5. Crystallography

Let $\mathbb{E}^n$ denote n-dimensional Euclidean space and let $R(n)$ be the group of rigid motions of $\mathbb{E}^n$. We observe that $R(n)$ contains the following elements:

(a) all translations. For each vector $v \in \mathbb{E}^n$ we will denote by t_v the translation through the vector v, and since these translations compose the same way as the vectors add we see that the group of all translations is isomorphic to $\mathbb{E}^n$. It is sometimes useful to maintain a distinction between the space $\mathbb{E}^n$ and the isomophic group whose elements are all translations t_v, but frequently we will identify them.

(b) orthogonal vector space transformations fixing the origin, i.e. the group $O(n, \mathbb{R})$, which we will abbreviate as $O(n)$.

In fact $R(n) = \mathbb{E}^n \rtimes O(n)$, since any rigid transformation is the product of a translation and a rotation, clearly $\mathbb{E}^n \lhd R(n)$ and $O(n) \cap \mathbb{E}^n = 1$. We also define the *affine group* $Aff(n)$, which is the group of transformations of $\mathbb{E}^n$ generated by $R(n)$ together with all scalar multiplications, and has the structure $Aff(n) = \mathbb{E}^n \rtimes GL(n, \mathbb{R})$. The affine group may be realized as the group of $(n+1) \times (n+1)$ block matrices of the form

$$\{\begin{pmatrix} A & v \\ 0 & 1 \end{pmatrix} \mid A \in GL(n, \mathbb{R}), v \in \mathbb{E}^n\}$$

since any affine transformation has the form $w \mapsto Aw + v$ for some invertible linear map A and vector v, and bijection which associates this transformation to the matrix $\begin{pmatrix} A & v \\ 0 & 1 \end{pmatrix}$ is a group isomorphism. This identification of $Aff(n)$ with a group of matrices puts a topology on $Aff(n)$, and $R(n)$ inherit the subspace topology as a subgroup of the affine group.

There are actions of $O(n)$ and $GL(n, \mathbb{R})$ on $\mathbb{E}^n$ given by conjugation within $R(n)$ and $Aff(n)$, and these are the same as the usual actions of $O(n)$ and $GL(n, \mathbb{R})$ on $\mathbb{E}^n$. Thus if $A \in GL(n, \mathbb{R})$ and $t_v \in R(n)$ is translation by the vector $v \in \mathbb{E}^n$ then $At_vA^{-1} = t_{Av} \in Aff(n)$.

We define a *crystal structure* in dimension n to be a subset $\mathcal{C}$ of n-dimensional real Euclidean space $\mathbb{E}^n$ such that

(i) Among the rigid motions of $\mathbb{E}^n$ which send $\mathcal{C} \to \mathcal{C}$, there exist n linearly independent translations.

(ii) There exists a number $d > 0$ such that any translation preserving $\mathcal{C}$ has magnitude at least d.

We let $S(\mathcal{C})$ denote the group of rigid motions $\mathbb{E}^n \to \mathbb{E}^n$ which preserve $\mathcal{C}$. This is the *space group* corresponding to $\mathcal{C}$, and in general we will say that G is a *space group* or *crystallographic group* in dimension n if it is the space group of some crystal structure in dimension n. The subgroup $T = \{t \in S(\mathcal{C}) \mid t \text{ is a translation}\} = S(\mathcal{C}) \cap \mathbb{E}^n$ is called the *translation subgroup*. It is a normal subgroup since as computed earlier a conjugate of a translation is a translation, and the quotient $P = S(\mathcal{C})/T$ is called the *point group*. There is a module action of P on T (and hence of $\mathbb{E}^n$) given by conjugation within $S(\mathcal{C})$, and by considering the embedding

$$P = S(\mathcal{C})/S(\mathcal{C}) \cap \mathbb{E}^n \cong \mathbb{E}^n \cdot S(\mathcal{C})/\mathbb{E}^n \hookrightarrow R(n)/\mathbb{E}^n = O(n)$$

we see that the action on T is orthogonal.

It is tempting to think that in the action of $S(\mathcal{C})$ on $\mathbb{E}^n$, the point group is a group of orthogonal transformations fixing some point, but this need not be the case. In fact it will happen precisely when the extension $1 \to T \to S(\mathcal{C}) \to P \to 1$ is split, since then the realization of P as a subgroup of $S(\mathcal{C})$ provides a splitting. In general this subtle point means that one genuinely has to work with quotient groups in the definition and calculation of the point group, and also that although we frequently identify T with a subgroup of $\mathbb{E}^n$, the conjugation action of P on T is not the same as an action of P on $\mathbb{E}^n$.

