra and isomorphic to A^{Δ}_G.

The associativity of B: let $a, b, c \in M_{n\times n}$ and $1 \leq i, j, k \leq s$, then:

$$(ag_ibg_j)cg_k = ab^{g_i}\Delta(n_{ij})g_{\delta(i,j)}cg_k = ab^{g_i}\Delta(n_{ij})c^{g_{\delta(i,j)}}\Delta(n_{\delta(i,j)k})g_{\delta(\delta(i,j),k)}$$
$$ag_i(bg_jcg_k) = ag_ibc^{g_j}\Delta(n_{jk})g_{\delta(j,k)} = a(bc^{g_j}\Delta(n_{jk}))^{g_i}\Delta(n_{i\delta(j,k)})g_{\delta(i,\delta(j,k)}$$

Now

$$c^{g_{\delta(i,j)}} = c^{n_{ij}^{-1}g_ig_j} = \Delta(n_{ij})^{-1}c^{g_ig_j}\Delta(n_{ij})$$

and by the associativity of the group multiplication:

$$n_{ij}n_{\delta(i,j)k} = g_in_{jk}g_i^{-1}n_{i\delta(j,k)}$$
$$g_{\delta(\delta(i,j),k)} = g_{\delta(i,\delta(j,k))}$$

Thus $(ag_ibg_j)cg_k = ag_i(bg_jcg_k)$. Therefore B is an associative algebra.
For $g \in G$ define $i(g)$ and $n_g \in N$ such that $g = n_g g_{i(g)}$.
Define $\phi : M^{\Delta}_{n\times n}G \to B$, by $\phi(\sum_{g\in G} a_g g) := \sum_{g\in G} a_g \Delta(n_g) g_{i(g)}$.
It is clear that ϕ is additive. For the multiplicativity of ϕ:

$$\begin{aligned}\phi(agbh) &= \phi(ab^g gh) = ab^g \Delta(n_{gh}) g_{i(gh)} \\ \phi(ag)\phi(bh) &= a\Delta(n_g) g_{i(g)} b \Delta(n_h) g_{i(h)} = a\Delta(n_g)(b\Delta(n_h))^{g_{i(g)}} \Delta(n_{i(g)i(h)}) g_{\delta(i(g),i(h))}\end{aligned}$$

Now

$$b^{g_{i(g)}} = b^{n_g^{-1}g} = \Delta(n_g)^{-1} b^g \Delta(n_g)$$

and by the fact that $n_{gh} g_{i(gh)} = gh = n_g g_{i(g)} n_h g_{i(h)}$:

$$\begin{aligned}n_{gh} &= n_g g_{i(g)} n_h g_{i(g)}^{-1} n_{i(g)i(h)} \\ g_{i(gh)} &= g_{\delta(i(g),i(h))}\end{aligned}$$

Thus $\phi(agbg) = \phi(ag)\phi(bh)$, concluding that ϕ is a ring homomorphism. Since $\phi(\Delta(n) - n) = 0$, $I \subset ker\,\phi$. It is clear that B as Abelian group can be embedded in $M^{\Delta}_{n\times n}G$ and $B/I = A^{\Delta}_{G}$. Thus $ker\,\phi = I$, so $B \cong A^{\Delta}_{G}$. □

Corollary 2. $\dim_K A^{\Delta}_{G} = (\dim_K \Delta)^2 |G/N|$

So the dimension of A^{Δ}_{G} is as desired.

Lemma 12. *Let Φ be a representation of G such that $\Phi|_N = e\Delta$, then Φ induces an A^{Δ}_{G}-representation.*

Let $M = \sum_{n\in N} a_n \Delta(n)$, then define $\Phi(M) := \sum_{n\in N} a_n \Phi(n)$. This is independent of the choice of the a_n's, since $\Phi|_N = e\Delta$. Let $L = \sum_{n\in N} b_n \Delta(n)$, then

$$\Phi(ML) = \sum_{n,m\in N} a_n b_m \Phi(nm) = \sum_{n\in N} a_n \Phi(n) \sum_{n\in N} b_n \Phi(n) = \Phi(M)\Phi(L).$$

Thus Φ is a ring homomorphism. Also

$$\Phi(M^g) = \Phi(\sum_{n\in N} a_n \Delta(gng^{-1})) = \sum_{n\in N} a_n \Phi(gng^{-1}) = \Phi(g)\Phi(M)\Phi(g)^{-1}$$

Now $\phi : M^{\Delta}_{n\times n}G \to End(W)$ is defined by:

$$\phi(\sum_{g\in G} a_g g) := \sum_{g\in G} \Phi(a_g)\Phi(g).$$

It is clear that ϕ is additive. The multiplication:

$$\phi(\sum_{g\in G} a_g g)\phi(\sum_{g\in G} b_g g) = \sum_{g\in G} \Phi(a_g)\Phi(g) \sum_{g\in G} \Phi(b_g)\Phi(g) = \sum_{g.h\in g} \Phi(a_g)\Phi(g)\Phi(b_h)\Phi(h)$$

$$\begin{aligned}\phi((\sum_{g\in G} a_g g)(\sum_{g\in G} b_g g)) &= \sum_{g,h\in G} \Phi(a_g b_h^g)\Phi(gh) = \sum_{g,h\in G} \Phi(a_g)\Phi(g)\Phi(b_h)\Phi(g)^{-1}\Phi(gh) \\ &= \sum_{g.h\in g} \Phi(a_g)\Phi(g)\Phi(b_h)\Phi(h)\end{aligned}$$

So ϕ is a ring homomorphism. Now $I \subset ker\,\phi$, since $\phi(n) = \Phi(n) = \phi(\Delta(n))$. Thus ϕ factors through I. □

Thus the irreducible KG-modules that have Δ as constituent are also A^{Δ}_{G}-modules.

Lemma 13. *Let W be an A^{Δ}_{G}-module, then $W =_{KN} \bigoplus_{i=1}^{r} V$.*

W is also a $M_{n\times n}$-module. Since $M_{n\times n}$ is semisimple and V is its only simple module, $W =_{M_{n\times n}} \bigoplus_{i=1}^r V$. Because W is an A_G^Δ-module, $KNv = M_{n\times n}v$ for every $v \in W$. Thus $W =_{KN} \bigoplus_{i=1}^r V$. □

By lemma 12 and lemma 13 the ring A_G^Δ is the correct ring for the representations that have restricted to N only Δ as constituent.

Lemma 14. *Let W be a A_G^Δ-module, then W is also a KG-module and $U <_{A_G^\Delta} W$ iff $U <_{KG} W$.*
Also if V is a A_G^Δ-module, then $Hom_{A_G^\Delta}(V, W) = Hom_{KG}(V, W)$.
E.g. the morphisms of modules and the submodules of a module are the same when consideerd as A_G^Δ-modules or as KG-modules.

Since $KG < M_{n\times n}^\Delta G$, W is a KG-module. For $g \in G$ define $g \cdot v := (g + I)v$. Thus the image is the same, since $\Delta(n)$ spans $M_{n\times n}$.
Let $\phi : V \to W$, then $\phi(gv) = g\phi(v)$ iff $\phi((g + I)v) = (g + I)\phi(v)$. □

Corollary 3. *A_G^Δ is a semisimple ring.*

Theorem 14. *Let $N \triangleleft G$ and V a G-invariant KN-module with representation Δ.*
The KG-modules that as KN-modules have only V as constituent are in one-to-one correspondence to the A_G^Δ-modules.
Moreover the simple KG-modules that as KN-modules have V as constituent are in one-to-one correspondence to the simple A_G^Δ-modules.

The theorem is a direct consequence of the lemmas 12, 13 and 14 and Clifford's theorem. □

The theorem 11 follows now from corollary 2 and 3 and theorem 14.

The theorem is also a direct consequence of the following theorem of Karpilovsky in the projective representation theory.

Theorem 15. *[Ka85] Let V be a G-invariant absolutely irreducible projective representation. Then there is a projective representation $ext(V)$ of G on the same vector space. Moreover if $\{U_1, \ldots, U_m\}$ is a full set of non-isomorphic irreducible projective representations of G/N of a certain factor system, dependent of V, then $\{U_i \otimes ext(V)\}$ is the full set of non-isomorphic irreducible projective representations whose restriction to N is a direct sum of copies of V.*

Just like in regular representation theory one has in projective representation theory that the sum of the squares of the dimensions of the irreducible representations is equal to the order of the group. Thus

$$\sum_{i=1}^{n}(dim\ U_i \otimes ext(V))^2 = \sum_{i=1}^{n}(dim\ U_i)^2(dim\ V)^2 = |G/N|(dim\ V)^2$$

4 Calculating Orbit Representatives

To have a picture of the irreducible representations of a space group it is natural to categorize them by the linear characters occurring in the restrictions to T. The goal of finding all irreducible representations of a space group is of course a little vague. With the method described in the previous chapters it is possible to calculate all the irreducible representations. But the set of irreducible representations contains isomorphic representations. The representations are isomorphic because their linear characters lie in one orbit under the symmorphic space group with point group G^*. The goal is to find a set of orbit representatives for the affine action of the space group. The orbit representatives are found with the theory of fundamental domains.

4.1 G-actions and fundamental domains

Definition 16. *Let $X \subset \mathbb{R}^n$ be a G-space and let $F \subset X$, then F is a* fundamental domain *of X with respect to G iff:*

1. *F is closed and convex*
2. *for all $x \in X$ there exists a $(g, y) \in G \times F$ with $gy = x$*
3. *F^0 has for each orbit at most one representative.*

The second part of the definition says that a fundamental domain contains a set of orbit representatives. Thus for each orbit there is at least one point in the orbit that is also in the fundamental domain. The third one says that a point in the interior of a fundamental domain has in its orbit no other points that are also in the interior. However, the boundary of a fundamental domain can have multiple points of the same orbit. A fundamental domain is an approximation of the set of orbit representatives.

Theorem 16 (Voronoi-Dirichlet)**.** *Let d be a G-invariant metric on X. For $x, y \in X$ define $H(x, y) := \{z \in X \,|\, d(x, z) \le d(y, z)\}$. Let $x \in X$, such that the stabilizer $Stab_G(x)$ of x is trivial and the orbit x^G is discrete in X. Then $D(x, x^G) := \bigcap_{g \in G} H(x, gx)$ is a fundamental domain. i.e. the intersection of the halfspaces of points which are closer to x than to any other orbit point is a fundamental domain.*

Since $H(x, y)$ is closed and convex for all $x.y \in X$, also $D(x, x^G)$ is closed and convex. Let $g \in G$, then $gH(x, y) = H(gx, gy)$. Since

$$\begin{aligned} gH(x,y) = \{gz \in X \,|\, d(x,z) \le d(y,z)\} &= \{z \in X \,|\, d(x, g^{-1}z) \le d(y, g^{-1}z)\} \\ &= \{z \in X \,|\, d(gx, z) \le d(gy, z)\} = H(gx, gy). \end{aligned}$$

Let $z \in X$. There is a point y in the orbit of x, such that z is as close or closer to y as to any other point in the orbit of x. Let $g \in G$ be such that $y = gx$. Now $g^{-1}z \in D(x, x^G)$. Thus $D(x, x^G)$ contains a set of orbit representatives.
Let $y \in D(x, x^G)^0$, then for all $z \in x^G$, one has $y \in H(x, z)^0$. Thus $d(x, y) < d(z, y)$, for all $z \in x^G - x$. Let $g \in G - id$. One has $d(x, gy) = d(g^{-1}x, y) > d(x, y) = d(gx, gy)$, therefore $gy \notin D(x, x^G)$. Concluding that $D(x, x^G)^0$ has for each orbit at most one representative. □

Corollary 4. *Let $x \in X$, then*

$$D(x, x^G)^0 \cap gD(x, x^G)^0 = \begin{cases} \emptyset & \text{if } x \neq gx \\ D(x, x^G)^0 & \text{if } x = gx \end{cases}$$

$$X = \bigcup_{y \in x^G} D(y, y^G)$$

Building a fundamental domain for the whole group from fundamental domains of subgroups is more difficult. There is however a special case where this can be done.

Theorem 17. *Let $x \in X$ and $S := Stab_G(x)$. Assume that S has a complement T in G, i.e $G = ST$ and $S \cap T = \{e\}$. If $y \in X$ such that $Stab_S(y)$ is trivial, then $D(y, y^S) \cap D(x, x^T)$ is a fundamental domain. Thus the points that are closer to y than any other orbit point of y^S and also closer to x than any other orbit point of x^T are a fundamental domain.*

The fist step is to show that $sD(x, x^T) = D(x, x^T)$ for $s \in S$. For $t \in T$ define $s_t \in S$ and $u_t \in T$ such that $st = u_t s_t$. Notice that $t \mapsto u_t$ is a bijection. Now

$$\begin{aligned} sD(x, x^T) &= s \bigcap_{t \in T} H(x, tx) = \bigcap_{t \in T} H(sx, stx) \\ &= \bigcap_{t \in T} H(x, sts_t^{-1} x) = \bigcap_{t \in T} H(x, u_t x) = D(x, x^T) \end{aligned}$$

If $z \in X$, then there is one $t \in T$ such that $tz \in D(x, x^T)$. For tz there is one s such that $stz \in D(y, y^S)$. Since $D(x, x^T)$ is S invariant $stz \in D(y, y^S) \cap D(x, x^T)$.
Assume that $z \in (D(y, y^S) \cap D(x, x^T))^0$. Assume also $gz \in (D(y, y^S) \cap D(x, x^T))^0$. Now $z, gz \in D(y, y^S)^0$ and $z, gz \in D(x, x^T)^0$, because $A \subset B \Rightarrow A^0 \subset B^0$. Take $s' \in S$ and $t' \in T$, such that $g = s't'$. Then $t'z \in s^{-1} D(x, x^T)^0 = D(x, x^T)^0$. Thus $t' = id$. Now $s'(z) \in D(y, y^S)^0$, thus $s' = id$. Concluding that $g = id$. So $D(y, y^S) \cap D(x, x^T)$ is a fundamental domain. □

Corollary 5. *If $G = N \rtimes H$, with $Stab_G(x) = H$ and $Stab_H(y) = 1$, then $D(y, y^H) \cap D(x, x^N)$ is a fundamental domain.*

So for calculating fundamental domains of symmorphic space groups one can first calculate the Voronoi cell with respect to the translation lattice and then consider the action of the point group on the Voronoi cell. This is the usual way of finding a fundamental domain for the linear representations of T.
Since there is already an algorithm for calculating a Vonoroi cell the only question is to calculate a fundamental domain of the point group on hyperplanes.
In both theorems the G-space X is fixed.
The following method applies the concept of base and strong generating set from computational group theory to the construction of fundamental domains.

Definition 17. *Let $x_1, \ldots, x_n \in X$, then G_i and F_i for $0 \leq i \leq n$ are defined inductively:*

$$\begin{aligned} G_0 &:= G, \quad G_{i+1} := Stab_{G_i}(x_i) = Stab_G(x_1) \cap \ldots \cap Stab_G(x_i) \\ F_0 &:= X, \quad F_{i+1} := D_{F_i}(x_i, x_i^{G_i}) \end{aligned}$$

The sequence $(x_1, \ldots, x_n)$ is called a base *if $G_n = 1$. If also $G_i \neq G_{i+1}$ for $0 \leq i \leq n-1$, then it is called* non-redundant*.*

Thus G_i fixes the points $x_1, \ldots, x_i$. The set F_i is the set of points in X that for $0 \leq j \leq i-1$ are closer to x_{j+1} then to any other point in the orbit $x_{j+1}^{G_j}$.

Lemma 15. *Let $(x_1, \ldots, x_n)$ be a base, then F_n is a fundamental domain of X with respect to G.*

For every $x \in X$ there is a $(g, y) \in G \times F_n$ such that $gy = x$, since for every $x \in F_i$ there is a $(g_i, y_i) \in G_i \times F_{i+1}$ sucht that $g_i y_i = x$.
With induction on i one can prove that for $x, y \in F_i^0$ and $g, h \in G$ if $gx = hy$, then $g^{-1}h \in G_i$:
For $i = 0$, $G_0 = G$, thus the conclusion is obvious. Assume that if $x, y \in F_i^0$ and $gx = hy$, then $g^{-1}h \in G_i$
Assume that $x, y \in F_{i+1}^0$ and $gx = hy$, then by the induction hypothesis $g^{-1}h \in G_i$. Now $g^{-1}h(y) = g^{-1}gx = x$. Thus $g^{-1}h(F_{i+1}^0) = F_{i+1}^0$ (corollary 4). So $g^{-1}h(x_i) \in x_i^{G_i} \cap F_{i+1}^0 = \{x_i\}$. Combining this with $g^{-1}h \in G_i$ it follows that $g^{-1}h \in G_{i+1}$.
Because $G_n = 1$, since $(x_1, \ldots, x_n)$ is a base, F_n is a fundamental domain. □

The preceding lemma gives rise to an algorithm for finding a fundamental domain. The problem is to calculate the vertices of the objects given by inequalities. This can be done with linear algebra and will be considered in the next paragraph.

4.2 Polytopes

The goal of this section is to describe an algorithm that calculates vertices of spaces given as intersections of half-spaces.

Definition 18. *Let $X \subset \mathbb{R}^n$, then the* convex hull $C(X)$ *is defined as follows:*

$$C(X) := \bigcap_{X \subset V, V \ convex} V$$

Lemma 16. *[Ca11]* $C(X) = \{\sum_{i=1}^{m} \alpha_i x_i : m \in \mathbb{N}, x_i \in X, \alpha \in [0,1]^m, \sum_{i=1}^{m} \alpha_i = 1\}$
Thus a point $v \in \mathbb{R}^n$ is in the convex hull of X iff there is a finite set $S \subset X$ such that v is in the convex hull of S.

Definition 19. *A* polytope *is a convex hull of a finite set of points.*

Besides this definition a polytope is also often defined as an intersection of halfspaces. An intersection of finitely many halfspaces is a convex hull of a finite set of points if and only if it is bounded, see [GR67] 3.1.3. Since the fundamental domains of the space groups are bounded, this definition is chosen.

Definition 20. *Let $P \subset \mathbb{R}^n$ be non-empty then the* dimension *of P is defined as follows:*

$$Dim(P) := \inf\{\dim(V) | V \text{ linear subspace of } \mathbb{R}^n | \exists_{x \in \mathbb{R}^n} P \subset V + x\}$$

Notation: dim *is only used for vector spaces, but Dim for all subsets of $\mathbb{R}^n$.*

Lemma 17. *Let $X = \{x_1, \ldots, x_m\} \subset \mathbb{R}^n$ and $V := \langle x_1 - x_i | 1 \le i \le m \rangle$. Then $Dim(X) = \dim(V)$.*
Assume that V, W are linear spaces and $x, y \in \mathbb{R}^n$ such that $P \subset V + x$ and $P \subset W + y$. If $\dim(V) = \dim(W) = Dim(P)$, then $V + x = W + y$ and $V = W$.
Thus the dimension of P is the dimension of the smallest vector space V such that $P \subset V + x$ for a $x \in \mathbb{R}^n$.

The first statement is a consequence of the observation that $Dim(P) = Dim(P + x)$, for $x \in \mathbb{R}^n$. WLOG assume that $0 \in P$. Then $V + x = V$ and $W + y = W$. So $P \subset V \cap W$. Thus $\dim(V \cap W) = \dim(V) = \dim(W)$, so $V = W$. □

Definition 21. *Let P be a polytope and V a linear space such that $P \subset V + x$ and $Dim(P) = \dim(V)$. The* boundary *of P denoted by ∂P and the* interior *of P denoted by P^0 are defined as the boundary respectively the interior of P in the topology of $V + x$ induced by $\mathbb{R}^n$.*

Definition 22. *Let $p \in \mathbb{R}^n$ and $c \in \mathbb{R}$. Then:*

- $h_{p,c} := \{x \in \mathbb{R}^n \mid \langle x, p \rangle \le c\}$ *is called a* half space*,*
- $H_{p,c} := \{x \in \mathbb{R}^n \mid \langle x, p \rangle = c\}$ *is called a* hyperplane.