(5.0) LEMMA. *Any discrete subgroup T of $\mathbb{E}^n$ is isomorphic to $\mathbb{Z}^r$ for some $r \leq n$, generated by r independent vectors.*

Proof. We proceed by induction on n, the case $n = 0$ starting us off. Suppose that $n > 0$ and the result is true for smaller values of n. We may choose a non-zero element $v \in T$ for which $\|v\|$ is minimal. This can be done because if $d = \inf\{\|x\| \bigm| 0 \neq x \in T\}$ then $d > 0$ by discreteness, $B(0, d/2) \cap T = \{0\}$, so $B(x, d/2) \cap T = \{x\}$ for all $x \in T$. Therefore, in any compact region of $\mathbb{E}^n$ there are only finitely many elements of T. Now $T/\langle v \rangle$ embeds in $\mathbb{E}^n/\mathbb{R}v \cong \mathbb{E}^{n-1}$ as a discrete subgroup. This is because if $d(\mathbb{R}x, \mathbb{R}v) = u$ for some $x \in T$ then there exists $x' \in T$ and y on the line segment from o to v with $d(x', y) = u$. since this line segment is compact and T is discrete, there is x' in T closest to this line segment. Thus for some δ we have $B(\mathbb{R}v, \delta) \cap ((T + \mathbb{R}v)/\mathbb{R}v) = \mathbb{R}v$. By induction, $T/\langle v \rangle \cong \mathbb{Z}^{r-1}$ for some r, generated by the images of $r-1$ independent vectors $v_1, \ldots, v_{r-1}$, and so $T = \langle v_1, \ldots, v_{r-1}, v \rangle$ is generated by r independent vectors. □

(5.1) LEMMA. *Let $S(\mathcal{C})$ be a space group. Then $T \cong \mathbb{Z}^n$, P acts faithfully on T and $|P| < \infty$.*

Proof. We identify T with a discrete subgroup X of $\mathbb{E}^n$ which contains n independent elements. We show that $X \cong \mathbb{Z}^n$ by induction on n. When $n = 0$ we have the trivial group. Now suppose that $n > 0$ and the result is true for smaller values of n. Let $0 \neq v \in X$ be a vector which cannot be expressed as $v = \lambda w$ for any $w \in X$ with $\lambda > 1$. Then $\langle v \rangle = X \cap \mathbb{R}v$ and $X/\langle v \rangle \cong (X + \mathbb{R}v)/\mathbb{R}v$ is a discrete subgroup of $\mathbb{E}^{n-1}$ containing $n-1$ independent elements, so by induction it is isomorphic to $\mathbb{Z}^{n-1}$, generated by vectors $v_1 + \langle v \rangle, \ldots, v_{n-1} + \langle v \rangle$. Now $v_1, \ldots, v_{n-1}, v$ generate X, which is a torsion free abelian group, so it is isomorphic to $\mathbb{Z}^n$.

Since P embeds in $O(n)$ which acts faithfully on $\mathbb{E}^n$, P also acts faithfully on $\mathbb{E}^n$. But now $\mathbb{E}^n = \mathbb{R} \otimes_{\mathbb{Z}} T$ and so P must act faithfully on T since any element which acted trivially would also act trivially on $\mathbb{E}^n$.

Let $T = \langle t_1, \ldots, t_n \rangle$. We write the set of all images of these generators under the action of P as $P\{t_1, \ldots, t_n\}$, which we regard as a subset of $\mathbb{E}^n$. P permutes this set of points faithfully. They lie inside a ball of finite radius, since P acts as a subgroup of $O(n)$. Since the distance between any two of them is at least d, there exist only finitely many of these points, and so $|P| < \infty$. □

(5.2) PROPOSITION. *G is a space group in dimension n if and only if G is a discrete subgroup of $R(n)$ which contains n linearly independent translations.*

Proof. If G is a space group then $T \leq \mathbb{E}^n$ is discrete and P is finite, so G is discrete.

Conversely, if G is discrete then $G \cap \mathbb{E}^n$ and $G/G \cap \mathbb{E}^n$ are discrete so $G \cap \mathbb{E}^n \cong \mathbb{Z}^n$ and $G/G \cap \mathbb{E}^n$ is finite since it embeds in $O(n)$ which is compact. Now to produce a crystal structure $\mathcal{C}$ for G, take an unsymmetric pattern so small and so positioned that it does not meet any of its images under G. This can be done because the points in $\mathbb{E}^n$ which have non-identity stabilizer are a finite union of proper subspaces, hence not the whole of $\mathbb{E}^n$. Let $\mathcal{C}$ be the orbit of the pattern. □

(5.3) THEOREM. *If G is an abstract group with a normal subgroup $T \cong \mathbb{Z}^n$ such that the quotient $P = G/T$ is finite and acts faithfully on T then G is (isomorphic to) a space group of dimension n.*

Proof. Embed T in $\mathbb{R}^n$ in any way and form the extension pushout

$$\begin{array}{ccccccccc} 1 & \longrightarrow & T & \xrightarrow{\theta} & G & \longrightarrow & P & \longrightarrow & 1 \\ & & {\scriptstyle\phi}\downarrow & & \downarrow & & \| & & \\ 1 & \longrightarrow & \mathbb{R}^n & \longrightarrow & E & \longrightarrow & P & \longrightarrow & 1 \end{array}$$

where $E = \mathbb{R}^n \rtimes G/\{(-\phi t, \theta t) \mid t \in T\}$. Since $\mathbb{R}^n$ is uniquely divisible by $|P|$ we have $H^2(P, \mathbb{R}^n) = 0$ and the lower extension splits.

Since $|P| < \infty$ we may put an inner product on $\mathbb{R}^n$ which is preserved by P. This is done by taking any inner product $\langle \;\; , \;\; \rangle_1$ and defining

$$\langle u, v \rangle = \sum_{g \in P} \langle gu, gv \rangle_1.$$

Now P acts orthogonally, so there exists an isomorphism $\sigma : \mathbb{R}^n \to \mathbb{E}^n$ and a map $\tau : P \to O(n)$ such that $\sigma(g \cdot v) = \tau(g) \cdot \sigma(v)$. The diagram

$$\begin{array}{ccccccccc}
1 & \longrightarrow & \mathbb{R}^n & \longrightarrow & \mathbb{R}^n \rtimes P & \longrightarrow & P & \longrightarrow & 1 \\
 & & {\scriptstyle\sigma}\big\downarrow & & & & {\scriptstyle\tau}\big\downarrow & & \\
1 & \longrightarrow & \mathbb{E}^n & \longrightarrow & \mathbb{E}^n \rtimes O(n) & \longrightarrow & O(n) & \longrightarrow & 1 \\
 & & & & \Big\| & & & & \\
 & & & & R(n) & & & &
\end{array}$$

may thus be completed to a commutative diagram by a map $\mathbb{R}^n \rtimes P \to R(n)$, which must necessarily be a monomorphism. Then the composite $G \hookrightarrow \mathbb{R}^n \rtimes P \hookrightarrow R(n)$ embeds G as a discrete subgroup of $R(n)$ with $G \cap \mathbb{E}^n \cong \mathbb{Z}^n$. □

(5.4) LEMMA. *Let G be any group which is an extension $1 \to T \to G \to P \to 1$ where $T \cong \mathbb{Z}^n$, $|P| < \infty$ and P acts faithfully on T, Then T is a maximal abelian subgroup of G, and is the unique such isomorphic to $\mathbb{Z}^n$.*

Proof. If $T < H \leq G$ and $h \in H - T$ then h acts non-trivially on T, so H is non-abelian.

Suppose $X \cong \mathbb{Z}^n$ is any subgroup isomorphic to $\mathbb{Z}^n$. Then

$$1 \to X \cap T \to X \to X/X \cap T \cong XT/T \to 1$$

is exact and XT/T is a subgroup of P which is finite, so $|X/X \cap T| < \infty$ and hence $X \cap T \cong \mathbb{Z}^n$. If there were $x \in X - T$ then x would act non-trivially on T and hence on $X \cap T$, so X would be non-abelian – a contradiction. Therefore $X = X \cap T \subseteq T$. This shows that T is the unique maximal subgroup isomorphic to $\mathbb{Z}^n$. □

We will show how to classify crystal structures in terms of their symmetries, but to do this we evidently need to introduce an equivalence relation so that two crystal structures are regarded as the same under certain circumstances. Specifically, they will be equivalent if the space group of one is obtained from the other after a combination of a rigid motion of space and a scalar magnification. These transformations generate the *affine group*, which is the group of transformations of $\mathbb{E}^n$ generated by $R(n)$ together with all scalar multiplications, and has the structure $\mathbb{E}^n \rtimes GL(n, \mathbb{R})$. Since we are only interested in the symmetries a crystal structure has, we work with its space group. Here is the formal definition: two space groups are *equivalent* if they are conjugate in the affine group. Sometimes the term *affinely equivalent* is used. We also say that two crystal structures are equivalent if their space groups are equivalent.