Definition 23. *Let $P := C(X)$ be an n-dimensional polytope. $Q \subset P$ is called a* face *of P if $Q \subset \partial P$ and there is a hyperplane H such that $H \cap P = Q$.*

- *0-dimensional faces are called* vertices*. $V(P)$ is the set of vertices of P.*
- *1-dimensional faces are called* edges.
- *$(n-1)$-dimensional faces are called* facets.

The faces of P are themselves also polytopes, since a face is equal to the convex hull of the points of X that are on that face.

Theorem 18. *[St35] Let $X = (x_1, \ldots, x_m)$ such that $P = C(X)$, then $C(V(P)) = P$. So the set of vertices of P is the smallest set $Y \subset P$, such that P is the convex hull of Y.*

Definition 24. *Let P be a polytope, the* boundary hyperplanes *$Pl(P)$ are defined as follows:*

$$Pl(P) := \{(p, c) : p \in \mathbb{R}^n, c \in \mathbb{R} \mid P \cap H_{p,c} \text{ is a facet of } P\}$$

Lemma 18. *The following statements are equivalent:*

- $(p, c) \in Pl(P)$
- $Dim(C(\{v \in V(P) | \langle v, p \rangle = c\})) = n - 1$ *and* $P \subset \{x \in \mathbb{R}^n | \langle x, p \rangle \le c\}$ *or* $P \subset \{x \in \mathbb{R}^n | \langle x, p \rangle \ge c\}$.

Thus (p, c) is a boundary hyperplane iff P is on one side of the hyperplane $H_{p,c}$ and the intersection $P \cap H_{p,c}$ is $(n-1)$-dimensional.

$\Rightarrow$: Let Q be the facet such that $Q \subset \{x \in \mathbb{R}^n | \langle x, p \rangle = c\}$. Then $Dim(Q) = n - 1$ and $V(Q) \subset V(P)$, so $Dim\, C(\{v \in V(P) | \langle v, p \rangle = c\}) = Dim\, C(V(Q)) = Dim\, Q = n - 1$, by theorem 18. Let $v, w \in P$ such that $\langle v, p \rangle < c$ and $\langle v, p \rangle > c$. Then the line segment vw intersects Q, which is a contradiction with $Q \subset \partial P$.
$\Leftarrow$: The intersection $P \cap H_{p,c}$ is $(n-1)$-dimensional. Also $P \cap H_{p,c}$ is on the boundary of P, since P is on one side of the half space $h_{p,c}$. □

Theorem 19. *Let P be an n-dimensional polytope and $x \in \mathbb{R}^n$. Then $x \in P$ iff $\langle x, p \rangle \leq c$ for all $(p, c) \in Pl(P)$. Thus polytopes are intersections of half spaces.*

See [GR67] 3.1.1 blz 31. $\square$

Definition 25. *Let $P \subset \mathbb{R}^m$ be an n-dimensional polytope. A set $In(P) \subset \{(p, c) \mid p \in \mathbb{R}^m, c \in \mathbb{R}\} \subset \mathbb{R}^m \times \mathbb{R}$. $In(P)$ is called a* set of inequalities *for P if the following hold:*

1. *if $(p, c) \in In(P)$, then either $P \subset H_{p,c}$ or $P \cap H_{p,c}$ is a facet of P,*
2. *if Q is a facet of P then there is exactly one $(p, c) \in In(P)$ such that $Q = P \cap H_{p,c}$.*
3. *there are exactly $m - n$ elements $(p_i, c_i) \in In(P)$, such that $P \subset \bigcap_{1 \leq i \leq m-n} H_{p_i,c_i}$ and $Dim \bigcap_{1 \leq i \leq m-n} H_{p_i,c_i} = n$.*

If P is a polytope, $In(P)$ will denote a set of inequalities of P.

The set of inequalities of P defines the polytope as intersection of halfspaces. Thus $x \in P$ if and only if for all $(p, c) \in In(P)$ the following holds: $\langle x, p \rangle = c$ if $P \cap H_{p.c} = P$ or $\langle x, p \rangle \leq c$ if $P \cap H_{p,c}$ is a facet of P. The set of inequalities is useful for the calculation of intersections between polytopes.

Lemma 19. *A face of a face of a polytope P, is a face of P.*
Moreover, a facet of a facet of P is an intersection of two facets of P.

See for example [GR67] 3.1.5 blz 33. $\square$

Lemma 20. *If $In(P)$ is a set of inequalities and $(p, c) \in Pl(P)$. Then $In(P)$ contains a set of inequalities of $P \cap H_{p,c}$.*

This is a direct consequence of the fact that facets of facets are intersections of two facets. $\square$

Theorem 20. *Let $P \subset \mathbb{R}^m$ be an n-dimensional polytope and Q a k-dimensional polytope. TFAE:*

1. *Q is a face of P*
2. $\dim \langle p : (p, c) \in In(P) \mid \forall_{q \in Q} \langle q, p \rangle = c \rangle = m - k$ *and*

$$V(Q) = \{x \in V(P) \mid \forall_{(p,c) \in In(P)} [\forall_{q \in Q} [\langle q, p \rangle = c] \Rightarrow \langle x, p \rangle = c]\}$$

i.e. the vertices of Q are the vertices of P that are in the intersection of the facets of P that contain Q.

$\Rightarrow$ With induction on the dimension of P this will be proven. If $n = 0$, then $k = 0$ and

$$\dim \langle p : (p, c) \in In(P) \mid \forall_{q \in Q} \langle q, p \rangle = c \rangle = m.$$

Let R be a facet of P such that $Q \subset R$. Take $In(R) \subset In(P)$. Then by induction

$$\dim \langle p : (p, c) \in In(R) \mid \forall_{q \in Q} \langle q, p \rangle = c \rangle = m - k.$$

Now $\langle p : (p, c) \in In(R) \mid \forall_{q \in Q} \langle q, p \rangle = c > \rangle \subset \langle p : (p, c) \in In(P) \mid \langle Q, p \rangle \rangle$, thus
$\dim \langle p : (p, c) \in In(P) \mid \forall_{q \in Q} \langle q, p \rangle = c \rangle \geq m - k$. Because Q is k-dimensional, then
$\dim \langle p : (p, c) \in In(P) \mid \forall_{q \in Q} \langle q, p \rangle = c \rangle = m - k$.
Let $x \in V(P)$ such that $\forall_{(p,c) \in In(P)} [\forall_{q \in Q} [\langle q, p \rangle = c] \Rightarrow \langle x, p \rangle = c]$. Because $R = P \cap H_{p,c}$ for a $(p, c) \in In(P)$ and $Q \subset R$, then $x \in V(R)$. Thus by induction

$$V(Q) = \{x \in V(P) \mid \forall_{(p,c) \in In(P)} [\forall_{q \in Q} [\langle q, p \rangle = c] \Rightarrow \langle x, p \rangle = c]\}$$

$\Leftarrow$ Now Q is at least in the intersection N of $n - k$ facets. The intersection of facets is a face since faces of faces are faces. Looking at the vertices of N one sees that $V(N) = V(Q)$. Thus $N = Q$, so that Q is a face of P. $\square$

Theorem 21. *Let $P \subset \mathbb{R}^n$ be an n-dimensional polytope and $Q \subset P$ a polytope, then:*
Q is on a k- and not on a $(k - 1)$-dimensional face iff dim $\langle p : (p, c) \in In(P) \mid \forall_{q \in Q} \langle q, p \rangle = c \rangle = n - k$.

It is enough to prove that Q is on an k-dimensional face iff

$$\dim \langle p : (p, c) \in In(P) \mid \forall_{q \in Q} \langle q, p \rangle = c \rangle \geq n - k.$$

By the preceding theorem if $Q \subset R$ is an m-dimensional face of P, then

$$\dim \langle p : (p, c) \in In(P) \mid \forall_{r \in R} \langle r, p \rangle = c \rangle = n - m.$$

Let R be the intersection of the facets that contain Q, then R is at most k-dimensional and a face of P. $\square$

Corollary 6. *Let $x \in P$, then $x \in V(P)$ if and only if dim $\langle p : (p,c) \in In(P) \mid \langle x,p \rangle = c \rangle = n$.*

Lemma 21. *Let $P \subset \mathbb{R}^n$ be a polytope and $S := \{(p,c) \in \mathbb{R}^n \times \mathbb{R}\}$ a finite set such that $P = \bigcap_{(p,c)\in S} H_{p,c}$, then for all facets Q of P, there is a $(p,c) \in S$ such that $P \cap H_{p,c} = Q$*

WLOG P is an n-dimensional polytope. By the assumption $\partial P \subset \bigcup_{(p,c)\in S} H_{p,c}$. Let $v \in Q^0$, then take $(p,c) \in S$ such that $v \in H_{p,c}$. Now $R := P \cap H_{p,c}$ is a face of P. Since $v \in R \cap Q^0$, $R = Q$. So $P \cap H_{p,c} = Q$. □

Theorem 22. *Let $P \subset \mathbb{R}^m$ be a polytope and $h_{p,c}$ a half space, then $Q := P \cap h_{p,c}$ is a polytope with the following vertices:*
$V(P) \cap h_{p,c}$ and the points on the intersection of the hyperplane $H_{p,c}$ and the edges $e := C(\{x,y\})$, such that $x, y \in V(P)$, $x \in h_{p,c}$ and $y \notin h_{p,c}$.
The boundary hyperplanes of Q are the boundary hyperplanes (q,d) of P, such that $\dim\{v \in V(Q) \mid \langle v,q \rangle = d\} = Dim\ Q - 1$ *and the hyperplane $H_{p,c}$ if $Dim\{v \in V(Q) \mid \langle v,p \rangle = c\} = Dim\ Q - 1$*
The following polytopes are the edges of Q:

1. *The edges of P that are in $h_{p,c}$,*
2. *For the edges $C(\{x,y\})$ of P, with $x \in h_{p,c}$ and $y \notin h_{p,c}$. The segment xz, where z is the point in the intersection of $H_{p,c}$ and $C(\{x,y\})$.*
3. *The segments vw, where $v, w \in V(Q) \cap H_{p,c}$ and* $\dim\langle p : (p,c) \in In(Q) \mid \langle v,p \rangle = \langle w,p \rangle = c \rangle = m - 2$.

Let $v \in V(Q)$, then the normal vectors of the hyperplanes through v form an n-dimensional space. Remove from the normal vectors p, then the other vectors form an n-dimensional or an $(n-1)$-dimensional space. If it is n-dimensional then $v \in V(P)$. If it is $(n-1)$-dimensional then v is on an edge of P and $v \notin V(P)$. Thus there are $x, y \in V(P)$, such that $v \in C(x,y)$.
The points in both sets have the property that $Dim\{p | (p,c) \in Pl(Q) | \langle x,p \rangle = c\} = n$. Thus they are vertices of Q.
By lemma 21 the boundary hyperplanes of Q are in the set $S := Pl(P) \cup \{(p,c)\}$. By lemma 18 $(p,c) \in Pl(Q)$ if $\dim\{v \in V(Q) \mid \langle v,q \rangle = d\} = Dim\ Q - 1$.
Let $C(v,w)$ be an edge of Q.
If $v \notin H_{p,c}$, take (q,d) such that $C(v,w) = Q \cap H_{q,d}$. Then there is a $z \in P$, such that w is on vz and $vz = P \cap H_{q,d}$:
Assume that $p \in P$ such that $p \in P \cap H_{q,d}$, then $C(p,v) \cap Q \subset Q \cap H_{q,d}$. Thus $C(p,v) \cap Q \subset C(v,w)$. Since $v \notin H_{p,c}$, $C(p,v) \cap Q$ is 1-dimensional. Therefore p is on the line through v and w. Take z to be the other point than v on the line through v and w that is on the boundary of P.

If also $w \notin H_{p,c}$, then the z above is equal to w.
Thus the edges with a vertex not in $H_{p,c}$ are in the first and second set of edges. The edges with both vertices in $H_{p,c}$ are the third set by theorem 20. □

So a polytope defined as intersection of halfspaces can be calculated by starting with a polytope that contains the intersection and then intersect the halfspaces one by one with the polytope. By keeping track of the vertices, edges and hyperplanes one can calculate the intersection by using the preceding theorem.
For calculating a fundamental domain for the symmorphic group one calculates first the Voronoi cell with respect to the translation lattice and then takes a point in the Voronoi cell with trivial stabilizer. The Voronoi Dirichlet construction will give a fundamental domain. To calculate $D(x, x^G)$ one slices one half space at the time from the polytope as described in the preceding theorem. In every step one calculates the edges, vertices and the facets of the new polytope.

4.3 From fundamental domain to set of representatives

For calculating the orbit representatives the fundamental domain is an approximation of a set of orbit representatives. Only the boundary of the fundamental domain can have multiple representatives for the orbits. The following goes about the problem of choosing the set of orbit representatives on the boundary of a fundamental domain.

The problem of finding a set of orbit representatives on the boundary of a fundamental domain will be investigated for two types of fundamental domains. The first one is a fundamental domain constructed

by taking first the Voronoi cell V of 0 wrt L with a G-invariant metric. The fundamental domain in $\mathbb{R}^n$ is then the fundamental domain in V of G for a point in general position in V.
For a fundamental domain constructed in such a way I have no working algorithm that calculates a set of orbit representatives.
The second construction of a fundamental domain is to take a Voronoi cell for a point in general position wrt its orbit of R in $\mathbb{R}^n$ and a G-invariant metric. This gives a fundamental domain for which I have a working algorithm that calculated a set of orbit representatives.
The following examples and statements indicate what can happen for fundamental domains.

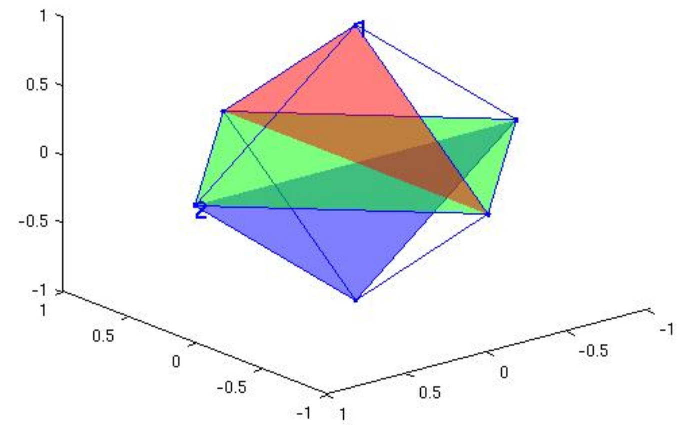
Definition 26. *Let F be a fundamental domain in X of G. F is face intersecting if for all $g \in G$ the intersection $gF \cap F$ is a face of F or empty.*

Not all fundamental domains are face intersecting. The following example shows that.

Example. The octahedron with group G generated by $g := \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$ and points

$$(1,0,0), (-1,0,0), (0,1,0), (0,-1,0), (0,0,1), (0,0,-1)$$

If one takes $x_1 := (0,0,1)$ and then $x_2 := (1,0,0)$ one has a fundamental domain F_2, where the intersections of the fundamental domains aren't faces. See the figure below. The points that are closer to x_1 than to gx_1 are in the pyramid with the green base. The points as close to x_2 as g^2x_2 chops this pyramid in half by the red triangle. F_2 is then the convex hull of the points $(1,0,0), (0,1,0), (0,-1,0), (0,0,1)$. The blue triangle is the polytope $gF_2 \cap g^3F_2$. One sees that $gF_2 \cap F_2$ is the triangle of the points $(1,0,0), 0, (0,1,0)$, which is the half of the facet with vertices $(1,0,0), (0,1,0), (0,-1,0)$.

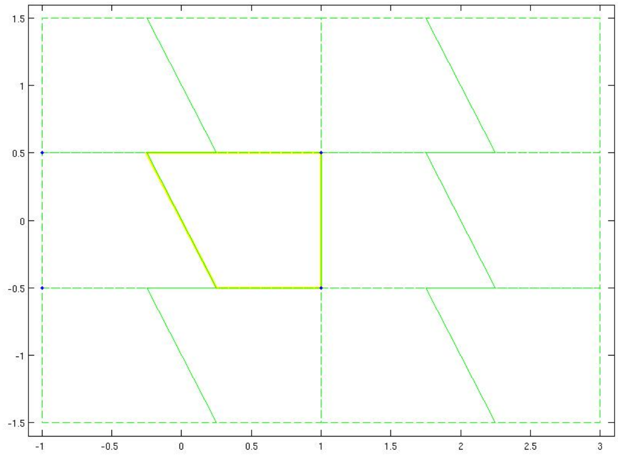


Theorem 23. *If P is a 2-dimensional polytope and G acts linearly on the polytope, thus P is invariant under the action of G, then every fundamental domain in P of G is face intersecting.*

Let F be a fundamental domain of P. Since F is convex $F \cap \partial P$ is a fundamental domain of ∂P (with the induced topology of ∂P). The center of the polytope $O := \frac{1}{|V(P)|} \sum_{v \in V(P)} v$ is an element of gF for all $g \in G$. Take the circle C around O for a G-invariant metric. The intersection $C \cap F$ is a fundamental domain of C. Now the only possible fundamental domains are arcs. The intersection of two arcs is empty or a point. If it is a point the intersection of $F \cap gF$ is the line through O and that point. If it is empty it is O. □

We now go back to the orbit representatives for the linear characters of T. Now the whole $\mathbb{R}^n$ plays a role and one has reduced it to the fundamental domain of the Voronoi cell of 0. But the faces of the Voronoi cell may have multiple representatives for an orbit of T. The following example shows that even in the 2-dimensional case $\{g \mid t\} F \cap F$ does not have to be a face of F, due to the affine action.

Example. Take $L = \langle 2e_1, e_2 \rangle$ and $g = -1$. The Voronoi cell of L has vertices $(\pm 1, \pm\frac{1}{2})$. The orbit of $(1, \frac{1}{2})$ contains also $(-1, -\frac{1}{2})$. The points closer to $(1, \frac{1}{2})$ are in the polytope F with the vertices $(-\frac{1}{4}, \frac{1}{2})$,$(\frac{1}{4}, -\frac{1}{2})$,$(1, \frac{1}{2})$ and $(1, -\frac{1}{2})$. Now $F \cap \{-1 \mid (0,1)\} F = C((-\frac{1}{4}, \frac{1}{2}), (\frac{1}{4}, \frac{1}{2}))$ is not a facet of F. A possible set of orbit representatives of the edges of F is $C((0,\frac{1}{2}),(1,\frac{1}{2})) \cup C((1,\frac{1}{2}),(1,0)) \cup C((0,0),(-\frac{1}{4},\frac{1}{2})) - \{(-\frac{1}{4},\frac{1}{2})\}$. In the figure below: the Voronoi cell is the rectangle with the blue corner points, the fundamental domain F is yellow and in green a couple of gF for $g \in R$.



Lemma 22. *Let F be an n-dimensional fundamental domain, $gF \cap F$ and $hF \cap F$ different $(n-1)$-dimensional polytopes. Then $gF \cap hF \cap F$ is on the boundary of $gF \cap F$.*

Else there is a point v that is not on the boundary of F but in both gF and hF. Then $gF \cap hF$ is n-dimensional which is in contradiction with F being a fundamental domain. □

For lower dimensional faces it is possible that the intersection of their interiors is not empty. If Q and P are intersections of F with a gF for some $g \in R$ and $Dim\ Q < Dim\ P$, it is also possible that $(P \cap Q)^0 \subset Q^0$ and $P \cap Q \neq Q$.