(5.5) PROPOSITION. *Let $1 \to T_1 \to G_1 \to P_1 \to 1$ and $1 \to T_2 \to G_2 \to P_2 \to 1$ be space groups acting on $\mathbb{E}^n$. The following are equivalent.*

(i) The space groups are equivalent.

(ii) There exists a commutative diagram

$$\begin{array}{ccccccccc} 1 & \to & T_1 & \to & G_1 & \to & P_1 & \to & 1 \\ & & \big\downarrow & & \cong\big\downarrow & & \big\downarrow & & \\ 1 & \to & T_2 & \to & G_2 & \to & P_2 & \to & 1. \end{array}$$

(iii) $G_1 \cong G_2$ as abstract groups.

Proof. (i) $\Rightarrow$ (iii) is clear.

(iii) $\Rightarrow$ (ii): If $\phi : G_1 \to G_2$ is an isomorphism then $\phi(T_1)$ must be the unique maximal abelian subgroup of G_2 isomorphic to $\mathbb{Z}^n$. Hence $\phi(T_1) = T_2$ by 6.4, and ϕ provides a commutative diagram as in condition (ii).

(ii) $\Rightarrow$ (i): Suppose we are given a commutative diagram

$$\begin{array}{ccccccccc} 1 & \to & T_1 & \to & G_1 & \to & P_1 & \to & 1 \\ & & \alpha\big\downarrow & & \beta\big\downarrow & & \gamma\big\downarrow & & \\ 1 & \to & T_2 & \to & G_2 & \to & P_2 & \to & 1. \end{array}$$

We will regard both of these extensions as being embedded in $\mathbb{R}^n \rtimes O(n)$ so we have containments

$$\begin{array}{ccccccccc} 1 & \to & T_i & \to & G_i & \to & P_i & \to & 1 \\ & & \big\downarrow & & \big\downarrow & & \big\downarrow & & \\ 1 & \to & \mathbb{R}^n & \to & \mathbb{R}^n \rtimes O(n) & \to & O(n) & \to & 1. \end{array}$$

In this manner we may assume that $T_i \leq \mathbb{R}^n$ and $P_i \leq O(n)$ for $i = 1, 2$. Since both T_1 and T_2 contain a basis of $\mathbb{R}^n$ they are conjugate within $GL(n, \mathbb{R})$, and so after applying such a conjugation we may assume $T_1 = T_2 = T$, say. Now $\gamma : P_1 \to P_2$ must be the identity, since for any element $g \in P_1$, $g^{-1}\gamma(g)$ must act as the identity on T, and hence on $\mathbb{R}^n$. This cannot happen unless $g = \gamma(g)$ since $O(n)$ acts faithfully on $\mathbb{R}^n$. We write P for the group $P_1 = P_2$. Let E denote the preimage of P in $\mathbb{R}^n \rtimes O(n)$, so that β extends to an automorphism $\tilde{\beta} : E \to E$ as follows:

$$\begin{array}{ccccccccc} & & & & E & & & & \\ & & & \nearrow & & \searrow & & & \\ 1 & \to & \mathbb{R}^n & & \tilde{\beta}\big\downarrow & & P & \to & 1 \\ & & & \searrow & & \nearrow & & & \\ & & & & E & & & & \end{array}$$

We show that $\tilde{\beta}$ is conjugation by some translation in $\mathbb{R}^n$. Firstly, both extensions here split, because $H^2(P, \mathbb{R}^n) = 0$; and now $\tilde{\beta}$ is conjugation by an element of $\mathbb{R}^n$ since $H^1(P, \mathbb{R}^n) = 0$. (As an alternative we may proceed geometrically. If C is a complement to $\mathbb{R}^n$ in E then $\beta(C)$ is another complement, and both are orthogonal groups fixing certain vectors $u, v \in \mathbb{E}^n$. Now conjugation by the translation from u to v induces $\tilde{\beta}$, and hence β.) □

As a summary of the results so far, we have now shown that to classify space groups of dimension n up to affine equivalence it is equivalent to classify extensions $1 \to T \to G \to P \to 1$ where $T \cong \mathbb{Z}^n$ and P is a finite group acting faithfully on T, up to equivalence by diagrams as in 6.5(ii).

Classification of 2-dimensional spacegroups.

We must determine:

(i) the finite groups P with a faithful action on $\mathbb{Z}^2$, i.e. the finite subgroups of $GL(2, \mathbb{Z})$,

(ii) for each such P the different faithful $\mathbb{Z}P$-modules T with $T \cong \mathbb{Z}^2$ as abelian groups. We need only determine T up to $\mathbb{Z}P$-isomorphism since if $T \cong T'$ we obtain isomorphic extensions using wither T or T',

(iii) the possible extensions for each P and T. Thus we calculate $H^2(P, T)$.

As in 6.3 we may always assume that T is a subgroup of $\mathbb{E}^n$ so that P acts as a group of orthogonal transformations of T.

(5.6) LEMMA. *If g is an automorphism of T of finite order then g has order 1, 2, 3, 4 or 6.*

Proof. We may suppose that g acts as an orthogonal transformation of T, and now g is either a rotation or a reflection. If it is a reflection, it has order 2. Suppose instead that g is a rotation and choose a vector $u \in T$ of minimal length. If g is rotation through an angle θ then $t_u g^{-1} t_{-u}$ is rotation through $-\theta$ centered on u. Let $v = t_u g^{-1} t_{-u}(0)$. Now the vector $v - gu$ lies in T and points in the same direction as u. By minimality of u, $v - gu$ is an integer multiple of u and so $\theta = 0, \frac{\pi}{3}, \frac{\pi}{2}, \frac{2\pi}{3}$, or π.

□

As a stepping stone in the determination of all possible faithful actions of a finite group on a n-dimensional lattice we introduce the notion of a Bravais lattice. We define a *Bravais lattice* in dimension n to be a subgroup $\mathbb{Z}^n \cong T \leq \mathbb{E}^n$ together with its full orthogonal automorphism group $Q = \{g \in O(n) \mid gT = T\}$ acting on it. Thus a Bravais lattice really consists of a pair (T, Q), but we may refer to just T as the lattice. We will refer to P as the *Bravais point group.* We consider two of these pairs (T_i, Q_i), $i = 1, 2$ equivalent if there is an automorphism $\alpha \in GL(n, \mathbb{R})$ so that $T_2 = gT_1$ and $Q_2 = {}^gQ_1$. Since every finite group subgroup of $GL(n, \mathbb{R})$ is conjugate to a subgroup of $O(n)$ we have immediately the following result.

(5.7) PROPOSITION. *Any faithful $\mathbb{Z}P$-module T with $T \cong \mathbb{Z}^n$ and P finite is $\mathbb{Z}P$-isomorphic to one of the Bravais lattices with P acting as a subgroup of the Bravais point group.*

It follows from this that to obtain all finite groups acting faithfully on lattices $\mathbb{Z}^n$ up to module isomorphism of the lattices, we get a complete list by enumerating the Bravais lattices (T, Q) and listing all subgroups of Q. We only need list these subgroups up to conjugacy, since conjugate subgroups will give isomorphic lattices. Even then we may obtain more than once the same group with an isomorphic lattice, so we should inspect our list to make sure such repetitions do not occur.

(5.8) PROPOSITION. *The Bravais lattices in dimension 2 are given in the accompanying list.*

Proof. We let P be a Bravais point group, assume that P contains either a certain rotation or a reflection and reconstruct the embedding of T in $\mathbb{E}^n$. We start with rotations. Choose a non-zero element of T which is closest to the origin. Clearly, up to linear transformation of $\mathbb{E}^n$, this could have been any non-zero vector. Now if P contains a rotation through $\frac{\pi}{3}$ or $\frac{2\pi}{3}$ we recover a triangular lattice, and if P contains a rotation through $\frac{\pi}{2}$ we recover a square lattice. We continue the argument in this way, assuming P contains a rotation through π, and finally that P contains a reflection. With these last possibilities an inappropriate choice of embedding for T would allow a larger automorphism group than that shown in the list, but then this Bravais lattice would have to be one of the earlier ones given on the list. Note that the two lattices with automorphism group $C_2 \times C_2$ are non-isomorphic for the reason that on one of them generators of T may be chosen along the reflection lines, and in the other this is not possible. □

P contains:	T embeds in $\mathbb{E}^2$ as:	Maximum P:
rotation $\frac{\pi}{3}$ or $\frac{2\pi}{3}$		D_{12}
rotation $\frac{\pi}{2}$		D_8
rotation π		C_2
reflection	generators of T can be chosen along reflection lines	$C_2 \times C_2$
reflection	generators of T cannot be chosen along reflection lines	$C_2 \times C_2$

TABLE: the Bravais Lattices in 2 dimensions.