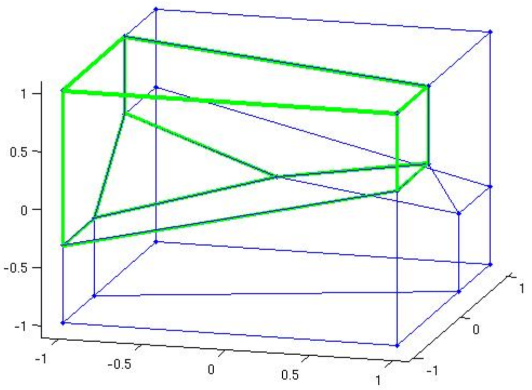
Example. Let R be a symmorphic space group with point group G generated by:

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

The Voronoi cell of the lattice $L = \langle 2e_1, 2e_2, 2e_3 \rangle$ is the cube with vertices $(\pm 1, \pm 1, \pm 1)$. Let $x := (-\frac{1}{3}, -1, 1)$ and F the set of points that are closer to x than to any other point in the orbit x^G. Then F has the following vertices:

$$0,\ (-1,-1,1),\ (1,-1,1),\ (1,-1,\frac{1}{3}),\ (-1,-1,-\frac{1}{3})$$
$$(-1,\frac{1}{3},1)\ ,(-1,\frac{1}{3},\frac{1}{3}),\ (-1,-\frac{1}{3},-\frac{1}{3}),\ (1,-\frac{1}{3},1),\ (1,-1,\frac{1}{3})$$

The Voronoi cell and the F are in the figure below. The green lines are the edges of F, the blue lines are the edges of polytopes in the orbit of F.
One sees that $F \cap \{g \mid (2,2,0)\} F$ is the edge $(-1,-1,1),(-1,-1,-\frac{1}{3})$ and $F \cap \{g \mid (0,2,0\} F$ the convex hull of the points $(-1,-1,1),(-1,-1,\frac{1}{3}),(1,-1,1),(1,-1,\frac{1}{3}),(0,0,-1)$. So their intersection is the segment $(-1,-1,1),(-1,-1,\frac{1}{3})$. This is half of the edge $F \cap \{g \mid (2,2,0)\} F$.



If one wants to calculate a set of orbit representatives in the boundary of a fundamental domain, one must somehow find out which points are in the same orbit. One idea to handle this problem is to calculate all the non-empty intersections of F with rF for all $r \in R$. Then one knows which polytopes in the boundary of the fundamental domain are mapped to each other. This doesn't work well, since a point on the boundary could be in multiple polytopes of the same dimension. To avoid this one can calculate also the intersections of the polytopes and their orbits, but this may require a large computational efford. At this point, I have no working algorithm that calculates a set of the orbit representatives in the general case. However if the fundamental is face intersecting there is an algorithm. There are also other arguments for choosing a face intersecting fundamental domain. Besides that the description of the set of orbit representatives is in general not very nice, the filling of the space with the fundamental domain is nicer if it is face intersecting. So it is better to choose the fundamental domain such that it is face intersecting.

Lemma 23. *Let $x \in X$, such that $Stab_G(x) = 1$ and $F := D(x, x^G)$, then F is face intersecting.*

The points that are in $F \cap gF$ are the points that are in F and are as close to x as to gx. So $F \cap gF$ is an intersection of a hyperplane with F. Since F is a fundamental domain the intersection is on the boundary of F. Thus $F \cap gF$ is a face of F. □

If a fundamental domain is face intersecting, then a set of orbit representations on the boundary can be found as follows. One first looks which facets are in the same orbit and selects facet representatives. One looks at the stabilizer of the facet representatives and calculate their set of representatives. From these facet representatives one calculates the facets. One calculates the orbit representatives of these facets of facets and goes so on.

A couple of lemmas which can be useful for the calculation of a set of orbit representatives when the fundamental domain is face intersecting are given below.

Definition 27. *Let P be a polytope then the* barycenter *of P, denoted by $B(P)$, is defined as follows:*

$$B(P) := \frac{1}{|V(P)|} \sum_{v \in V(P)} v$$

Lemma 24. *Let P be a polytope, then the mapping $Q \to B(Q)$ is a bijection between $\{Q : Q \text{ a face of } P\}$ and $\{B(Q) : Q \text{ a face of } P\}$.*

Let $b = B(Q) = B(R)$, then $b \in R \cap Q$. Assume $R \neq Q$, $Dim(Q) \geq Dim(R)$. Since $R \neq Q$, $R \cap Q$ is a face of Q. But then $b \in Q^0$ and $b \in R \cap Q = \partial Q$, which is a contradiction. So $B(R) \neq B(Q)$. □

Lemma 25. *Let g be an affine map and P, P' be polytopes with $gP = P'$. Let b be the barycenter of the face Q of P. Then gb is the barycenter of a face gQ of P'.*

Affine maps preserve hyperplanes, therefore also the faces of a polytope. So $Q' := gQ$ is a face of P'. Also $V(Q') = gV(Q)$, so the barycenter of Q' is gb. □

Corollary 7. *If F is face intersecting, then the barycenters of the faces of F are mapped to each other. For $g \in R$ and Q, Q' faces of F with barycenters b, b' respectively, $gQ = Q'$ iff $gb = b'$. The stabilizer of a face is the stabilizer of its center.*

A couple of lemmas which could be useful for calculating a fundamental domain of a point in general position and a Voronoi cell of 0 with respect to a lattice are given below.

In the following V is the Voronoi cell of 0 with respect to a lattice.

Lemma 26. *If $(V+t) \cap V$ is non-empty then $\frac{1}{2}t \in V$.*

Let $v, w \in V$ such that $v + t = w$. Now also $-v \in V$, thus $\frac{1}{2}t = \frac{w-v}{2} \in V$. □

So for calculating the Voronoi cell of a lattice one can look at the points of the lattice $\frac{1}{2}L$ in a polytope which contains the Voronoi cell.

Theorem 24. *Let x be a point in general position and V the Voronoi cell of 0 wrt L. The points of the orbit of x that are neighbors of x are in $2V + x$.*

Let y and x be in general position such that the intersection of their fundamental domains is non-empty. Since the fundamental domain of y resp x are in $V + y$ resp. $V + x$, the set $V + (y - x) \cap V$ is non-empty. By lemma 26 $\frac{y-x}{2} \in V$. So $y \in 2V + x$. □

In general, 2 is the lowest number r such that the relevant orbit points are in rV. For calculating the fundamental domain with x, a point in general position. The points that are closer to x than the orbit points of x that are in $2V + x$ is the fundamental domain by preceding theorem.

Theorem 25. *Let F be a face intersecting fundamental domain of a space group R in $\mathbb{R}^n$. Then a facet has either a stabilizer of order 2 or is in an orbit with only one other facet of F.*

Let P be a facet of F. Since the orbit of F covers the whole space, there is a unique $g \in G$, such that $P = gF \cap F$. Now if $gP = P$, then P has stabilizer of order 2. If $P \neq gP$, then it is in an orbit with $g^{-1}P$. □

Lemma 27 (special case fundamental theorem of stereohedra)**.** *The maximal number of hyperplanes of a Voronoi cell wrt a lattice in $\mathbb{R}^n$ is $2^{n+1} - 2$.*

The center of a hyperplane is in $\frac{1}{2}L$. A point in the interior of the hyperplane is represented twice in the Voronoi cell. $[L : \frac{1}{2}L] = 2^n$ and 0 is not on a hyperplane, thus the maximum number of points that are on a hyperplane is $2^n - 1$. So the maximum number of hyperplanes of a Voronoi cell is $2^{n+1} - 2$. □

So the algorithm begins with a point in general position. The shape of the fundamental domain depends on the position of this point. For the calculation and description of the fundamental domain it is better that is has as little hyperplanes and vertices as possible. By studying some 2-dimensional cases a general rule emerges: the more closest lattice points a point in general position has, the less hyperplanes and vertices its fundamental domain has. This is purely an educated guess. I have no idea if it is in general true and how it could be proven. The number of closest lattice points is much faster calculated, than a fundamental domain of a point in general position. The following lemmas give small hints to the general rule.

Lemma 28. *Let v be a point in general position and F its fundamental domain. If $t \in L$ is a closest lattice point of v, then $t \in F$.*
Assume that 0 is a closest lattice point of v and that $\mathbb{R}^n = \langle gv : g \in G\rangle$, then $0 \in V(F)$.
Thus if K is a subfield of $\mathbb{R}$, such that $v \in K^n$ and K^n is as KG-module irreducible, then $0 \in V(F)$.

Define $d(L, p) := \min\{d(t, p) : t \in L\}$ to be the closest distance of p to the lattice L.
Because both the metric and L are R-invariant, the action of the space group respects the closest distance of a point to L: for all $\{g \mid t\} \in R$, $d(L, p) = d(L, \{g \mid t\}\, p)$.
Take $\{g \mid s\} \in R$, such that $t \in \{g \mid s\}\, F$. Then $d(t, \{g \mid s\}\, v) \geq d(L, \{g \mid s\}\, v) = d(L, v) = d(t, v)$. Thus $t \in F$.
Assume that 0 is a closest lattice point of v. The polytope $P := \cap_{g \in G} gF$ contains of course 0. Since $\dim\langle gv : g \in G\rangle = n$, $P = \{0\}$.
Another proof for the last case. The polytope $P := \cap_{g \in G} gF$ is of course G-invariant. Since F is a fundamental domain $Dim(P) \leq n - 1$. Thus the G-invariant vectorspace generated by $P \cap K^n$ is not equal to K^n. Since K^n is irreducible, $P \cap K$ must be equal to $\{0\}$. Since $v \in K^n$, one has $V(P) \subset K^n$. So $V(P) = \{0\}$ and therefore $P = \{0\}$. Since F is face intersecting, P is an intersection of faces and therefore a face of F. So $0 \in V(F)$. □

Example. The following example shows that it is necessary for v to be in K such that K^n is an irreducible KG-module to have that $0 \in V(F)$. Let G be the group generated by

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

As $\mathbb{Q}G$-module, $\mathbb{Q}^n$ is irreducible. So for every $v \in \mathbb{Q}^n$ in general position the fundamental domain $F := D(v, v^R)$, one has $0 \in V(F)$. As $\mathbb{R}G$-module, $\mathbb{R}^4$ is reducible. With a change of the basis g acts like:

$$\begin{pmatrix} \cos(\phi) & -\sin(\phi) & 0 & 0 \\ \sin(\phi) & \cos(\phi) & 0 & 0 \\ 0 & 0 & \cos(2\phi) & -\sin(2\phi) \\ 0 & 0 & \sin(2\phi) & \cos(2\phi) \end{pmatrix}$$

where $\phi = \frac{2\pi}{5}$. Let $v \in \mathbb{R}^4$, such that the $\mathbb{R}G$-module generated by v is 2-dimensional. Take $w := \lambda v$ such that $0 < ||w|| \leq \frac{1}{3}$. Now $gw \neq w$ for all $g \in G$, since the $\mathbb{R}G$-module generated by w is 2-dimensional. For $t \in L - 0$ and $g \in G$, one has $d(\{g \mid t\}\, w, w) \geq \frac{1}{3}$, since $||w|| \leq \frac{1}{3}$ and $||t|| \geq 1$. So w is in general position. Since $||w|| \leq \frac{1}{3}$, 0 is a closest lattice point of w. To check in what kind of face 0 lies, the points in the orbit of w that have the same distance to 0 as w must be calculated. Since $||w|| \leq \frac{1}{3}$, these are only the points in w^G. Since these points span a 2-dimensional space, 0 is on an 2-dimensional face of F and not on a lower dimensional face. So 0 is not a vertex of F.

Lemma 29. *The point $t \in L$ is a closest lattice point of v iff $t \in V + v$.*
If there are two or more closest lattice points of v then they are all on the boundary of $V + v$.

If t is a closest lattice point of v then certainly $t \in V + v$.
Assume that $s \in L$ and $s \in V + v$. Since t is a closest lattice point of v, s is a closest lattice point of $v + (s - t)$. Thus $s \in V + (v + (s - t)) \cap V + v$. So s is as close to v as to $v + (s - t)$, therefore s is also a closest lattice point of v. If $s \neq t$, then s is on the boundary of $V + v$. □

4.4 Counting the representations

Counting the representations of R/mT of a particular kind can be seen as counting the number of orbits in $\frac{1}{m}\mathbb{Z}$ that have an element that is fixed by a particular subgroup. This section is actually about counting the number of linear representation of T/mT that have a particular inertia group. First some statements about counting orbits which an element fixed by a subgroup in general. Later the application to the counting of the representations.

Definition 28. *Let $H, L < G$, then $e_{HL} := \#\{gLg^{-1} : g \in G \mid H < gLg^{-1}\}$.*
Let X be a finite G-space, then

$$\begin{aligned} Fix(H) &:= \{x \in X \mid x^H = x\} \\ n_H &:= \#\{x \in X \mid G_x = H\} \\ o_H &:= \#\{x^G : x \in X \mid G_x = H\} \end{aligned}$$

If $L_0 := H, L_1, \ldots, L_n$ has the property that for each $L > H$ there is a unique i such that there is a $g \in G$ so that $L = gL_ig^{-1}$, then $L_1, \ldots, L_n$ is called a set of supergroup representatives above H.

The definition of e_{HL} is the opposite of the table of marks, in the sense that the table of marks goes about the number of to H conjugated subgroups in L and e_{HL} about the number of to L conjugated supergroups of H.
If $X = (\frac{1}{m}\mathbb{Z}^n)/\mathbb{Z}^n$ then o_H is the number of orbits in $\frac{1}{m}\mathbb{Z}^n$ in the Wyckoff positions with stabilizer H.
The goal of this sections is calculating o_H. The number of orbits in X of the whole group can be calculated with Burnside's lemma:

Theorem 26 (Burnside)**.** *The number of orbits is equal to $\sum_{g \in G} Fix(g)$.*

Lemma 30. *Assume that H is the stabilizer of both x and y. If $gx = y$, then $g \in N_G(H)$.*
Also $N_G(H)$ acts on the points with stabilizer H.
So o_H, the number of orbits with a point with stabilizer H, is equal to $\frac{n_H}{[N_G(H):H]}$.

Take $g \in G$ such that $gx = y$, then $G_y = gHg^{-1}$. Since $G_y = H$, one has $g \in N_G(H)$. Assume $g \in N_G(H)$, then $G_{gx} = gHg^{-1} = H$. □

Lemma 31. *Let $L_1, \dots, L_n$ be a set of supergroups representatives, then*

$$n_H = |Fix(H)| - \sum_{i=1}^{n} e_{HL_i} n_{L_i}$$

If L and L' are conjugated subgroups, then $n_L = n_{L'}$. Also $|Fix(H)| = \sum_{L>H} n_L$. □

Let $m \in \mathbb{N}$ and $H < G$. The goal of this paragraph is to calculate the number of representations that come from linear representations of T/mT that have H as stabilizer.

Lemma 32. *Let $H < G$ and $m \in \mathbb{N}$. Then take $X = \mathbb{Z}^n/(m\mathbb{Z}^n)$. Let $D := (d_1, \dots, d_r, 0, \dots, 0)$ be the Smith normal form for the calculation of the Wyckoff positions of H. Then:*

$$|Fix(H)| = m^{n-r} \prod_{i=1}^{r} gcd(m, d_i)$$

If N is the number of H-irreducible representations in ϕ^H, where ϕ is a linear representation of T/mT with inertia group H, then the number of representations that come from linear representations of T/mT that have H as stabilizer is $N \cdot o_H$.

In the section about Wyckoff positions, a point x is fixed by H if $Ax \cong 0 \mod \mathbb{Z}^n$. The number of points of this congruence in $\frac{1}{m}\mathbb{Z}^n/\mathbb{Z}^n$ is equal to the number of points in $\mathbb{Z}^n/(m\mathbb{Z}^n)$ that are fixed by H. Now the number of points in $\frac{1}{m}\mathbb{Z}^n/\mathbb{Z}^n$ of $Ax \cong 0 \mod \mathbb{Z}^n$ is the same as the number of points in $\frac{1}{m}\mathbb{Z}^n/\mathbb{Z}^n$ of $Dx \cong 0 \mod \mathbb{Z}^n$. The last congruence is just a couple of congruences: for $1 \le i \le n$, then $d_i x_i \cong 0 \mod \mathbb{Z}^n$. Now the number of $x \in \frac{1}{m}\mathbb{Z}$ such that $0 \le x < 1$ and $d_i x \in \mathbb{Z}$ is equal to $gcd(d_i, m)$. □

5 Conjugacy Classes of Space Groups

The conjugacy classes of space groups are interesting for at least two reasons. Elements of the same conjugacy class have as affine maps the same geometric property. The conjugacy classes are also important in the representation theory, since they are in one-to-one correspondence with the irreducible representations. The periodic boundary condition gives representations of the group R/mT for a large $m \in \mathbb{N}$. The goal is to calculate the conjugacy classes for all the factor groups R/mT for $m \in \mathbb{N}$.

The conjugacy classes are orbits of the conjugacy action of the group. Therefore first a useful lemma about actions.

Lemma 33. *Let G be a group acting on $X \times Y$, $\pi : X \times Y \to X$ the projection map onto X. Assume that the action factors through Y, ie $\pi(g(x,y)) = \pi(g(x,y'))$ for all $x \in X$ and $y, y' \in Y$. Then G acts on X by $gx := g(\pi(x,y))$. For $x \in X$, the stabilizer G_x of x acts on $\{x\} \times Y$.*
Let Y_x be a set of representatives for the orbits of G_x on $\{x\} \times Y$. If S is a set of representatives for the orbits of G on X then $\bigcup_{x \in S} Y_x$ is a set of representatives for the action of G on $X \times Y$.

Preceding lemma splits the problem of finding orbit representatives into subproblems where the space is smaller and the group is typically smaller. This method applied to conjugacy classes and group homomorphisms gives the following lemma.

Lemma 34. *Let $\phi : G \to H$ a surjective group homomorphism, $N := ker\,\phi$. Let $h \in H$ and g_h such that $\phi(g_h) = h$, then*

1. *the pre-image $C := \phi^{-1}C_H(h)$ of the centralizer of h acts on N by $n \mapsto g_h^{-1} g g_h n g^{-1}$ for $g \in C$*

2. *for $n, m \in N$, $g_h n$ is conjugated with $g_h m$ if and only if n and m are in the same orbit of C*

3. *define $\langle h \rangle_G := \phi^{-1}(\langle h \rangle)$, then $\langle h \rangle_G \lhd C$ and $QC := C/\langle h \rangle_G \cong C_H(h)/\langle h \rangle$ acts on the set of orbits of $\langle h \rangle_G$ on N*

4. *the orbits of $\langle h \rangle_G$ on N are the same as the orbits of N on N*

Moreover if $h_1, \dots, h_m$ is a set of representatives for the conjugacy classes of H, R_{h_i} a set of representatives for the orbits of $\phi^{-1}C_H(h_i)$ on N and $g_1, \dots, g_m$ a set of pre-images in G of $h_1, \dots, h_m$, then $\{g_i n \mid 1 \le i \le m, n \in R_{h_i}\}$ is a set of representatives for the conjugacy classes of G.