(5.9) CORLLARY (Leonardo da Vinci). *Any finite group of real* 2×2 *matrices is either cyclic or dihedral.*

The attribution of this corollary is given by Hermann Weyl in his book ‘Symmetry’.

(5.10) THEOREM. *The possible faithful actions of a finite group* P *on* $\mathbb{Z}^2$ *up to* $\mathbb{Z}P$*-isomorphism are given on the accompanying table.*

Proof. We examine all the subgroups of the Bravais point groups. □

At this point we mention a further piece of terminology, which we shall not have occasion to use. For each point group P and each $\mathbb{Z}P$-isomorphism class of lattices T there may be several space groups which are extensions of P by T. We call the collection of such space groups an *arithmetic crystal class.* There is a weaker equivalence relation on space groups which arises by grouping together all those space groups with the same point group P and such that the $\mathbb{Q}P$-modules $\mathbb{Q} \otimes_{\mathbb{Z}} T$ are isomorphic. We obtain in this way a *geometric crystal class* of space groups. For example in dimension 2, pm and pg constitute an arithmetic crystal class, and cm is also in the same geometric crystal class.

Computation of $H^2(P,T)$.

We turn now to the final ingredient in the classification of crystal structures. Having determined the possibilities for the point group and the translation lattice, we compute the possible extensions that there may be.

In the case of wallpaper patterns we have seen that the point group is either cyclic or dihedral, and as far as the cyclic groups are concerned we may quote a formula for the cohomology: $H^2(P,T) = T^P / \sum_{g\in P} g \cdot T$. In case P is C_3, C_4 or C_6 it is clear that there are no non-zero fixed points on T , so $T^P = 0$, and the only extension of P by T is split. In case $P = C_2$ there are three possible actions, giving lattices T_1, T_2 and T_3 listed in the table of possible actions. These lattices have the structure

$$T_1 = \tilde{\mathbb{Z}} \oplus \tilde{\mathbb{Z}}, \quad T_2 = \mathbb{Z} \oplus \tilde{\mathbb{Z}}, \quad T_3 = \mathbb{Z}C_2$$

as $\mathbb{Z}C_2$-modules, where $\tilde{\mathbb{Z}}$ denotes a copy of $\mathbb{Z}$ with the generator of C_2 acting as -1. Since $T_1^P = 0$ and T_3 is the regular representation we get zero cohomology in these cases. By direct calculation $H^2(C_2, T_2) = \mathbb{Z}/2\mathbb{Z}$. We conclude that for all the cyclic point groups in two dimensions $H^2(P,T) = 0$, except $H^2(C_2,T_2) = \mathbb{Z}/2\mathbb{Z}$, and there is one non-split extension in this case.

For the remaining point groups we follow a general procedure which is due to Zassenhaus.

(5.11) THEOREM. *Let P be a finite group given by a presentation*

$$P = \langle g_1, \ldots, g_d \,\big|\, r_1, \ldots, r_t \rangle.$$

We will regard this presentation also as an exact sequence $1 \to R \to F \to P \to 1$ where F is the free group on $g_1, \ldots, g_d$. Let T be a $\mathbb{Z}P$-module such that $T \cong \mathbb{Z}^n$ as an abelian group, and let $\rho : P \to GL(n,\mathbb{Z})$ be the corresponding representation of P. Form the $nt \times nd$ matrix

$$\Lambda = (\rho\left(\frac{\partial r_i}{\partial g_j}\right)) \in M_{nt,nd}(\mathbb{Z})$$

where the elements $\frac{\partial r_i}{\partial g_j} \in \mathbb{Z}F$ are defined by

$$r_i - 1 = \sum_{j=1}^{d} \frac{\partial r_i}{\partial g_j}(g_j - 1).$$

Then $H^2(P,T) \cong \mathbb{Z}/b_1\mathbb{Z} \oplus \cdots \oplus \mathbb{Z}/b_u\mathbb{Z}$ where $b_1, \ldots, b_u$ are the non-zero invariant factors of Λ.

In connection with this result we recall the following theorem of H.J.S. Smith from 1861, which is equivalent to the structure theorem for finitely generated abelian groups.