1. C acts on $\phi^{-1}(h)$ by conjugation and $n \mapsto g_h n$ is a set isomorphism from N to $g_h N = \phi^{-1}(h)$. Thus C acts on N by $n \mapsto g_h^{-1} g g_h n g^{-1}$.
2. Assume $g g_h n g^{-1} = g_h m$, then $\phi(g) h \phi(g)^{-1} = h$ and $g_h^{-1} g g_h n g^{-1} = m$.
Assume $g_h^{-1} g g_h n g^{-1} = m$, then $g g_h n g^{-1} = g_h m$.
So $g_h n$ is conjugated with $g_h m$ if and only if n and m are in the same orbit under $C_G(h)$.
3. The group $\langle h \rangle \lhd C_H(h)$, since h is in the center of $C_H(h)$. The pre-images of $\langle h \rangle$ and $C_H(h)$ are respectively $\langle h \rangle_G$ and C, thus $\langle h \rangle_G \lhd C$ and $C/\langle h \rangle_G \cong C_H(h)/\langle h \rangle$. Because $\langle h \rangle_G \lhd C$, the group $C/\langle h \rangle_G$ acts on the sets of orbits of $\langle h \rangle_G$ on N.
4. Let $g \in \langle h \rangle_G$, then take $k \in \mathbb{N}$ and $n \in N$ such that $g = g_h^k n$. Then

$$\begin{aligned}(g_h^k n) g_h m (g_h^k n)^{-1} &= (g_h^k n (g_h m)^{-k} (g_h m)^k) g_h m (g_h^k n (g_h m)^{-k} (g_h m)^k)^{-1} \\ &= (g_h^k n (g_h m)^{-k}) (g_h m)^k g_h m (g_h m)^{-k} (g_h^k n (g_h m)^{-k})^{-1} \\ &= (g_h^k n (g_h m)^{-k}) (g_h m) (g_h^k n (g_h m)^{-k})^{-1}\end{aligned}$$

Now $g_h^k n (g_h m)^{-k} \in N$, since $\phi(g_h^k n (g_h m)^{-k}) = h^k h^{-k} = e$. Thus the orbits of $\langle h \rangle_G$ on N are the same as the orbits of N on N.

By lemma 33 and the second point of this lemma $\{g_i n \mid 1 \le i \le m, n \in R_{h_i}\}$ is a set of representatives for the conjugacy classes of G. □

The conjugacy classes of G can now be calculated through the conjugacy classes of H. For calculating the conjugacy classes of a space group it is natural to divide the elements of R first by the conjugacy classes of the point group G. Since the point group is finite its conjugacy classes can be calculated by standard methods. Let $g_1, \dots, g_m$ be representative for the conjugacy classes of G. For the conjugacy classes of the space group R the lemma is applied to the morphism $\Pi : R \to G$. Thus

$\{\{g \mid t_g + t\} : g \in C_G(g_i), t \in T\}$ acts on $\{\{g_i \mid t_{g_i} + t\} : t \in T\}$ by conjugation. The representatives for the orbits of $\{\{g \mid t_g + t\} : g \in C_G(g_i), t \in T\}$ on $\{\{g_i \mid t_{g_i} + t\} : t \in T\}$ are then the representatives for the conjugacy classes of R. For the space group it is more natural to ask when $\{g \mid t_g + t\} = \{id \mid t\}\{g \mid t_g\}$ is conjugated to $\{g \mid t_g + t'\} = \{id \mid t'\}\{g \mid t_g\}$ with $t, t' \in T$, the translation subgroup, because the group's elements are written that way. Therefore the action of $\Pi^{-1}(C_G(g))$ on T by $\{id \mid t\} \mapsto \{h \mid t_h\}\{id \mid t\}\{g \mid t_g\}\{h^{-1} \mid -h^{-1}t_h\}\{g^{-1} \mid -g^{-1}t_g\}$ is examined for the conjugacy classes of g. The element $\{g \mid t_g + t\}$ is conjugated by $\{h \mid t_h\}$ for the conjugacy action. The resulting element is multiplied by the inverse of $\{g \mid t_g\}$ to get an element of T again.

Definition 29. *Let $g \in G$, define $M_g := T/(id - g)T$. The group M_g is as set exactly the set of orbits of T on T by the action of conjugacy on $\{g \mid t_g + s\}$ by $\{id \mid t\}$:*

$$\{id \mid s\} \mapsto \{id \mid t\}\{g \mid t_g + s\}\{id \mid -t\}\{-g^{-1} \mid -g^{-1}t_g\}$$

For $m \in \mathbb{N}$ define the following set

$$H_g^m := \{(h, x) : h \in C_G(g), x \in M_g \mid \exists_{t \in M_g}\ x = (1 - g)t_h + (h - 1)t_g + mt\}$$

Let $(h, x) \in H_g^m$. Because $h(id - g)T = (id - g)T$, (h, x) denotes an affine function on M_g by

$$(h, x + (id - g)T)t + (id - g)T = ht + x + (id - g)T$$

Lemma 35. *H_g^m is a group isomorphic to $C_G(g) \ltimes mM_g$ and $C_G(g) \cong H_g^0 < H_g^m$.*

Since $\{id \mid t\}\{g \mid t_g + s\}\{id \mid -t\}\{g^{-1}1 \mid -g^{-1}t_g\} = \{id \mid s + (id - g)t\}$, the orbits of T on T are $\{t + (id - g)T \mid t \in T\} = M_g$. The action of $C_G(g)$ on M_g corresponds with the action of H_g^m on M_g:

$$\{h \mid t_h\}\{g \mid t_g\}\{id \mid t\}\{h^{-1} \mid -h^{-1}t_h\}\{g^{-1} \mid -g^{-1}t_g\} = \{id \mid ht + (1 - g)t_h + (h - 1)t_g\}$$

Thus by lemma 34 the set $H_g^0 = \{(h, (1 - g)t_g + (h - 1)t_h) \mid h \in C_G(g)\}$ is isomorphic to $C_G(g)$. Because $mM_g \triangleleft H_g^m$ and H_g^0 is a transversal of mM_g, the group $H_g^m = C_G(g) \ltimes mM_g$. □

Theorem 27. *The group elements $\{g \mid t_g + t\}$ and $\{g \mid t_g + t'\}$ are conjugated in R/mT iff $t + (id - g)T$ and $t' + (id - g)T$ in M_g are in the same orbit of H_g^m.*

Assume $\{g \mid t_g + t\}$ and $\{g \mid t_g + t'\}$ are conjugated in R/mT then there is a $\{h \mid t_h + s\} \in R$ and a $r \in T$ such that

$$\{h \mid t_h + s\}\{g \mid t_g + t\}\{h^{-1} \mid -h^{-1}(t_h + s)\} = \{id \mid mr\}\{g \mid t_g + t'\}$$

Thus $h \in C_G(g)$ and $\{id \mid (1 - g)(t_h + s) + (h - 1)t_g + ht\} = \{id \mid mt + t'\}$. So

$$(h, (1 - g)t_h + (h - 1)t_g - mr)(t + (id - g)T) = t' + (id - g)T.$$

Thus $t + (id - g)T$ and $t' + (id - g)T$ are in the same orbit of H_g^m.
Assume that $t + (id - g)T$ and $t' + (id - g)T$ are in the same orbit of H_g^m. Take a $h \in C_G(g)$ and $r \in T$ such that:

$$(h, (1 - g)t_h + (h - 1)t_g + mr)(t + (id - g)T) = t' + (id - g)T$$

Now take a $s \in T$ such that:

$$\{h \mid (1 - g)t_h + (h - 1)t_g + mr\}\{id \mid t\} = \{id \mid t\}\{id \mid (g - 1)s\}$$

But then $\{h \mid t_h + s\}\{g \mid t_g + t\}\{h^{-1} \mid -h^{-1}(t_h + s)\} = \{id \mid -mr\}\{g \mid t_g + t'\}$. Thus $\{g \mid t_g + t\}$ and $\{g \mid t_g + t'\}$ are conjugated in R/mT. □

Thus by preceding theorem the problem of representatives of conjugacy classes is replaced by a problem of finding orbit representatives of H_g^m in M_g. If $P, D, Q \in GL_n(\mathbb{Z})$ are such that $D = P(id - g)Q$ is the Smith normal form of $(id - g)$, then $PM_g \cong T/DT \cong \oplus_{i=1}^n \mathbb{Z}_{d_i}$. It turns out that if m and m' are the same modulo $\max_{i=1}^n d_i$, the conjugacy classes can be described in the same way. That is the reason to put the translations (id, mt) in the group H_g^m instead of defining a space like $M_g^m = T/((id - g)T + mT)$. The group M_g has a torsion and a free part. To look how to deal with the free part the conjugacy classes of R lying in T and of R/mT lying in T/mT are considered.

5.1 The conjugacy classes of R lying in T and of R/mT lying in T/mT

Definition 30. *The dual group G^* of G is defined as follows $G^* := \{(g^{-1})^{tr} \mid g \in G\}$. The dual group also acts on T and hence on the linear characters of T.*

The conjugacy classes having as linear part the identity have a connection with the linear representations of space groups with the dual group as point group.

Theorem 28. *The orbits of G^* on the linear characters of T/mT are in one-to-one correspondence to the representatives of the conjugacy classes of R/mT lying in T.*

One can see that the conjugacy classes of T in R/mT are in one to one correspondence to the orbits of G in T/mT. It is well known that the group of linear characters of T/mT is isomorphic to T/mT. The orbits are exactly the orbits of G^* on the linear characters of T/mT. □

A fundamental domain of the Voronoi cell of 0 with respect to $\mathbb{Z}^n$ and a G-invariant metric on $\mathbb{R}^n$ defines the set of orbit representatives on the linear characters. That gives the following theorem.

Theorem 29. *Let R be a space group with point group G. Let Φ be a set of orbit representatives on $\mathbb{R}^n$ of $G \ltimes T$.*
The set $\{mx \mid x \in \Phi \cap \frac{1}{m}\mathbb{Z}^n\}$ is a set of representatives for the conjugacy classes of R/mT with $m > 0$.

Since $C_G(id) = G$ and $M_{id} = T$, the group $H_g^m = G \ltimes mT$. The group H_g^m acts on $\mathbb{R}^n$. The intersection of a set of orbit representatives in $\mathbb{R}^n$ and T is a set of representatives for the conjugacy classes of R lying in T. The linear map: $L_m : x \mapsto \frac{1}{m}x$ for $x \in \mathbb{R}^n$ maps $\mathbb{Z}^n$ to $\frac{1}{m}\mathbb{Z}^n$. Now $L_m H_g^m L_m^{-1} = G \ltimes T$. Thus the set $\{mx \mid x \in \Phi \cap \frac{1}{m}\mathbb{Z}^n\}$ is a set of representatives for the conjugacy classes of R/mT with $m > 0$. □

When studying the representations of certain space groups it is almost always the case that space groups with point group G and space groups with point group G^* are both examined. The representations are grouped by the orbits of the linear characters on T/mT and hence already calculated.

5.2 Calculating representatives of the conjugacy classes

For calculation of $M_g = T/(id-g)T$ there will be chosen a different basis for T. Take $P, Q \in GL_n(\mathbb{Z})$ such that $D := P(id-g)Q$ is the Smith normal form of $id-g$. Change the coordinates by $v \mapsto Pv$. Now $PT/P(id-g)T = PT/DT \cong T/DT$. The situation depends strongly on the form of D. Let d_i be the elements on the diagonal of D. Thus $M_g \cong \bigoplus_{i=1}^n (\mathbb{Z}/d_i\mathbb{Z})$. Let r be the lowest i such that $d_i = 0$. So $d_r, \ldots, d_n = 0$. Let $h \in C_G(g)$, then h acts on T with $v \mapsto PhP^{-1}v + P((1-g)t_h + (h-1)t_g)$. This action factors through DT, hence $PhP^{-1} = \begin{pmatrix} A_h & C_h \\ 0 & B_h \end{pmatrix}$, with A_h an $r-1 \times r-1$, B_h an $n+1-r \times n+1-r$ and C_h an $r-1 \times n+1-r$ matrix. Thus the action of $C_G(g)$ factors through $M_g^t := \bigoplus_{i=1}^{r-1} \mathbb{Z}_{d_i}$. Now the method of lemma 33 will be used. $C_G(g)$ acts on $\mathbb{Z}^{n+1-r} = M_g/M_g^t$ and therefore also on $\mathbb{R}^{n+1-r}$. The action of h on $\mathbb{R}^{n+1-r}$ is the action of the affine map $\{B_h \mid s_h\}$ with $(s_h)_i = P((1-g)t_h + (h-1)t_g)_{r+i-1}$ on $\mathbb{R}^{n+1-r}$. Since $C_G(g)$ is finite it has a fixed point: $\frac{1}{|C_G(g)|}\sum_{h \in C_G(g)} h \cdot w$ for $w \in \mathbb{R}^{n+1-r}$. So with a translation in $\mathbb{R}^{n+1-r}$ the action of h is B_h for all $h \in C_G(g)$. Take a set of orbit representatives and one has in the same way as in the case of the conjugacy classes of T representatives for the orbits of H_g^m in $\mathbb{Z}^{n+1-r}$. The stabilizers of the orbit representatives must be calculated. This is done by calculating the Wyckoff positions of the symmorphic space group $\{\{B_h \mid t\} \mid h \in C_G(g), t \in \mathbb{Z}^n\}$ on $\mathbb{R}^{n+1-r}$. The stabilizer of a point p of $M_g/(M_g^t + mM_g^t)$ acts on M_g^t. Assume that h is in the stabilizer of p, then h acts on $M_g^t \times \{p\}$ as follows:

$$\begin{pmatrix} A_h & C_h \\ 0 & B_h \end{pmatrix} \begin{pmatrix} v \\ p \end{pmatrix} + \begin{pmatrix} w \\ u \end{pmatrix} = \begin{pmatrix} A_h v + C_h p + w \\ p + mt \end{pmatrix}$$

So the action of the stabilizer of p on M_g^t only depends on p modulo $d_{r-1}M_g/M_g^t$. Since M_g^t is finite the representatives for the orbits of the stabilizer can be calculated by standard methods.

Example. The conjugacy classes with linear part $b = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ in the point group V_4 generated by b and $c := \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$ will be calculated. The image of $(b-id)\mathbb{Z}^2$ is $(0, 2x)$. Thus $M_g = \mathbb{Z} \oplus \mathbb{Z}_2$. Since

$C_{V_4}(b) = V_4$, V_4 acts on M_g. The action of b is of course trivial, but the action of c is $(u, i_2) \mapsto (-u, i_2)$. So the representatives of the conjugacy classes are $\{b \mid (u, i_2)\}$, with $i_2 \in \{0, 1\}$ and $u \in \mathbb{N}$. The Voronoi cell in M_g/M_g^t is $0 \le x \le \frac{1}{2}$. Both 0 and $\frac{1}{2}$ are fixed points. If m is odd the second coordinate doesn't matter and the representatives are $\{b \mid (u, 0)\}$, with $0 \le u \le \frac{m-1}{2}$. If m is even then the representatives are $\{b \mid (u, i_2)\}$, with $0 \le u \le \frac{m}{2}$ and $i_2 \in \{0, 1\}$.

For the space group generated by $C := \left\{c \mid (\frac{1}{2}, 0)\right\}, B := \left\{b \mid (\frac{1}{2}, 0)\right\}$ the action of C is $(u, i_2) \mapsto (-u-1, i_2)$. Again the representatives of the conjugacy classes are $\{b \mid (u, i_2)\}$, with $i_2 \in \{0, 1\}$ and $u \in \mathbb{N}$. The action of C has fixed point $-\frac{1}{2}$. Thus the domains are translated by $\frac{1}{2}$ to the left. If m is odd the representatives are $\left\{b \mid (u + \frac{1}{2}, 0)\right\}$ with $0 \le u \le \frac{m-1}{2}$. If m is even then the representatives are $\left\{b \mid (u + \frac{1}{2}, i_2)\right\}$ with $0 \le u \le \frac{m-2}{2}$ and $i_2 \in \{0, 1\}$.

For the space group generated by $C := \left\{c \mid (\frac{1}{2}, \frac{1}{2})\right\}, B := \left\{b \mid (\frac{1}{2}, \frac{1}{2})\right\}$ the action of C is $(u, i_2) \mapsto (-u-1, i_2-1)$. Thus C has fixed point $-\frac{1}{2}$. Thus if m is odd the representatives are $\left\{b \mid (u + \frac{1}{2}, \frac{1}{2})\right\}$ with $0 \le u \le \frac{m-1}{2}$. If m is even the representatives are $\left\{b \mid (u + \frac{1}{2}, i_2 + \frac{1}{2})\right\}$ with $0 \le u \le \frac{m-2}{2}$ and $i_2 \in \{0, 1\}$.

Example. Look at a cubic group generated by:

$$R_3 := \begin{pmatrix} 0 & 1 & -1 \\ -1 & 1 & 0 \\ 0 & 2 & -1 \end{pmatrix}, R_4 := \begin{pmatrix} 0 & -1 & 1 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, S := \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, E := \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & 0 & -1 \end{pmatrix}.$$

The conjugacy class of elements with linear part $R_4^2 := \begin{pmatrix} -1 & 0 & 1 \\ 0 & -1 & 1 \\ 0 & 0 & 1 \end{pmatrix}$ are calculated.

The Smith normal form of $R_4^2 - id$ is $D := (1, 2, 0)$ and $P := \begin{pmatrix} 1 & 0 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$. So the image of $R_4^2 - id$ is $(x, x-2y, 0)$. Thus $(0, i_2, u)$ with $0 \le i_2 \le 1, u \in \mathbb{Z}$ are representatives of $M_{R_4^2}$ in T. The centralizer of R_4^2 is generated by R_4, S, E. For the action of the generators on M_{R_4} conjugated them with P: $PR_4P^{-1} = \begin{pmatrix} -1 & 1 & 1 \\ -2 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix}, PSP^{-1} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, PEP^{-1} = \begin{pmatrix} -1 & 0 & 0 \\ -2 & 1 & 1 \\ 0 & 0 & -1 \end{pmatrix}$. The action on the representatives is then the 2×2 matrix in the bottom right corner. So (i_2, u) is mapped by R_4, S, E respectively to $(i_2 + u, u), (i_2, -u), (i_2 + u, -u)$. The action on $\mathbb{Z}$ are thus $u, -u, -u$. Therefore $0 \le u$ is a set of representatives in $\mathbb{Z}$ of that action. If $u = 0$ then the stabilizer is the centralizer. If $u \ne 0$ then the stabilizer of u is generated by $R_4, S \cdot E$, which both have the action $(i_2, u) \mapsto (i_2 + u, u)$ on $\mathbb{Z}_2 \times \mathbb{Z}$. Thus the representatives are $\left\{R_4^2 \mid (0, 0, u)\right\}$ for $0 \le u$ and $\left\{R_4^2 \mid (0, 1, 2u)\right\}$ for $0 \le u$. Now the calculation of the conjugacy classes of R/mT. Note that $0 \le u \le \frac{1}{2}$ is a Voronoi cell for the action on $\mathbb{Z}$. If $gcd(m, 2) = 1$, then $(0, u)$ and $(1, u)$ are in one orbit under $H_{R_4}^m$. So if m is odd the representatives are $\left\{R_4^2 \mid (0, 0, u)\right\}$ for $0 \le u \le \frac{m-1}{2}$. If m is even, then the representatives are $\left\{R_4^2 \mid (0, 0, u)\right\}$ for $0 \le u \le \frac{m}{2}$ and $\left\{R_4^2 \mid (0, 1, 2u)\right\}$ for $0 \le u \le \frac{m}{2}$.

For the group generated by $\{R_3 \mid 0\}, \left\{R_4 \mid (\frac{1}{2}, 0, \frac{1}{2})\right\}, \left\{R_4^2 \mid (0, \frac{1}{2}, 0)\right\}, \{S \mid 0\}, \left\{E \mid (\frac{1}{2}, 0, 0)\right\}$, the conjugacy classes with linear part R_4^2 are calculated. Now the actions of R_4, S, E are respectively: $(i_2 + u + 1, u)$, $(i_2 + 1, -u)$, $(i_2 + u + 1, -u)$. Again the action on $\mathbb{Z}$ are $u, -u, -u$. So $0 \le u$ is a set of representatives. If $u = 0$, then the stabilizer is the centralizer. If $u \ne 0$ then the stabilizer is generated by $R_4, S \cdot E$, which have the action $(i_2 + u + 1, u), (i_2 + u, u)$. Thus the representatives are $\left\{R_4^2 \mid (0, \frac{1}{2}, u)\right\}$ for $0 \le u$. If m is odd, then again the representatives are $\left\{R_4^2 \mid (0, \frac{1}{2}, u)\right\}$ for $0 \le u \le \frac{m-1}{2}$. If m is even, then the representatives are $\left\{R_4^2 \mid (0, \frac{1}{2}, u)\right\}$ for $0 \le u \le \frac{m}{2}$.

6 Data for A_5

A summary of the group theoretic data of A_5 is given in this section.
The presentation used throughout this master thesis is $\langle a, b | a^3, b^2, (ab)^5 \rangle$.
The letters a, b, c, d, e, f stands for the following elements of A_5:

a	b	c	d	e	f
(123)	(14)(25)	(12)(45)	(13245)	(124)	(13254)

The permutations c, d, e are chosen such that the following series is a composition series of A_4:

$$\langle c \rangle \triangleleft \langle c, b \rangle \triangleleft \langle c, b, e \rangle$$

For D_3 the composition series is $\langle a \rangle \triangleleft \langle a, c \rangle$
For D_5 the composition series is $\langle d \rangle \triangleleft \langle d, c \rangle$
For the representatives of the conjugacy classes is besides d another 5-cycle needed, there is chosen for f.

6.1 The irreducible representations of A_5

The alternating group of degree 5 has 60 elements. The character table of A_5 is stated below:

$C_G(g_i)$	60	4	3	5	5
$\lvert C_i \rvert$	1	15	20	12	12
g_i	id	b	a	d	f
χ_1	1	1	1	1	1
χ_2	3	-1	0	$\frac{1+\sqrt{5}}{2}$	$\frac{1-\sqrt{5}}{2}$
χ_3	3	-1	0	$\frac{1-\sqrt{5}}{2}$	$\frac{1+\sqrt{5}}{2}$
χ_4	4	0	1	-1	-1
χ_5	5	1	-1	0	0

For the character and the representation the same symbol is used. Thus the representation of χ_i is a representation with character χ_i. The $\mathbb{Q}$-irreducible representations are $\chi_1, \chi_2 + \chi_3, \chi_4$ and χ_5. The representation χ_2 comes from the action of A_5 on the dodecahedron. The algebraic conjugate of χ_2 is χ_3. The representation $\chi_2 + \chi_3$ is equivalent to the linear representation of D_5, $d \mapsto 1, c \mapsto -1$ induced to the whole group. The representation $\chi_4 + \chi_1$ is the permutation action on the cosets of A_4, the natural representation on 5 elements. The representation $\chi_5 + \chi_1$ is the permutation action on the cosets of D_5. The irreducible representations over $\mathbb{Z}$ are given in the appendix.
The representation of χ_2 and χ_3 are from the isomorphism of A_5 with the symmetry group of the dodecahedron:

$$\chi_2 : a \mapsto \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, b \mapsto \begin{pmatrix} 0 & 1 & \frac{\sqrt{5}-1}{2} \\ 1 & 0 & \frac{\sqrt{5}-1}{2} \\ 0 & 0 & -1 \end{pmatrix}$$

$$\chi_3 : a \mapsto \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, b \mapsto \begin{pmatrix} 0 & 1 & \frac{-\sqrt{5}-1}{2} \\ 1 & 0 & \frac{-\sqrt{5}-1}{2} \\ 0 & 0 & -1 \end{pmatrix}$$

The projective representations of A_5 for $a^3 = 1, b^2 = -1, (ab)^5 = 1$. This are the faithful ordinary representations of $2.A_5 \cong SL_2(5)$. Each representation is given by two matrices: a is mapped to the matrix on the left and b is mapped to the matrix on the right.
The 2-dimensional representations

$$\begin{pmatrix} -\zeta_5 - 1 & \zeta_5^3 \\ \zeta_5 + 1 & \zeta_5 \end{pmatrix}, \begin{pmatrix} \zeta_5^2 & \zeta_5^3 \\ -\zeta_5^2 - \zeta_5 & -\zeta_5^2 \end{pmatrix}$$

and

$$\begin{pmatrix} -\zeta_5^2 - 1 & \zeta_5 \\ \zeta_5^2 + 1 & \zeta_5^2 \end{pmatrix}, \begin{pmatrix} \zeta_5^4 & \zeta_5 \\ -\zeta_5^4 - \zeta_5^2 & -\zeta_5^4 \end{pmatrix}$$

The 4-dimensional representation

$$\begin{pmatrix} i+1 & i-1 & -i+1 & -i \\ -1 & -i & i+1 & 1 \\ -i+1 & i+1 & -1 & i \\ -1 & -2i & i+1 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 & -i+1 \\ 0 & i & 0 & 0 \\ 1 & i-1 & -2i & -i-1 \\ -i-1 & 1 & i-1 & i \end{pmatrix}$$

The 6-dimensional representation

$$\begin{pmatrix} 0 & 0 & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & i & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -i & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & i \end{pmatrix}$$

6.2 The subgroups and their representations

In this section all the data needed for the subgroups of A_5 are given. First the subgroups are given. The normalizers of the subgroups and the numbers e_{HL} are given in the following two tables. These two tables are needed for the calculation of the number of representations of R/nT as described in section 4.4. For the induction of the irreducible representations of the inertia group the irreducible representations and irreducible projective representations of the subgroups are induced.
The subgroups of A_5 up to conjugacy are the following:

H	gen	ord
C_2	$(12)(34)$	2
C_3	(123)	3
V_4	$(12)(34), (13)(24)$	4
D_3	$(123), (12)(45)$	6
C_5	(12345)	5
D_5	$(12345), (25)(34)$	10
A_4	$(12)(34), (13)(24), (123)$	12
A_5	$(12)(34), (135)$	60

The normalizers of the subgroups of A_5 are:

$group$	$Normalizer$	$[N_G(H) : H]$
C_2	V_4	2
C_3	D_3	2
V_4	A_4	3
D_3	D_3	1
C_5	D_5	2
D_5	D_5	1
A_4	A_4	1

The extension table for the subgroups of A_5 is below. In the cell of the row of subgroup H and the column of subgroup L is stated how many subgroups of A_5 which are conjugate to L contain H, ie in (H, L) is the number e_{HL}. A $-$ indicates that there is no to L conjugated subgroup that contains H, ie $e_{HL} = 0$.

$H\backslash L$	e	C_2	C_3	V_4	D_3	C_5	D_5	A_4	A_5
e	1	15	10	5	10	6	6	5	1
C_2	$-$	1	$-$	1	2	$-$	2	1	1
C_3	$-$	$-$	1	$-$	1	$-$	$-$	2	1
V_4	$-$	$-$	$-$	1	$-$	$-$	$-$	1	1
D_3	$-$	$-$	$-$	$-$	1	$-$	$-$	$-$	1
C_5	$-$	$-$	$-$	$-$	$-$	1	2	$-$	1
D_5	$-$	$-$	$-$	$-$	$-$	$-$	1	$-$	1
A_4	$-$	$-$	$-$	$-$	$-$	$-$	$-$	1	1
A_5	$-$	$-$	$-$	$-$	$-$	$-$	$-$	$-$	1

To induce the irreducible representation of the inertia group one must calculate a transversal and the action of a and b on the elements written on the transversal. Therefore the theory of presentation sequences as described in section 3.3 is used.

Example. For the group A_5, the sequence e, b, c, d with $3, 2, 2, 5$ is a presentation sequence.
The coset representatives of $D_5 = \langle c, d \rangle$ and the action of a on the coset representatives are:

i	1	2	3	4	5	6
$T_{D_5}(i)$	id	b	e	eb	e^2	e^2b
$aT_{D_5}(i)$	$ebcd^4$	e^2bcd^2	cd	ed^3	bd^2	e^2cd^4

Since $aT_{D_5}(1) = a = ebcd^4$, $\rho_a^{D_5}(1) = T_{D_5}^{-1}(eb) = 4$. If one goes on, one sees that $\rho_a^{D_5} = (143)(265)$. For the induction of the representation $\phi : d \mapsto 1, c \mapsto -1$ one has already the permutation, but the sequence of matrix blocks must be found. Now the i-th matrix block is equal to $\phi(T_{D_5}(\rho(i))^{-1} aT_{D_5}(i)$. Since $aT_{D_5}(1) = ebcd^4$, $T_{D_5}(\rho(i))^{-1} aT_{D_5}(i) = cd^4$. Thus the first matrix block is equal to $\phi(cd^4) = -1$. So

$$\phi^{A_4}(a) = [4, 6, 1, 3, 2, 5], B(-1, -1, -1, 1, 1, -1) = \begin{pmatrix} 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & -1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

A transversal for A_4 is d^i. A transversal for V_4 in A_4 is e^k. A transversal for C_2 in V_4 is b^l and a transversal for id in C_2 is c^m. So the elements of A_5 can be written uniquely as $d^ie^kb^lc^m$ with $i \in \{0, 1, 2, 3, 4\}, k \in \{0, 1, 2\}, l, m \in \{0, 1\}$. So d, e, b, c with $5, 3, 2, 2$ is a presentation sequence for A_5. The permutations $\rho_a, \rho_a^{C_2}, \rho_a^{V_4}, \rho_a^{A_4}$ are given in the 2-nd up to 5-th table below as sequences. ie the i-th element of the sequence is $\rho(i)$. The sequences are written from left to right and then from top to bottom. eg the sequence $S_1, \ldots S_9$ is given as follows:

S_1	S_2	S_3
S_4	S_5	S_6
S_7	S_8	S_9

The first table is $E^{-1}\rho_a$. The first column gives aT_{A_4}, thus the elements $a \cdot d^i$ written on the transversal. The columns with on both sides lines give aT_{V_4} (join the columns horizontally to get the table for aT_{V_4}), thus the elements $a \cdot d^ie^k$ and the odd columns give $aT_{C_2}(i)$, thus the elements $a \cdot d^ie^kb^l$.

d^4e^2b	d^4e^2bc	d^4e^2	d^4e^2c	d^4c	d^4	d^4bc	d^4b	d^4ebc	d^4eb	d^4ec	d^4e
ebc	eb	ec	e	e^2b	e^2bc	e^2	e^2c	c		bc	b
d^2ec	d^2e	d^2ebc	d^2eb	d^2e^2bc	d^2e^2b	d^2e^2c	d^2e^2	d^2b	d^2bc	d^2	d^2c
d^3e^2c	d^3e^2	d^3e^2bc	d^3e^2b	d^3bc	d^3b	d^3c	d^3	d^3eb	d^3ebc	d^3e	d^3ec
db	dbc	d	dc	dec	de	$debc$	deb	de^2bc	de^2b	de^2c	de^2

	59	60	57	58	50	49	52	51	56	55
	54	53	8	7	6	5	11	12	9	10
$1 \to A_5$	2	1	4	3	30	29	32	31	36	35
	34	33	27	28	25	26	46	45	48	47
	40	39	38	37	43	44	41	42	15	16
	13	14	18	17	20	19	24	23	22	21

	30	29	25	26	28	27	4	3	6	5
$C_2 \to A_5$	1	2	15	16	18	17	14	13	23	24
	20	19	22	21	8	7	9	10	12	11

	15	13	14	2	3
$V_4 \to A_5$	1	8	9	7	12
	10	11	4	5	6

$A_4 \to A_5$	5	1	3	4	2

The same tables, but then for b.

b	bc		c	ec	e	ebc	eb	e^2bc	e^2b	e^2c	e^2
d^3e^2b	d^3e^2bc	d^3e^2	d^3e^2c	d^3c	d^3	d^3bc	d^3b	d^3ebc	d^3eb	d^3ec	d^3e
d^4ebc	d^4eb	d^4ec	d^4e	d^4e^2b	d^4e^2bc	d^4e^2	d^4e^2c	d^4c	d^4	d^4bc	d^4b
dec	de	$debc$	deb	de^2bc	de^2b	de^2c	de^2	db	dbc	d	dc
d^2e^2c	d^2e^2	d^2e^2bc	d^2e^2b	d^2bc	d^2b	d^2c	d^2	d^2eb	d^2ebc	d^2e	d^2ec

$1 \to A_5$

3	4	1	2	6	5	8	7	12	11
10	9	47	48	45	46	38	37	40	39
44	43	42	41	56	55	54	53	59	60
57	58	50	49	52	51	18	17	20	19
24	23	22	21	15	16	13	14	34	33
36	35	28	27	26	25	31	32	29	30

$C_2 \to A_5$

2	1	3	4	6	5	24	23	19	20
22	21	28	27	30	29	25	26	9	10
12	11	8	7	17	18	14	13	16	15

$V_4 \to A_5$

1	2	3	12	10
11	14	15	13	5
6	4	9	7	8

$A_4 \to A_5$ 1 4 5 2 3

For the induction of the representations of D_5 and C_5, the following presentation sequence of A_5 is chosen: e, b, c, d with $3, 2, 2, 5$. This gives the same tables for D_5 as for A_5: $E^{-1}\rho, \rho^{C_5}$ and ρ^{D_5}. The columns in the first table for C_5 are between the lines and the first column is the sequence for D_5.

For a:

$ebcd^4$	ebc	$ebcd$	$ebcd^2$	$ebcd^3$	ebd	ebd^2	ebd^3	ebd^4	eb
e^2bcd^2	e^2bcd^3	e^2bcd^4	e^2bc	e^2bcd	e^2bd^3	e^2bd^4	e^2b	e^2bd	e^2bd^2
cd	cd^2	cd^3	cd^4	c	d^4		d	d^2	d^3
ed^3	ed^4	e	ed	ed^2	ecd^2	ecd^3	ecd^4	ec	ecd
bd^2	bd^3	bd^4	b	bd	bcd^3	bcd^4	bc	bcd	bcd^2
e^2cd^4	e^2c	e^2cd	e^2cd^2	e^2cd^3	e^2d	e^2d^2	e^2d^3	e^2d^4	e^2

$C_5 \to A_5$

8	7	12	11	2	1
5	6	3	4	10	9

$D_5 \to A_5$ 4 6 1 3 2 5

For b:

b	bd	bd^2	bd^3	bd^4	bc	bcd	bcd^2	bcd^3	bcd^4
	d	d^2	d^3	d^4	c	cd	cd^2	cd^3	cd^4
ec	ecd	ecd^2	ecd^3	ecd^4	e	ed	ed^2	ed^3	ed^4
ebc	$ebcd$	$ebcd^2$	$ebcd^3$	$ebcd^4$	eb	ebd	ebd^2	ebd^3	ebd^4
e^2bc	e^2bcd	e^2bcd^2	e^2bcd^3	e^2bcd^4	e^2b	e^2bd	e^2bd^2	e^2bd^3	e^2bd^4
e^2c	e^2cd	e^2cd^2	e^2cd^3	e^2cd^4	e^2	e^2d	e^2d^2	e^2d^3	e^2d^4

$C_5 \to A_5$

3	4	1	2	6	5
8	7	12	11	10	9

$D_5 \to A_5$ 2 1 3 4 6 5

For the induction of the representations of D_3 and C_3 the following presentation sequence of A_5 is chosen: d, b, c, a with $5, 2, 2, 3$. The second and third table are respectively ρ^{C_3} and ρ^{D_3}. The first table is $E^{-1}\rho$. This time the columns between the lines are for C_3 and the first column is the sequence for D_3.

For a:

a	a^2		ca^2	c	ca
d^3ca	d^3ca^2	d^3c	d^3a^2	d^3	d^3a
d^2bca	d^2bca^2	d^2bc	d^2ba^2	d^2b	d^2ba
d^3bca^2	d^3bc	d^3bca	d^3ba	d^3ba^2	d^3b
bca^2	bc	bca	ba	ba^2	b
d^4bca	d^4bca^2	d^4bc	d^4ba^2	d^4b	d^4ba
d^2a^2	d^2	d^2a	d^2ca	d^2ca^2	d^2c
d^4ca^2	d^4c	d^4ca	d^4a	d^4a^2	d^4
db	dba	dba^2	dbc	$dbca$	$dbca^2$
d	da	da^2	dc	dca	dca^2

$C_3 \to A_5$	1	2	14	13	12	11	16	15	4	3
	20	19	9	10	18	17	7	8	5	6
$D_3 \to A_5$	1	7	6	8	2	10	5	9	4	3

For b:

b	ba	ba^2	bc	bca	bca^2
	a	a^2	c	ca	ca^2
d^4a	d^4a^2	d^4	d^4ca^2	d^4c	d^4ca
d^2ca	d^2ca^2	d^2c	d^2a^2	d^2	d^2a
$dbca$	$dbca^2$	dbc	dba^2	db	dba
d^2bca^2	d^2bc	d^2bca	d^2ba	d^2ba^2	d^2b
d^4bca^2	d^4bc	d^4bca	d^4ba	d^4ba^2	d^4b
d^3bca	d^3bca^2	d^3bc	d^3ba^2	d^3b	d^3ba
da^2	d	da	dca	dca^2	dc
d^3ca^2	d^3c	d^3ca	d^3a	d^3a^2	d^3

$C_3 \to A_5$	3	4	1	2	17	18	10	9	8	7
	12	11	20	19	16	15	5	6	14	13
$D_3 \to A_5$	2	1	9	5	4	6	10	8	3	7

The matrix blocks of the induced representations.

The representations of the subgroups of A_5 are induced to A_5. The permutations are given above. The sequence of matrix blocks is given for every representation first for a and then for b. There are also a couple of projective representations that are induced in the same way as the regular representations. The precise definition of the matrix blocks listed for the projective representations will be made clear for each projective representation separately.

$\mathbf{C_2}$

$c \mapsto 1$

1	1	1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1	1	1

1	1	1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1	1	1

$c \mapsto -1$

1	1	−1	−1	−1	−1	−1	−1	1	1
−1	−1	−1	−1	−1	−1	1	1	−1	−1
−1	−1	1	1	1	1	−1	−1	−1	−1

1	1	−1	−1	−1	−1	1	1	−1	−1
−1	−1	−1	−1	1	1	−1	−1	−1	−1
−1	−1	1	1	−1	−1	−1	−1	1	1

$\mathbf{V_4}$

$c, b \mapsto 1$

1	1	1	1	1
1	1	1	1	1
1	1	1	1	1

1	1	1	1	1
1	1	1	1	1
1	1	1	1	1

$c \mapsto 1, b \mapsto -1$

−1	1	−1	−1	−1
1	1	−1	−1	1
−1	−1	−1	1	−1

−1	1	−1	−1	1
−1	−1	−1	1	1
−1	−1	1	−1	−1

$c \mapsto -1, b \mapsto 1$

$$\begin{matrix} 1 & -1 & -1 & -1 & 1 \\ -1 & -1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & -1 \end{matrix}$$

$$\begin{matrix} 1 & -1 & -1 & 1 & -1 \\ -1 & -1 & 1 & -1 & -1 \\ -1 & 1 & -1 & -1 & 1 \end{matrix}$$

$c \mapsto -1, b \mapsto -1$

$$\begin{matrix} -1 & -1 & 1 & 1 & -1 \\ -1 & -1 & 1 & -1 & -1 \\ 1 & -1 & -1 & -1 & 1 \end{matrix}$$

$$\begin{matrix} -1 & -1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 & -1 \end{matrix}$$

A projective representation of V_4 with the following relations $c^2, b^2 = -1, b^{-1}cb = -c$.
$c \mapsto \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, b \mapsto \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ For $(E_{V_4}^{-1}(\rho_h^{V_4}(i)))^{-1} h E_{V_4}(i) = b^{i_2} c^{i_1}$, the matrix block $\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}^{i_2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}^{i_1}$ is given.