(5.12) THEOREM (Smith normal form). *Let $A \in M_{m,n}(\mathbb{Z})$. There exist matrices $P \in GL(m,\mathbb{Z})$ and $Q \in GL(n,\mathbb{Z})$ such that PAQ is a diagonal matrix*

$$\begin{pmatrix} b_1 &&&&&& \\ & b_2 &&&&& \\ && \ddots &&&& \\ &&& b_u &&& \\ &&&& 0 && \\ &&&&& \ddots & \\ &&&&&& 0 \end{pmatrix}$$

with $b_1 \mid b_2 \mid \cdots \mid b_u \neq 0$. The b_i are called the invariant factors of A.

Proof of 5.11. We embed T in the n-dimensional real vector space $\mathbb{R}T = \mathbb{R} \otimes_{\mathbb{Z}} T$, which becomes a $\mathbb{Z}P$-module through the action on T. Since $\mathbb{R}$ is uniquely divisible, we have $H^2(P,\mathbb{R}T) = 0$. From the resolution

$$\begin{array}{ccccccccccc} \mathbb{Z}P^t & & \rightarrow & & \mathbb{Z}P^d & & \rightarrow & & \mathbb{Z}P & \rightarrow & \mathbb{Z} & \rightarrow & 0 \\ & \searrow & & \nearrow & & \searrow & & \nearrow & & & & & \\ & & R/R' & & & & IP & & & & & & \end{array}$$

we obtain the following commutative diagram in which the rows are the sequences used to calculate $H^2(P,T)$ and $H^2(P,\mathbb{R}T) = 0$:

$$\begin{array}{ccccccccc} & & 0 & & 0 & & & & \\ & & \downarrow & & \downarrow & & & & \\ \mathrm{Hom}(IP,T) & \longrightarrow & \mathrm{Hom}(\mathbb{Z}P^d,T) & \longrightarrow & \mathrm{Hom}(R/R',T) & \rightarrow & H^2(P,T) & \rightarrow & 0 \\ \downarrow & & \downarrow & & \downarrow & & & & \\ \mathrm{Hom}(IP,\mathbb{R}T) & \xrightarrow{\beta} & \mathrm{Hom}(\mathbb{Z}P^d,\mathbb{R}T) & \xrightarrow{\alpha} & \mathrm{Hom}(R/R',\mathbb{R}T) & \rightarrow & 0 & & \end{array}$$

All the rows and columns here are exact and β is injective. We see that α is surjective. Let

$$X = \{\phi : \mathbb{Z}P^d \rightarrow \mathbb{R}T \mid \phi(R/R') \subseteq T\}.$$

Then

$$0 \to \mathrm{Hom}(IP, \mathbb{R}T) \to X \to \mathrm{Hom}(R/R', T) \to 0$$

is exact, and so the composite surjection $X \to \mathrm{Hom}(R/R', T) \to H^2(P, T)$ has kernel $\beta(\mathrm{Hom}(IP, \mathbb{R}T)) + \mathrm{Hom}(\mathbb{Z}P^d, T)$.

Now $\mathbb{Z}P^d$ is a free module, so homomorphisms $\phi : \mathbb{Z}P^d \to \mathbb{R}T$ biject with d-tuples $(v_1, \ldots, v_d)$ of elements of $\mathbb{R}T$, where v_i is the image of the ith basis vector of $\mathbb{Z}P^d$. The generators of R/R' have coordinates which the the rows of the matrix $\left(\frac{\partial r_i}{\partial g_j}\right)$, and so the images of the generators of R/R' form a t-tuple of vectors in $\mathbb{R}T$

$$\Lambda \begin{pmatrix} v_1 \\ \vdots \\ v_d \end{pmatrix} \in \mathbb{R}T^t.$$

From this we see that

$$X \cong \{\underline{x} \in \mathbb{R}T^d \bigm| \Lambda(\underline{x}) \in T^t\}.$$

In a similar way

$$\begin{aligned} \mathrm{Hom}(IP, T) &\cong \{\phi : \mathbb{Z}P^d \to T \bigm| \phi(R/R') = 0\} \\ &= \{\underline{x} \in \mathbb{R}T^d \bigm| \Lambda(\underline{x}) = 0\} \\ &= \mathrm{Ker}\,\Lambda \end{aligned}$$

and $\mathrm{Hom}(\mathbb{Z}P^d, T) \cong T^d$. We conclude that

$$H^2(P, T) \cong \{\underline{x} \in \mathbb{R}T^d \bigm| \Lambda(\underline{x}) \in T^t\}/(\mathrm{Ker}\,\Lambda + T^d).$$