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

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

$\mathbf{A_4}$

$c, b, e \mapsto 1$

$$1, 1, 1, 1, 1$$

$$1, 1, 1, 1, 1$$

$c, b \mapsto 1, e \mapsto \zeta_3$

$$\zeta_3^2, \zeta_3, \zeta_3, \zeta_3^2, 1$$

$$1, \zeta_3^2, \zeta_3, \zeta_3, \zeta_3^2$$

$c, b \mapsto 1, e \mapsto \zeta_3^2$

$$\zeta_3, \zeta_3^2, \zeta_3^2, \zeta_3, 1$$

$$1, \zeta_3, \zeta_3^2, \zeta_3^2, \zeta_3$$

$c \mapsto \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, b \mapsto \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, e \mapsto \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$

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

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

The projective representation with

$$c^2 = 1, b^2 = -1, b^{-1}cb = -c, e^{-1}ce = -cb, e^{-1}be = ic, e^3 = 1.$$

$c \mapsto \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, b \mapsto \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, e \mapsto \frac{1}{2} \begin{pmatrix} i-1 & -i+1 \\ -i-1 & -i-1 \end{pmatrix}$

For $g_{\rho_h(i)}^{-1} h g_i = e^{i_3} b^{i_2} c^{i_1}$ the matrix block

$$\left(\frac{1}{2} \begin{pmatrix} i-1 & -i+1 \\ -i-1 & -i-1 \end{pmatrix}\right)^{i_3} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}^{i_2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}^{i_1}$$

is given.

$\frac{1}{2} \begin{pmatrix} -i+1 & -i-1 \\ -i+1 & i+1 \end{pmatrix}, \frac{1}{2} \begin{pmatrix} i-1 & -i+1 \\ i+1 & i+1 \end{pmatrix}, \frac{1}{2} \begin{pmatrix} i-1 & i-1 \\ -i-1 & i+1 \end{pmatrix}, \frac{1}{2} \begin{pmatrix} -i-1 & -i+1 \\ i+1 & -i+1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \frac{1}{2} \begin{pmatrix} -i+1 & -i-1 \\ -i+1 & i+1 \end{pmatrix}, \frac{1}{2} \begin{pmatrix} i-1 & -i+1 \\ i+1 & i+1 \end{pmatrix}, \frac{1}{2} \begin{pmatrix} i-1 & i-1 \\ -i-1 & i+1 \end{pmatrix}, \frac{1}{2} \begin{pmatrix} -i-1 & -i+1 \\ i+1 & -i+1 \end{pmatrix}$

$\mathbf{C_5}$

$d \mapsto 1$

$$\begin{matrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{matrix}$$

$$\begin{matrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{matrix}$$

$d \mapsto \zeta_5$

$$\begin{matrix} \zeta_5^4 & \zeta_5 & \zeta_5^2 & \zeta_5^3 & \zeta_5 & \zeta_5^4 \\ \zeta_5^3 & \zeta_5^2 & \zeta_5^2 & \zeta_5^3 & \zeta_5^4 & \zeta_5 \end{matrix}$$

$$\begin{matrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{matrix}$$

$d \mapsto \zeta_5^2$

$$\begin{matrix} \zeta_5^3 & \zeta_5^2 & \zeta_5^4 & \zeta_5 & \zeta_5^2 & \zeta_5^3 \\ \zeta_5 & \zeta_5^4 & \zeta_5^4 & \zeta_5 & \zeta_5^3 & \zeta_5^2 \end{matrix}$$

$$\begin{matrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{matrix}$$

$d \mapsto \zeta_5^3$

$$\begin{matrix} \zeta_5^2 & \zeta_5^3 & \zeta_5 & \zeta_5^4 & \zeta_5^3 & \zeta_5^2 \\ \zeta_5^4 & \zeta_5 & \zeta_5 & \zeta_5^4 & \zeta_5^2 & \zeta_5^3 \end{matrix}$$

$$\begin{matrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{matrix}$$

$d \mapsto \zeta_5^4$

$$\begin{matrix} \zeta_5 & \zeta_5^4 & \zeta_5^3 & \zeta_5^2 & \zeta_5^4 & \zeta_5 \\ \zeta_5^2 & \zeta_5^3 & \zeta_5^3 & \zeta_5^2 & \zeta_5 & \zeta_5^4 \end{matrix}$$

$$\begin{matrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{matrix}$$

$\mathbf{D_5}$

$d, c \mapsto 1$

$$1, 1, 1, 1, 1, 1$$

$$1, 1, 1, 1, 1, 1$$

$d \mapsto 1, c \mapsto -1$

$$-1, -1, -1, 1, 1, -1$$

$$1, 1, -1, -1, -1, -1$$

$d \mapsto \begin{pmatrix} \zeta_5 & 0 \\ 0 & \zeta_5^4 \end{pmatrix}, c \mapsto \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

$$\begin{pmatrix} 0 & \zeta_5 \\ \zeta_5^4 & 0 \end{pmatrix}, \begin{pmatrix} 0 & \zeta_5^3 \\ \zeta_5^2 & 0 \end{pmatrix}, \begin{pmatrix} 0 & \zeta_5^2 \\ \zeta_5 & 0 \end{pmatrix}, \begin{pmatrix} \zeta_5^3 & 0 \\ 0 & \zeta_5^2 \end{pmatrix}, \begin{pmatrix} \zeta_5^2 & 0 \\ 0 & \zeta_5^3 \end{pmatrix}, \begin{pmatrix} 0 & \zeta_5 \\ \zeta_5^4 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$d \mapsto \begin{pmatrix} \zeta_5^2 & 0 \\ 0 & \zeta_5^3 \end{pmatrix}, c \mapsto \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

$$\begin{pmatrix} 0 & \zeta_5^2 \\ \zeta_5^3 & 0 \end{pmatrix}, \begin{pmatrix} 0 & \zeta_5 \\ \zeta_5^4 & 0 \end{pmatrix}, \begin{pmatrix} 0 & \zeta_5^3 \\ \zeta_5^2 & 0 \end{pmatrix}, \begin{pmatrix} \zeta_5 & 0 \\ 0 & \zeta_5^4 \end{pmatrix}, \begin{pmatrix} \zeta_5^4 & 0 \\ 0 & \zeta_5 \end{pmatrix}, \begin{pmatrix} 0 & \zeta_5^2 \\ \zeta_5^3 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$\mathbf{C_3}$

$a \mapsto 1$

$$\begin{array}{cccccccccc} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{array}$$

$$\begin{array}{cccccccccc} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{array}$$

$a \mapsto \zeta_3$

$$\begin{array}{cccccccccc} \zeta_3 & \zeta_3^2 & \zeta_3 & \zeta_3^2 & \zeta_3 & \zeta_3^2 & \zeta_3^2 & \zeta_3 & \zeta_3^2 & \zeta_3 \\ \zeta_3 & \zeta_3^2 & \zeta_3^2 & \zeta_3 & \zeta_3^2 & \zeta_3 & 1 & 1 & 1 & 1 \end{array}$$

$$\begin{array}{cccccccccc} 1 & 1 & 1 & 1 & \zeta_3 & \zeta_3^2 & \zeta_3 & \zeta_3^2 & \zeta_3 & \zeta_3^2 \\ \zeta_3^2 & \zeta_3 & \zeta_3^2 & \zeta_3 & \zeta_3 & \zeta_3^2 & \zeta_3^2 & \zeta_3 & \zeta_3^2 & \zeta_3 \end{array}$$

$a \mapsto \zeta_3^2$

$$\begin{array}{cccccccccc} \zeta_3^2 & \zeta_3 & \zeta_3^2 & \zeta_3 & \zeta_3^2 & \zeta_3 & \zeta_3 & \zeta_3^2 & \zeta_3 & \zeta_3^2 \\ \zeta_3^2 & \zeta_3 & \zeta_3 & \zeta_3^2 & \zeta_3 & \zeta_3^2 & 1 & 1 & 1 & 1 \end{array}$$

$$\begin{array}{cccccccccc} 1 & 1 & 1 & 1 & \zeta_3^2 & \zeta_3 & \zeta_3^2 & \zeta_3 & \zeta_3^2 & \zeta_3 \\ \zeta_3 & \zeta_3^2 & \zeta_3 & \zeta_3^2 & \zeta_3^2 & \zeta_3 & \zeta_3 & \zeta_3^2 & \zeta_3 & \zeta_3^2 \end{array}$$

$\mathbf{D_3}$

$a, c \mapsto 1$

$$\begin{array}{ccccc} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{array}$$

$$\begin{array}{ccccc} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{array}$$

$a \mapsto 1, c \mapsto -1$

$$\begin{array}{ccccc} 1 & -1 & -1 & -1 & -1 \\ -1 & 1 & -1 & 1 & 1 \end{array}$$

$$\begin{array}{ccccc} 1 & 1 & 1 & -1 & -1 \\ -1 & -1 & -1 & 1 & -1 \end{array}$$

$a \mapsto \begin{pmatrix} \zeta_3 & 0 \\ 0 & \zeta_3^2 \end{pmatrix}, c \mapsto \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

$$\begin{array}{ccccc} \begin{pmatrix} \zeta_3 & 0 \\ 0 & \zeta_3^2 \end{pmatrix} & \begin{pmatrix} 0 & \zeta_3^2 \\ \zeta_3 & 0 \end{pmatrix} & \begin{pmatrix} 0 & \zeta_3^2 \\ \zeta_3 & 0 \end{pmatrix} & \begin{pmatrix} 0 & \zeta_3 \\ \zeta_3^2 & 0 \end{pmatrix} & \begin{pmatrix} 0 & \zeta_3 \\ \zeta_3^2 & 0 \end{pmatrix} \\ \begin{pmatrix} 0 & \zeta_3^2 \\ \zeta_3 & 0 \end{pmatrix} & \begin{pmatrix} \zeta_3^2 & 0 \\ 0 & \zeta_3 \end{pmatrix} & \begin{pmatrix} 0 & \zeta_3 \\ \zeta_3^2 & 0 \end{pmatrix} & \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{array}$$

$$\begin{array}{ccccc} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & \begin{pmatrix} \zeta_3 & 0 \\ 0 & \zeta_3^2 \end{pmatrix} & \begin{pmatrix} 0 & \zeta_3^2 \\ \zeta_3 & 0 \end{pmatrix} & \begin{pmatrix} 0 & \zeta_3^2 \\ \zeta_3 & 0 \end{pmatrix} \\ \begin{pmatrix} 0 & \zeta_3 \\ \zeta_3^2 & 0 \end{pmatrix} & \begin{pmatrix} 0 & \zeta_3 \\ \zeta_3^2 & 0 \end{pmatrix} & \begin{pmatrix} 0 & \zeta_3^2 \\ \zeta_3 & 0 \end{pmatrix} & \begin{pmatrix} \zeta_3^2 & 0 \\ 0 & \zeta_3 \end{pmatrix} & \begin{pmatrix} 0 & \zeta_3 \\ \zeta_3^2 & 0 \end{pmatrix} \end{array}$$

7 Manual for the appendix

In the appendix the irreducible representations over $\mathbb{C}$ of the space groups with point group A_5 are described. Also the conjugacy classes are described in the appendix. For each space group there are a couple of tables that describe the space group and the representations.

1. point group table
2. space group table
3. relations table
4. representations table
5. conjugacy class table
6. the induction tables

Throughout the tables, $\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}, \mathbf{e}, \mathbf{f}$ will be the following elements of A_5: $(123), (14)(25), (12)(45), (13245), (124), (13254)$.
The following generators are chosen for the subgroups:

C_2	C_3	V_4	D_3	C_5	D_5	A_4	A_5
c	a	c, b	a, c	d	d, c	c, b, e	a, b

In the point group table and space group table the different space group are defined. In the relations and representations table the irreducible representations up to the inertia group are calculated. In the induction tables the irreducible representations of the space groups are given as a list of factors. In the conjugacy class table the conjugacy classes of the space groups which are not in the translation subgroup are calculated.

Point group table

The point group table gives the relevant point group elements for the representations. For the elements a, b, c, d, e the image of the representation $\phi : A_5 \to G$ is given. In the second row the image of the dual representation $\phi^{tr} : A_5 \to G^*$ is given.

Space group table

The space group table gives the different space groups for the point group given in the point group table up to conjugacy with translations in $\mathbb{R}^n$. The space groups are listed by R_i. So for every space group R with the given point group there is a $t \in \mathbb{R}^n$ and a space group R_i, such that $\{id \mid t\}\, R\, \{id \mid -t\} = R_i$. In the column headed R_i the translation vectors of $\phi(a)$ and $\phi(b)$ are given in the rows of respectively a and b. In the column headed R_1 the translation vectors that give the symmorphic space group are given by the general coordinates x, y, z, u, v, w. This is done by translating the origin with t, a vector in general coordinates ie conjugating the space group with $\{id \mid t\}$. In the column headed a stands the translation part of $\{id \mid t\}\,\{a \mid 0\}\,\{id \mid -t\}$ and in the column headed b the translation part of $\{id \mid t\}\,\{b \mid 0\}\,\{id \mid -t\}$. If the space groups R_i and R_j are isomorphic, then that will be indicated below the table with $\mathbf{R_i} \cong \mathbf{R_j}$. The Zassenhaus algorithm [Za48] described in section 2.3 gives the different space groups for a point group.

Example. In the point group table of the first 4-dimensional group stands:

g	a	b	$\cdots$
$\phi(g)$	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 0 & 1 \\ 0 & -1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 1 & -1 & 0 & 0 \end{pmatrix}$	$\cdots$

The space group table is:

	R_1	R_2	R_3
a	$(x-y, y-z, -x+z, 0)$	$(0, 0, 0, \frac{1}{3})$	$(0, 0, 0, \frac{2}{3})$
b	$(x+y-u, 2y, y, -x+y+u)$	0	0

Thus space group R_2 is generated by the translation subgroup and the following representatives of the point group in the space group:

$$\left\{\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \mid (0,0,0,\frac{1}{3})\right\}, \left\{\begin{pmatrix} 0 & -1 & 0 & 1 \\ 0 & -1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 1 & -1 & 0 & 0 \end{pmatrix} \mid (0,0,0,0)\right\}$$

Relations table

In the relations table for each space groups for the generators of the subgroups pre-images are chosen and their relations are evaluated. In the first column the generators of the subgroups of A_5 are listed. For all except the last group, corresponding to A_5 itself, the generators are chosen such that they form a composition series. (e.g. g_1, g_2, g_3 stands for the composition series $\langle g_1\rangle \triangleleft \langle g_1, g_2\rangle \triangleleft \langle g_1, g_2, g_3\rangle$). In the following columns for each space group a pre-image of the last element of the sequence is chosen and denoted by their translation vector if there is not yet a pre-image chosen for this element. See the table below:

group	R	$\cdots$
g_1	t_1	$\cdots$
g_1, g_2	t_2	$\cdots$

In space group R, the pre-image of g_1 is $\{g_1 \mid t_1\}$ and the pre-image of g_2 is $\{g_2 \mid t_2\}$.
The column headed *rel* gives the defining relations for the subgroups. Only the relations with the last element are given, since the other relations are already given for smaller subgroups. So if g_i, g_j generates a subgroup, then the defining relations are the one given in the column headed *rel* which consist only of g_i and g_j. In the columns that follow the relations are evaluated in the space group for the pre-images. Let $w = u$ be a relation, then $t \in T$ is given so that $w = tu$ in R. If the relation is g^n, then $t \in T$ is given such that $\{g \mid t_g\}^n = t$.

group	R	*rel*	R
g	t_1	g^3	s_1
g, h	t_2	$h^2, h^{-1}gh = g^{-1}$	s_2, s_3

The pre-image in space group R for g is $\{g \mid t_1\}$ and the pre-image in R for h is $\{h \mid t_2\}$. The relation for the group generated by g and h are g^3 and $h^2, h^{-1}gh = g^{-1}$. In the second row of the last column one sees that $(\{g \mid t_1\})^3 = \{id \mid s_1\}$. In the third row of the last column one sees that: $(\{h \mid t_2\})^2 = \{id \mid s_2\}$ and $(\{h \mid t_2\})^{-1}\{g_1 \mid t_1\}\{h \mid t_2\} = \{id \mid s_3\}(\{g_1 \mid t_1\})^{-1}$.

Representation table

In the representation table the linear representations of T are extended to their inertia groups as described in section 3.2. For the linear representations of T the inertia groups are calculated and the representations extended to the inertia groups are given. The representations induced to the space group are given in the factor table for the non-symmorphic space groups. For each subgroup the points that are fixed by the dual group are given in the column headed Wyckoff. The conjugation action of G on the linear representations of T corresponds with the action of the dual group G^* on $\mathbb{R}^n$. The Wyckoff positions for G^* are given. A vector k corresponds with the representation $t \mapsto e^{2\pi i k \cdot t}$. For each space group the irreducible representations of the inertia group which restricted to T have the Wyckoff position as irreducible component are given. The representation is denoted by a sequence of matrices that are the images of the sequence of generators. (e.g. if $\phi : G \to GL_n$ is a representation of G and g_1, g_2, g_3 are the generators of G, then the representation will by denoted by $\phi(g_1), \phi(g_2), \phi(g_3)$.) The general coordinates are given with x, y, z, u. The representation depends on the general coordinates and these are given in the representation. Thus the linear representation $f(x, y, z, u)$ has been extended to the irreducible representation $\phi(x, y, z, u)$ of the inertia group. For the solvable subgroups, then the theory about induction and restriction is used to calculate the irreducible representations up to the inertia group. The inproduct of the vector that indicates the Wyckoff position and the vector of the relation in R gives the conjugacy action of the last element.

Explanation of the symbols $\mathbf{e}(\cdot), \pm, \zeta_3^i, \zeta_5^i$

If $r \in \mathbb{C}$, then $e(r) := exp(2\pi r)$. The symbols $\pm, \zeta_3^i, \zeta_5^i$ are introduced to write down representations that look very similar in one sequence. The generator can be mapped to the matrix after the symbol multiplied to any integral power of -1, ζ_3 respectively ζ_5 to get another irreducible representation. Let g_1, g_2, g_3 be generators of the group G and A_1, A_2, A_3 matrices, then the sequence $\pm A_1, \zeta_3^i A_2, \zeta_5^i A_3$ stands for $2 \times 3 \times 5$ representations, namely $(-1)^i A_1, \zeta_3^j A_2, \zeta_5^k A_y$ for $i = 0,1$, $j = 0,1,2$ and $k = 0,1,2,3,4$. Let $V_4 := \langle c, b\rangle$, then the 4 irreducible linear representations of V_4: $(1,1)$,$(1,-1)$,$(-1,1)$ and $(-1,-1)$ are abbreviated with $(\pm 1, \pm 1)$.

Example. See the tables below for the second space group of the third 5-dimensional group:

group	*R*	*rel*	*R*
c	$(0, \frac{3}{4}, 0\frac{1}{4}, \frac{1}{2})$	c^2	$(-1,1,-2,0,0)$
c, b	$(\frac{1}{2}, 0,0,0,0)$	$b^2, b^{-1}cb = c$	$(1,0,0,0,0), (-1,-1,1,0,-1)$
c, b, e	$(0, \frac{3}{4}, 0, \frac{1}{2}, \frac{3}{4})$	$e^3, e^{-1}ce = cb, e^{-1}be = c$	$(3,3,3,0,3), (-1,-3,-2,0,0), (0,-1,-1,1,-1)$

group	*Wyckoff*	*R*
C_2	$(z, -2z-y-2x, 0, y, x)$	$\pm e(\frac{-3z-y-2x}{2})$
V_4	$(-y-x+\frac{1}{2}, y, 0, y, x)$	$\begin{pmatrix} ie(\frac{2y+x}{2}) & 0 \\ 0 & -ie(\frac{2y+x}{2}) \end{pmatrix}, \begin{pmatrix} 0 & -e(-y-x) \\ 1 & 0 \end{pmatrix}$
A_4	$(\frac{1}{2}, \frac{1}{3}, 0, \frac{1}{3}, \frac{2}{3})$	$\begin{pmatrix} i\zeta_3^2 & 0 \\ 0 & -i\zeta_3^2 \end{pmatrix}, \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, -\zeta_3^i \frac{1}{2} \begin{pmatrix} -i-1 & i-1 \\ i+1 & i-1 \end{pmatrix}$

Define $C := \{\phi(c) \mid (0, \frac{3}{4}, 0\frac{1}{4}, \frac{1}{2})\}$, $B := \{\phi(b) \mid (\frac{1}{2}, 0,0,0,0)\}$ and $E := \{\phi(e) \mid (0, \frac{3}{4}, 0, \frac{1}{2}, \frac{3}{4})\}$.
The linear representation $k_1 := (z, -2z-y-2x, 0, y, x)$ has stabilizer C_2, thus inertia group of k_1 is $\langle C, T\rangle$. Let Γ be a to the inertia group extended representation of k_1. The first relation c^2 gives that $C^2 = \{id \mid t\}$, with $t := (-1,1,-2,0,0)$. Thus $\Gamma(C^2) = e^{2\pi i k_1 \cdot t} = e(-3z-y-2x)$. So $\Gamma : C \mapsto \pm e(\frac{-3z-y-2x}{2})$.

The linear representation $k_2 := (-y-x+\frac{1}{2}, y, 0, y, x)$ has stabilizer V_4, thus the inertia group of k_2 is $\langle B, C, T\rangle$. In the same way as for k_1 one extend the representation to $\langle C, T\rangle$. The representation k_2 has the following extended representations to $\langle C, T\rangle$: $\gamma_j : C \mapsto (-1)^j ie(\frac{2y+x}{2})$ for $j \in \{0,1\}$. Now one looks at the action of B on the representations γ_0 and γ_1 to get the representations of k_2 extended to $\langle B, C, T\rangle$. In the relation table one sees that $B^{-1}CB = \{id \mid (-1,-1,1,0,-1)\}\, C$, thus

$$\gamma_j^B(C) = \gamma_j(B^{-1}CB) = \gamma_j((-1,-1,1,0,-1))\gamma_j(C) = e(-1(-y-x+\frac{1}{2}) + -y + -x)\gamma_j(C) = -\gamma_j(C)$$

Thus $\gamma_0^B = \gamma_1$, so γ_0 is not invariant under B. Thus one must induce the representation γ_0 to get the irreducible representations of $\langle B, C, T\rangle$ that is the extension of the representation k_2. The irreducible representation sends C to $\begin{pmatrix} ie(\frac{2y+x}{2}) & 0 \\ 0 & -ie(\frac{2y+x}{2}) \end{pmatrix}$. Because $B^2 = \{id \mid (1,0,0,0,0)\}$, the irreducible representation sends B to $\begin{pmatrix} 0 & -e(-y-x) \\ 1 & 0 \end{pmatrix}$, where $-e(-y-x) = e(k_2 \cdot (1,0,0,0,0))$.

For A_4 and Wyckoff position $(\frac{1}{2}, \frac{1}{3}, 0, \frac{1}{3}, \frac{2}{3})$ the linear representation is first extended to V_4 in the same way as for k_2. The irreducible representation up to V_4 is $\Gamma : C, B \mapsto \begin{pmatrix} i\zeta_3^2 & 0 \\ 0 & -i\zeta_3^2 \end{pmatrix}, \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$. There must now be found a matrix M, such that: $M^3 = \Gamma(e^3) = -1$, $M^{-1}\Gamma(C)M = -\Gamma(C)\Gamma(B)$ and $M^{-1}\Gamma(B)M = \zeta_3\Gamma(C)$. It turns out that M is equal to $\frac{1}{2}\begin{pmatrix} -i-1 & i-1 \\ i+1 & i-1 \end{pmatrix}$.

Wyckoff position with stabilizer A_5

The Wyckoff positions with stabilizer A_5 are given by $\frac{i}{n}v$, where $n \in \mathbb{N}$ and $v \in L$. This means that there are n Wyckoff positions: $0, \frac{1}{n}v, \ldots, \frac{n-1}{n}v$. For every space group there are given two factors c_1, c_2, such that for every irreducible representation $a \mapsto A, b \mapsto B$ of A_5, the representations $\{a \mid t_a\} \mapsto c_1 A, \{b \mid t_b\} \mapsto c_2 B$ is an irreducible representation of the space group. If for all the Wyckoff positions the factors are equal to 1, then they are not given.

Example. The first 4-dimensional point group has in the relation table the following data:

group	*Wyckoff*	R_1	R_2
A_5	$\frac{i}{5}(1,1,1,1)$		$\zeta_5^{2i}, 1$

So there are 5 Wyckoff positions:

$$(0,0,0,0), (\frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}), (\frac{2}{5}, \frac{2}{5}, \frac{2}{5}, \frac{2}{5}), (\frac{3}{5}, \frac{3}{5}, \frac{3}{5}, \frac{3}{5}), (\frac{4}{5}, \frac{4}{5}, \frac{4}{5}, \frac{4}{5})$$

There are no constants in the column of the space group R_1, so for all these Wyckoff positions the representations are $\{a \mid 0\} \mapsto \phi(a), \{b \mid 0\} \mapsto \phi(b)$, for ϕ an irreducible representation of A_5. In the column of R_2 stands $\zeta_5^{2i}, 1$, so for the Wyckoff position $(\frac{2}{5}, \frac{2}{5}, \frac{2}{5}, \frac{2}{5})$ the irreducible representations are $\{a \mid t_a\} \mapsto \zeta_5^4\phi(a), \{b \mid t_b\} \mapsto \phi(b)$ for ϕ an irreducible representation of A_5.

Not all the irreducible representations differ by a factor from the irreducible representations of A_5. Sometimes the irreducible representations are projective representations of A_5. All the j such that $\frac{j}{n}v$ gives in the space group a projective representation are given by $\mathbf{P(j_1, j_2, j_3)}$. This stands in front of the factors. Thus if the factors for $\frac{j}{n}v$ are c_1, c_2, then:
If $j \in \{j_1, j_2, j_3\}$, then the irreducible representation are $\{a \mid t_a\} \mapsto c_1\Gamma(a), \{b \mid t_b\} \mapsto c_2\Gamma(b)$ for all irreducible projective representations Γ of A_5.
If $j \notin \{j_1, j_2, j_3\}$ then the irreducible representation are $\{a \mid t_a\} \mapsto c_1\phi(a), \{b \mid t_b\} \mapsto c_2\phi(b)$ for all irreducible representations ϕ of A_5

Example. The first 5-dimensional point group

group	*Wyckoff*	R_2
A_5	$\frac{i}{6}(1,1,1,1,1)$	$P(1,3,5) : \zeta_3^i, \zeta_6^{-i}$

The $P(1,3,5)$ means that for $(\frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}), (\frac{3}{6}, \frac{3}{6}, \frac{3}{6}, \frac{3}{6}, \frac{3}{6}), (\frac{5}{6}, \frac{5}{6}, \frac{5}{6}, \frac{5}{6}, \frac{5}{6})$ the projective representations are needed. The two constants mean the same as in the regular representations, but instead of the regular now the irreducible projective representations of A_5 must be used. So for $(\frac{3}{6}, \frac{3}{6}, \frac{3}{6}, \frac{3}{6}, \frac{3}{6})$, the constants are $1, -1$. Thus for every irreducible projective representation Γ of A_5 the representation $\{a \mid t_a\} \mapsto \Gamma(a), \{b \mid t_b\} \mapsto -\Gamma(b)$ is an irreducible representation for the space group.
For the Wyckoff positions $0, (\frac{1}{3}, \frac{1}{3}, \frac{1}{3}, \frac{1}{3}, \frac{1}{3}), (\frac{2}{3}, \frac{2}{3}, \frac{2}{3}, \frac{2}{3}, \frac{2}{3})$ the constants are respectively $1, 1$, ζ_3^2, ζ_3 and ζ_3, ζ_3^2. These constants must be multiplied with the regular representation.

The conjugacy class table

The representatives for the conjugacy classes of the space groups are found by the theory in chapter 5. The conjugacy classes are first listed by the conjugacy classes of the point group A_5. The representatives are a, b, d, f and of course id. For each representative except for the identity the conjugacy classes are described in the column below it. Let $g \in \{a, b, d, f\}$. The vector in the column headed g and in the row with alg is in general coordinates $t(x, y, z, u)$ and the vector in the column headed g and in row with rep is in general coordinates $s(u, w, v, i_m, j_m)$. The vectors t such that for $s \in T$, $\{g \mid t_g + s\}$ is in the same conjugacy class as $\{g \mid t_g + t + s\}$ by reason of conjugation of $\{g \mid t_g + s\}$ with T are the following:

$$\{t(x, y, z, u) + s(0, 0, 0, mi_m, mj_m) : x, y, z, u, i_m, j_m \in \mathbb{Z}\}$$

This set is the space $(id - g)T$. In the row with rep the representatives of $M_g = T/(id - g)T$ are given. The representatives are given in general coordinates u, v, w and bounded coordinates i_m, j_m for $m \in \mathbb{N}$. Let $t(u, v, w, i_m, j_m)$ be a vector written in these coordinates, then the representatives of M_g are:

$$\{t(u, v, w, i_m, j_m) : u, v, w \in \mathbb{Z},\ i_m, j_m \in \{0, \cdots, m-1\}\}$$

For $g \in \{a, d, f\}$ these are representatives for the conjugacy classes. These are the vectors such that $\{g \mid t_g + t\}$ are the representatives of the conjugacy classes that have a group element with g as linear part, since $C_{A_5}(g) = \langle g \rangle$. To get the conjugacy classes of g in R/nT one must also consider the actions $t \mapsto t + ns$ on M_g for $s \in T$. This results in taking the vectors modulo $\mathbb{Z}_n$. So the representatives of the conjugacy classes are:

$$\{\{g \mid t_g + t(u, v, w, i_m, j_m)\} : 0 \le u, v, w \le n - 1,\ 0 \le i_m, j_m \le gcd(m, n) - 1\}$$

For b the centralizer is equal to V_4 so c acts also on M_b. The action of c on M_b is given in the row headed a as action on the representatives. If for a space group the action of c is different than the action of c in the symmorphic group, the action is denoted with the point group in the first column. In the fourth row of the column headed b the representatives that represent elements of M_g that are fixed by the action of V_4 are listed. The vector could have a fraction $\frac{i}{2}$. For this fraction the numbers $m \in \mathbb{Z}_n$ that satisfies $2m \equiv i \mod n$ are inserted to get the representatives. Thus if $t(u, v, \frac{i}{2}, \frac{j}{2})$ is in the fourth row of the column headed b then the following representatives of M_g are fixed by conjugacy of C in M_g:

$$\{t(u, v, m, k) : u, v, m, k \in \mathbb{Z} \mid 2m = i\ 2k = j\}$$

In R/nT the elements $\{b \mid t_b + t\}$ that are mapped by C to an element that is also the conjugacy of $\{b \mid t_b + t\}$ with an element of T are the following:

$$\{\{b \mid t_b + t(u,v,m,k)\} : u,v,m,k \in \mathbb{Z} \mid 2m \equiv i \; 2k \equiv j \mod n\}$$

If however there are in the fifth column three polynomials, then only if $gcd(n,4) = 4$ there is inserted $\frac{n}{2}$. So then if $gcd(n,4) = 2$ the elements fixed by C in M_b are:

$$\{t(u,v,0,0) : u,v \in \mathbb{Z}\}$$

and if $gcd(n,4) = 4$ the elements fixed by C in M_b are:

$$\{t(u,v,m,k) : u,v \in \mathbb{Z}, m,k \in \{0, \frac{n}{2}\}\}$$

The representatives for b are given in the text below the table. The first inequality is for the whole space group and the next inequalities are for R/nT. For space groups with different representatives than the symmorphic space group the representatives will also be given.
The representatives with id as the point group element can be derived from the linear representations of the dual group. These are the representatives of the fundamental domain.
The number of conjugacy classes with an element with linear part g are in the last row as polynomials of n. With the i_m's the relevant numbers are described. The polynomial is the same for n's who have the same common divisor with m. The polynomials are listed in the order of the divisors of m from 1 up to m. For the conjugacy classes with b the polynomials are for $gcd(n,2) = 1$, then for $gcd(n,2) = 2$ and if necessary for $gcd(n,4) = 4$.

Example. The first 5-dimensional point group has the following conjugacy table.

g	a	b	d	f
alg	$(x,y,3z+2y+2x,z,2z+3y+3x)$	$(y,x,y,2y-x,2y)$	$(x,-z,v-4z-y,y-x,-v-z)$	$(x,-z,v-4z-y,y-x,-v-y)$
rep	$(0,0,u-i_3,0,2u-i_3)$	$(0,0,u,v,w)$	$(0,0,0,0,u)$	$(0,0,0,0,u)$
	$\{-u,v-2u,w-2u\}$	$(0,0,0,v,w)$		
	$n, 3n$	$\frac{1}{2}(n^3+n^2), \frac{1}{2}(n^3+2n^2)$	n	n
R_2	$\{-u-1,v-2u-1,w-2u-1\}$	$(0,0,\frac{-1}{2},v,w)$		
		$\frac{1}{2}(n^3+n^2), \frac{1}{2}n^3$		

$$0 \leq u, 0 \leq v, w \leq n-1, 0 \leq u \leq \frac{n}{2}$$

$$0 \leq u, 0 \leq v, w \leq n-1, 0 \leq u \leq \frac{n-1}{2}$$

For the symmorphic space group the table gives the following information.
The action of c on M_b is thus $(u,v,w) \mapsto (-u, v-2u, w-2u)$. The representatives for the conjugacy classes of t are:

$$\begin{array}{ll} \{a \mid t_a + (0,0,u-i,0,2u-i)\} & i \in \{0,1,2\} \\ \{b \mid t_b + (0,0,u,v,w)\} & 0 \leq u \\ \{d \mid t_d + (0,0,0,0,u)\} & \\ \{f \mid t_f + (0,0,0,0,u)\} & \end{array}$$

The description of the representatives for the conjugacy classes of R/nT depends on the value of $gcd(n,6)$. If the $gcd(n,6) = 1$, then the representatives are:

$$\begin{array}{ll} \{a \mid t_a + (0,0,u,0,2u)\} & 0 \leq u \leq n-1 \\ \{b \mid t_b + (0,0,u,v,w)\} & 0 \leq u \leq \frac{n-1}{2}, 0 \leq v \leq n-1, 0 \leq w \leq n-1 \\ \{d \mid t_d + (0,0,0,0,u)\} & 0 \leq u \leq n-1 \\ \{f \mid t_f + (0,0,0,0,u)\} & 0 \leq u \leq n-1 \end{array}$$

The number of elements in the conjugacy classes are respectively $n, \frac{1}{2}(n^3+n^2), n, n$
If the $gcd(n,6) = 3$, then the representatives are:

$$\begin{array}{ll} \{a \mid t_a + (0,0,u+i,0,2u+i)\} & 0 \leq u \leq n-1, 0 \leq i \leq 2 \\ \{b \mid t_b + (0,0,u,v,w)\} & 0 \leq u \leq \frac{n-1}{2}, 0 \leq v \leq n-1, 0 \leq w \leq n-1 \\ \{d \mid t_d + (0,0,0,0,u)\} & 0 \leq u \leq n-1 \\ \{f \mid t_f + (0,0,0,0,u)\} & 0 \leq u \leq n-1 \end{array}$$

The number of elements in the conjugacy classes are respectively $3n, \frac{1}{2}(n^3+n^2), n, n$
If the $gcd(n,6) = 2$, then the representatives are:

$$\begin{array}{ll} \{a \mid t_a + (0,0,u,0,2u)\} & 0 \leq u \leq n-1 \\ \{b \mid t_b + (0,0,u,v,w)\} & 0 \leq u \leq \frac{n}{2}, 0 \leq v \leq n-1, 0 \leq w \leq n-1 \\ \{d \mid t_d + (0,0,0,0,u)\} & 0 \leq u \leq n-1 \\ \{f \mid t_f + (0,0,0,0,u)\} & 0 \leq u \leq n-1 \end{array}$$

The number of elements in the conjugacy classes are respectively $n, \frac{1}{2}(n^3 + 2n^2), n, n$
And if the $gcd(6, n) = 6$, then the representatives are:

$$\begin{array}{ll} \{a \mid t_a + (0,0,u+i,0,2u+i)\} & 0 \le u \le n-1, 0 \le i \le 2 \\ \{b \mid t_b + (0,0,u,v,w)\} & 0 \le u \le \frac{n}{2}, 0 \le v \le n-1, 0 \le w \le n-1 \\ \{d \mid t_d + (0,0,0,0,u)\} & 0 \le u \le n-1 \\ \{f \mid t_f + (0,0,0,0,u)\} & 0 \le u \le n-1 \end{array}$$

The number of elements in the conjugacy classes are respectively $3n, \frac{1}{2}(n^3 + 2n^2), n, n$

The action of c on M_b is for space group R_2 the following: $(u, v, w) \mapsto (-u-1, v-2u-1, w-2u-1)$. The representatives for R_2 are the same as for R_1 up to the t_g except for the representatives with linear part b. For the space group R_2 the representatives with linear part b are the following:

$$\begin{array}{lll} gcd(n,6) & rep & \\ 1,3 & \{b \mid t_b + (0,0,u,v,w)\} & 0 \le u \le \frac{n-1}{2}, 0 \le v \le n-1, 0 \le w \le n-1 \\ 2,6 & \{b \mid t_b + (0,0,u,v,w)\} & 0 \le u \le \frac{n-2}{2}, 0 \le v \le n-1, 0 \le w \le n-1 \end{array}$$

If the $gcd(n, 6)$ is equal to 1 or 3, then the number of conjugacy classes with linear part b is equal to $\frac{1}{2}(n^3 + 2n^2)$.
If the $gcd(n, 6)$ is equal to 2 or 6, then the number of conjugacy classes with linear part b is equal to $\frac{1}{2}n^3$.

Example. The third 6-dimensional space group has the following values relevant for b in the conjugacy class table:

$$\begin{array}{ccc} g & a & b \\ alg & (x, y, -x-y, z, u, -z-y) & (-2y, -x, 0, x, y+x, -x) \\ rep & (0,0,w,0,0,v) & (i_2 + 2j_2 + u, 0, -i_2, v, 0, -j_2) \\ & \{i_2 + 2j_2 + u, -j_2 - u - v, -u, -v\} & (i_2, j_2, \frac{0}{2}, \frac{0}{2}) \\ & n^2 & \frac{1}{2}(n^2+1), \frac{1}{2}(4n^2+4), \frac{1}{2}(4n^2+16) \\ R_2 & \{i_2 + 2j_2 + u, -j_2 - u - v - 2, -u, -v\} & (i_2, j_2, \frac{0}{2}, \frac{0}{2}) \\ & & \frac{1}{2}(n^2+1), \frac{1}{2}(4n^2+4), \frac{1}{2}(4n^2+16) \end{array}$$

If $(u, v) \equiv (0, 0) \mod 2$

$$0 \le u, \quad 0 \le u \le \frac{n}{2}, 0 \le v \le n-1$$

If $(u, v) \equiv (1, 1) \mod 2$

$$i_2 = 0, \quad 0 \le u \le \frac{n}{2}, 0 \le v \le n-1$$

If $(u, v) \equiv (0, 1), (1, 0) \mod 2$

$$j_2 = 0, \quad 0 \le u \le \frac{n}{2}, 0 \le v \le n-1$$

In the column headed a the fourth row gives the action of c on M_b for the symmorphic space group. So the action of c on $M_b \cong \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z} \times \mathbb{Z}$ in the symmorphic space group is:

$$(i_1, j_2, u, v) \mapsto (i_2 + 2j_2 + u, -j_2 - u - v, -u, -v)$$

In the following column stands $(i_2, j_2, \frac{0}{2}, \frac{0}{2})$ and three polynomials of n. This means that $(0, 0)$ is fixed by c if $gdc(n, 4) = 1$, $(i_2, j_2, 0, 0)$ is fixed by c if $gcd(n, 2) = 2$ and $(i_2, j_2, \frac{n}{2}, \frac{n}{2})$ is fixed by c if $gcd(n, 4) = 4$.
For the space group one has the following representative for the conjugacy classes with b:
For $\mathbb{Z} \times \mathbb{Z}$ the representatives are (u, v) with $0 \le u$.
For (u, v) with $u \equiv v \equiv 0 \mod 2$ the representatives are:

$$\{b \mid t_b + (u,0,0,v,0,0)\}, \{b \mid t_b + (1+u,0,-1,v,0,0)\},$$

$$\{b \mid t_b + (2+u,0,0,v,0,-1)\}, \{b \mid t_b + (3+u,0,-1,v,0,-1)\}$$

For $u \equiv v \equiv 1 \mod 2$ the representatives are:

$$\{b \mid t_b + (u,0,0,v,0,0)\}, \{b \mid t_b + (1+u,0,-1,v,0,0)\}$$

And for $u \equiv v \equiv 1 \mod 2$ the representatives are:

$$\{b \mid t_b + (u, 0, 0, v, 0, 0)\}, \{b \mid t_b + (2 + u, 0, 0, v, 0, -1)\}$$

For the group R/nT with $gcd(n, 2) = 1$ one has the representatives $\{b \mid t_b + (u, 0, 0, v, 0, 0)\}$ for $0 \leq u \leq \frac{n}{2}, 0 \leq v \leq n - 1$.
For the group R/nT with $gcd(n, 2) = 2$ one has the same representatives as for the whole space group except that $0 \leq u \leq \frac{n}{2}$ and $0 \leq v \leq n-1$. The number of conjugacy classes with b in R/nT are $\frac{1}{2}(n^2+1)$ if $gcd(n, 4) = 1$, $\frac{1}{2}(4n^2 + 4)$ if $gcd(n, 4) = 2$, and $\frac{1}{2}(4n^2 + 16)$ if $gcd(n, 4) = 4$.

The number of orbits in a Wyckoff position

For the Wyckoff positions of the dual space group $R^* = G^* \ltimes T$ the number of orbits on $\mathbb{Z}_n^m$ with that Wyckoff position is calculated with lemma 32 in section 4.4. For each group the number of orbits in a Wyckoff position with that group as stabilizer is given as polynomial of n. The polynomial depends on the $gcd(60, n)$ and is given for all these cases. The number of representations can be calculated by multiplying the number of orbits in a Wyckoff position for a subgroup with the number of extended representations of one linear representation in the Wyckoff position, see again lemma 32.

The induction tables

The irreducible representations of the inertia groups are induced to the space group as described in section 3.3. For every Wyckoff position the orbit of the vector is given. The orbit is given in the order in which the transversal for the induction is chosen. Thus if $w_1, w_2, w_3, w_4, w_5 \in \mathbb{R}^n$ are given, then the induced representation ϕ has on the translation subgroup the following matrix:

$$\phi(\{id \mid t\}) := \begin{pmatrix} e^{2\pi i w_1 \cdot t} & 0 & 0 & 0 & 0 \\ 0 & e^{2\pi i w_2 \cdot t} & 0 & 0 & 0 \\ 0 & 0 & e^{2\pi i w_3 \cdot t} & 0 & 0 \\ 0 & 0 & 0 & e^{2\pi i w_4 \cdot t} & 0 \\ 0 & 0 & 0 & 0 & e^{2\pi i w_5 \cdot t} \end{pmatrix}$$

For every non-symmorphic subgroup the induced representation is the same as a one of the standard representations given in section 6.2 up to a constant with absolute value 1 for every matrix block. For every Wyckoff position the logarithm of these constants are given by two sequences. The first sequence is for $\{a \mid t_a\}$ and the second for $\{b \mid t_b\}$. So if $A_1, \ldots, A_m$ is the sequence of matrix blocks, ρ the permutation of the induction and $c_1, \ldots, c_m$ the sequence of constants, then $e^{2\pi i c_1} A_1, \ldots, e^{2\pi i c_m} A_m, \rho$ is the image of $\{a \mid t_a\}$ of the irreducible representation.

Example. The Wyckoff position of $(x, -2x, 0, 0, 0)$ has stabilizer D_5. The orbit of $(x, -2x, 0, 0, 0)$ is:

$$\begin{matrix} (x, -2x, 0, 0, 0) & (x, 0, 0, -2x, 0) & (x, 0, -2x, 0, 0) \\ (-5x, 2x, 2x, 2x, 2x) & (x, 0, 0, 0, -2x) & (x, 0, 0, 0, 0) \end{matrix}$$

The sequence of constants are:

$$-\tfrac{13}{2}x \quad -\tfrac{7}{2}x \quad \tfrac{1}{2}x \quad 5x \quad -2x \quad \tfrac{13}{2}x$$

$$0 \quad x \quad \tfrac{1}{2}x \quad -\tfrac{5}{2}x \quad -\tfrac{11}{2}x \quad \tfrac{13}{2}x$$

These tables stands for 4 representations. For example the induced representation of the representation $d \mapsto 1, c \mapsto -1$. $\phi(\{id \mid (t_1, t_2, t_3, t_4, t_5)\} :=$

$$\begin{pmatrix} e^{2\pi i(xt_1 - 2xt_2)} & 0 & 0 & 0 & 0 & 0 \\ 0 & e^{2\pi i(xt_1 - 2xt_4)} & 0 & 0 & 0 & 0 \\ 0 & 0 & e^{2\pi i(xt_1 - 2xt_3)} & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{2\pi i(-5xt_1 + 2x(t_2 + t_3 + t_4 + t_5))} & 0 & 0 \\ 0 & 0 & 0 & 0 & e^{2\pi i(xt_1 - 2xt_5)} & 0 \\ 0 & 0 & 0 & 0 & 0 & e^{2\pi i x t_1} \end{pmatrix}$$

The permutation of a is:

$$4 \quad 6 \quad 1 \quad 3 \quad 2 \quad 5$$

and the sequence of matrix blocks is:

$$-1, -1, -1, 1, 1, -1$$

so $\phi(\{a \mid t_a\}) :=$

$$\begin{pmatrix} 0 & 0 & -e^{2\pi i \frac{1}{2} x} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & e^{-2\pi i 2x} & 0 \\ 0 & 0 & 0 & e^{2\pi i 5x} & 0 & 0 \\ -e^{-2\pi i \frac{13}{2} x} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -e^{2\pi i \frac{13}{2} x} \\ 0 & -e^{-2\pi i \frac{7}{2} x} & 0 & 0 & 0 & 0 \end{pmatrix}$$

The permutation of b is:

$$2 \quad 1 \quad 3 \quad 4 \quad 6 \quad 5$$

and the sequence of matrix blocks is:

$$1, 1, -1, -1, -1, -1$$

so $\phi(\{b \mid t_b\}) :=$

$$\begin{pmatrix} 0 & e^{2\pi i x} & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -e^{2\pi i \frac{1}{2} x} & 0 & 0 & 0 \\ 0 & 0 & 0 & -e^{-2\pi i \frac{5}{2} x} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & e^{2\pi i \frac{13}{2} x} \\ 0 & 0 & 0 & 0 & e^{-2\pi i \frac{11}{2} x} & 0 \end{pmatrix}$$

Since the translations, $\{a \mid t_a\}$ and $\{b \mid t_b\}$ generate the space group this determines the irreducible representation.

If the inertia group is V_4 or A_4 it is possible that the representations are projective. This can be seen from the dimension of the induced representation. One has the projective case iff the representation is 2-dimensional. In that case one must take the sequence of matrices for the projective case.

Example. The second space group of the third integral group of dimension 5 has Wyckoff position $(\frac{1}{2}, \frac{1}{3}, 0, \frac{1}{3}, \frac{2}{3})$. The orbit is:

$$(\tfrac{1}{2}, \tfrac{2}{3}, 0, \tfrac{2}{3}, \tfrac{1}{3}) \quad (\tfrac{1}{2}, 0, \tfrac{2}{3}, \tfrac{1}{3}, \tfrac{2}{3}) \quad (\tfrac{1}{2}, \tfrac{2}{3}, \tfrac{1}{3}, \tfrac{1}{3}, 0) \quad (\tfrac{1}{2}, \tfrac{1}{3}, \tfrac{2}{3}, 0, \tfrac{1}{3}) \quad (\tfrac{1}{2}, \tfrac{1}{3}, \tfrac{1}{3}, \tfrac{2}{3}, \tfrac{2}{3})$$

The sequence of constants are:

$$\begin{matrix} \frac{1}{6} & \frac{5}{12} & \frac{3}{4} & \frac{7}{12} & \frac{1}{3} \\ 0 & 0 & \frac{3}{4} & \frac{1}{4} & \frac{3}{4} \end{matrix}$$

Let ϕ be the irreducible representation. The representation extended to the inertia group is 2-dimensional, thus $\phi(\{id \mid (t_1, t_2, t_3, t_4, t_5)\}$ is equal to the diagonal matrix with on the diagonal:

$$\begin{matrix} (-1)^{t_1}\zeta_3^{2t_2+2t_4+t_5} & (-1)^{t_1}\zeta_3^{2t_2+2t_4+t_5} & (-1)^{t_1}\zeta_3^{2t_3+t_4+2t_5} & (-1)^{t_1}\zeta_3^{2t_3+t_4+2t_5} \\ (-1)^{t_1}\zeta_3^{2t_2+t_3+t_4} & (-1)^{t_1}\zeta_3^{2t_2+t_3+t_4} & (-1)^{t_1}\zeta_3^{t_2+2t_3+t_5} & (-1)^{t_1}\zeta_3^{t_2+2t_3+t_5} \\ (-1)^{t_1}\zeta_3^{t_2+t_3+2t_4+2t_5} & (-1)^{t_1}\zeta_3^{t_2+t_3+2t_4+2t_5} & & \end{matrix}$$

The permutation of a is:

$$5 \quad 1 \quad 3 \quad 4 \quad 2$$

and the sequence of matrix blocks is:

$$\begin{matrix} A_1 & A_2 & A_3 & A_4 & A_5 \\ \frac{1}{2}\begin{pmatrix} -i+1 & -i-1 \\ -i+1 & i+1 \end{pmatrix} & \frac{1}{2}\begin{pmatrix} i-1 & -i+1 \\ i+1 & i+1 \end{pmatrix} & \frac{1}{2}\begin{pmatrix} i-1 & i-1 \\ -i-1 & i+1 \end{pmatrix} & \frac{1}{2}\begin{pmatrix} -i-1 & -i+1 \\ i+1 & -i+1 \end{pmatrix} & \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \end{matrix}$$

So $\phi(\{a \mid t_a\}) :=$

$$\begin{pmatrix} 0 & -i\zeta_3 A_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \zeta_3 A_5 \\ 0 & 0 & -iA_3 & 0 & 0 \\ 0 & 0 & 0 & i\zeta_3 A_4 & 0 \\ -\zeta_3 A_1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

The permutation of b is:

$$1 \quad 4 \quad 5 \quad 2 \quad 3$$

and the sequence of matrix blocks is:

$$\underset{B_1}{\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}} \quad \underset{B_2}{\frac{1}{2}\begin{pmatrix} -i+1 & -i-1 \\ -i+1 & i+1 \end{pmatrix}} \quad \underset{B_3}{\frac{1}{2}\begin{pmatrix} i-1 & -i+1 \\ i+1 & i+1 \end{pmatrix}} \quad \underset{B_4}{\frac{1}{2}\begin{pmatrix} i-1 & i-1 \\ -i-1 & i+1 \end{pmatrix}} \quad \underset{B_5}{\frac{1}{2}\begin{pmatrix} -i-1 & -i+1 \\ i+1 & -i+1 \end{pmatrix}}$$

So $\phi(\{b \mid t_b\}) :=$

$$\begin{pmatrix} B_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & iB_4 & 0 \\ 0 & 0 & 0 & 0 & -iB_4 \\ 0 & B_2 & 0 & 0 & 0 \\ 0 & 0 & -iB_3 & 0 & 0 \end{pmatrix}$$

7.1 A set of orbit representatives

For each point group a set of orbit representatives for the symmorphic group is calculated as described in chapter 4 especially section 4.3. A fundamental domain F is calculated by calculation a Voronoi cell of a point v with respect to the points in its orbit. The fundamental domain is given by a sequence of inequalities for the facets and the vertices of the domain. The inequalities are given by a vector $p \in \mathbb{R}^n$ and a constant c. The p and c are given such that $\forall_{x \in F} \langle x, p \rangle \leq c$. The inproduct is the standard inproduct on $\mathbb{R}^n$ NOT a G-invariant one. Thus the inequality $x_1 + 2x_2 + 3x_3 \leq 4$ in $\mathbb{R}^3$ is denoted by $(1, 2, 3) \quad 4$. The vector p and the constant c are chosen such that they are both integral.

It is possible that there are multiple points of one orbit on the boundary. For the boundary a set of representatives is chosen by looking at the orbits of the faces of the fundamental domain. For each dimension m there is a set of orbit representatives chosen for the m-faces. For the chosen m-faces a set of orbit representatives for the stabilizer for that m-face is chosen. The inequalities necessary for a fundamental domain on the m-face are called *additional inequalities* and is sometimes abbreviated with *ad. ineq.*. A *additional facet* is a facet of a fundamental domain of an m-face that lies in the hyperplane of an additional inequality. Sometimes additional facet is abbreviated with *adfacet*. Only the interior points of the m-face in that set of orbit representatives for the stabilizer are in the set of orbit representatives for the symmorphic group. The facets are given by their number. The other faces are unless otherwise stated given by the numbers of the vertices that are on the face. An m-face P is **fixed** by $H < A_5$ if there is a group S in $G \rtimes T$ isomorphic to H such that $sP = P$ for all $s \in S$. The face P has **stabilizer** H if P is fixed by H.

Example. A set of orbit representatives for the symmorphic group with point group C_4:

$$\langle r := \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \rangle$$

is described by the following.

The fundamental domain is the Voronoi cell of the point $(\frac{1}{2}, \frac{1}{4})$.
The faces:

$$1. \quad (1, -1) \quad 0 \quad 2. \quad (0, -1) \quad 0 \quad 3. \quad (1, 1) \quad 1$$

The vertices:

$$1 \quad (0, 0) \quad 2 \quad (\frac{1}{2}, \frac{1}{2}) \quad 3 \quad (1, 0)$$

The incidence table in given below:

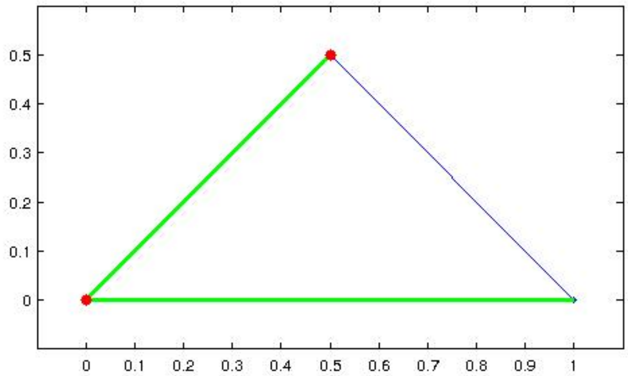
$v\backslash p$	1	2	3
1	×	×	
2	×		×
3		×	×

The representative facets are $1, 2$.
The facet 2 has stabilizer C_2.
The representative vertices are 2 and 3. The vertices $2, 3$ are fixed by C_4.

So the set of orbit representatives is the union of the following points:

1. The interior of the fundamental domain: $\{(x,y) \mid x-y<0, -y<0, x+y<1\}$
2. The interior of facet 1: $\{(x,y) \mid x-y=0, -y<0, x+y<1\}$
3. The interior of facet 2: $\{(x,y) \mid x-y<0, -y=0, x+y<1\}$
4. The vertices $(\frac{1}{2},\frac{1}{2})$ and $(1,0)$

In the next figure the points inside the triangle, the green lines and the red dots are in the set of orbit representatives.



Example. A set of orbit representatives for the symmorphic group with point group generated by

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

has the following description.

The fundamental domain is the Voronoi cell of the point $(\frac{1}{4},\frac{1}{4})$.
The faces:

1.	$(4,-4)$	-2	2.	$(4,4)$	4	3.	$(-4,4)$	-2	4.	$(-4,-4)$	0

The vertices:

$$1\ \ (-\frac{1}{4},\frac{1}{4})\quad 2\ \ (\frac{1}{4},\frac{3}{4})\quad 3\ \ (\frac{3}{4},\frac{1}{4})\quad 4\ \ (\frac{1}{4},-\frac{1}{4})$$

The incidence table:

$v\backslash p$	1	2	3	4
1	×			×
2	×	×		
3		×	×	
4			×	×

The representative facets are $1,2,3,4$. All are fixed by C_2. The fundamental domain on the facets are the following:

face	ver	ad. ineq.		vertices	vertices on adfacet
1	1	$(2,2)$	1	$1,(0,\frac{1}{2})$	$(0,\frac{1}{2})$
2	3	$(2,-2)$	0	$3,(\frac{1}{2},\frac{1}{2})$	$(\frac{1}{2},\frac{1}{2})$
3	3	$(-2,-2)$	-1	$3,(\frac{1}{2},0)$	$(\frac{1}{2},0)$
4	1	$(-2,2)$	0	$1,(0,0)$	$(0,0)$

The representative vertex is 1. This vertex has trivial stabilizer.

So the set of orbit representatives is the union of the following points:

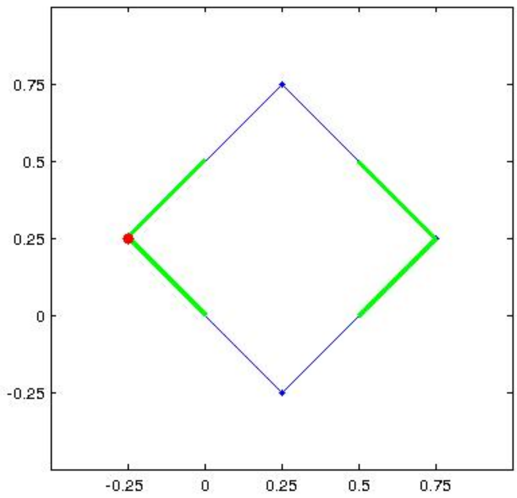
1. The interior of the fundamental domain:

$$\{(x,y) \mid 2x-2y<-1, x+y<1, -2x+2y<-1, -x-y<0\}$$

2. The interior for face 1: $\{(x,y) \mid 2x-2y=-1, 2x+2y\le 1, -x-y<0\}$

3. The interior for face 2: $\{(x, y) \mid x + y = 1, x - y \leq 0, -2x + 2y < -1\}$
4. The interior for face 3: $\{(x, y) \mid -2x + 2y = -1, -2x - 2y \leq -1, x + y < 1\}$
5. The interior for face 4: $\{(x, y) \mid -x - y = 0, -x + y \leq 0, 2x - 2y < -1\}$
6. The vertex $(-\frac{1}{4}, \frac{1}{4})$

The points $(0, 0), (\frac{1}{2}, 0), (\frac{1}{2}, \frac{1}{2})$ and $(0, \frac{1}{2})$ have stabilizer C_2.
In the next figure the orbit representatives are given. The points inside the square are in the set of orbit representatives. The green lines are the representatives for the facets. The red dot is the representative for the vertices.



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