At this stage we observe that our calculation will be independent of the choice of basis for the domain T^d and codomain T^t of Λ, so we will chose bases such that Λ is in Smith normal form. The result is now immediate since for a diagonal matrix $\mathrm{diag}(b_1, \ldots, b_q)$ we have

$$\{\underline{x} \in \mathbb{Z}^q \bigm| b_i x_i \in \mathbb{Z} \text{ for all } i\}/\mathbb{Z}^q = (\oplus \frac{1}{b_i}\mathbb{Z})/\mathbb{Z}^q = \oplus \mathbb{Z}/b_i\mathbb{Z}$$

and the zeros on the diagonal of Λ simply contribute to the kernel. □

Example. Let $P = \langle x, y \bigm| x^2 = y^2 = (xy)^2 = 1\rangle$ acting on $T = \mathbb{Z}^2$ via $A = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$ and $B = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. We have

$$\begin{aligned} x^2 - 1 &= (x+1)(x-1) \\ y^2 - 1 &= (y+1)(y-1) \\ (xy)^2 - 1 &= (xy+1)(xy-1) \\ &= (xy+1)x(y-1) + (xy+1)(x-1). \end{aligned}$$

So

$$\Lambda = \begin{pmatrix} x+1 & 0 \\ 0 & y+1 \\ xy+1 & (xy+1)x \end{pmatrix}_{\substack{x\mapsto A \\ y\mapsto B}}$$

$$= \begin{pmatrix} \begin{matrix} 0 & 0 \\ 0 & 2 \end{matrix} & 0 \\ 0 & \begin{matrix} 0 & 0 \\ 0 & 2 \end{matrix} \\ 0 & 0 \end{pmatrix}$$

and $H^2(C_2 \times C_2, T) = \mathbb{Z}/2\mathbb{Z} \oplus \mathbb{Z}/2\mathbb{Z}$. The following are homomorphisms $R/R' \to T$ which represent the elements of this group:

$$\begin{matrix} x^2 \\ y^2 \\ (xy)^2 \end{matrix} \begin{matrix} \mapsto \\ \mapsto \\ \mapsto \end{matrix} \left\{ \begin{matrix} (0,0) \\ (0,0) \\ (0,0) \end{matrix} \right. \underbrace{\left\{ \begin{matrix} (0,1) \\ (0,0) \\ (0,0) \end{matrix} \right. \left\{ \begin{matrix} (0,0) \\ (1,0) \\ (0,0) \end{matrix} \right.}_{\text{isomorphic extensions}} \left\{ \begin{matrix} (0,1) \\ (1,0) \\ (0,0) \end{matrix} \right.$$

where momentarily we represent vectors as row vectors. For example, the second extension has a presentation

$$\langle x, y, e_1, e_2 \mid x^2 = e_2,\ y^2 = (xy)^2 = [e_1, e_2] = 1,\ {}^{x}e_1 = e_1^{-1},\ {}^{x}e_2 = e_2,\ {}^{y}e_1 = e_1,\ {}^{y}e_2 = e_2^{-1} \rangle$$

and the third has the same presentation but with x and y interchanged and e_1 and e_2 interchanged, so is isomorphic.

When do two elements of $H^2(P,T)$ give extensions which are equivalent as space groups? It happens if and only if there is a commutative diagram

$$\begin{array}{ccccc} T & \longrightarrow & G_1 & \longrightarrow & P \\ \downarrow{\scriptstyle\alpha} & & \downarrow{\scriptstyle\cong} & & \downarrow{\scriptstyle\beta} \\ T & \longrightarrow & G_2 & \longrightarrow & P \end{array}$$

where $\alpha \in GL(T)$. Since T is the same P-module in the top and bottom extension we have for all $g \in P$, for all $t \in T$, ${}^{\beta(g)}(\alpha t) = \alpha({}^{g}t)$ so that ${}^{\beta(g)}(t) = \alpha\, {}^{g}(\alpha^{-1}t)$. We see from this that β has the same effect as conjugation by α within $GL(T)$, and since $\beta P = P$ we have $\alpha \in N_{GL(T)}(P)$. We may formalize this by observing that $N_{GL(T)}(P)$ acts on equivalence classes of extension, and hence on $H^2(P,T)$ in the following way. Given $\alpha \in N_{GL(T)}(P)$ and an extension $\mathcal{E} : T \xrightarrow{\phi} G_1 \xrightarrow{\theta} P$ we obtain an extension $\alpha\mathcal{E} : T \xrightarrow{\phi\alpha^{-1}} G_1 \xrightarrow{\beta\theta} P$ where β denotes conjugation by α within $GL(T)$. Using this action we may now state the following result, which we have already proved.

(5.13) PROPOSITION. *Two space groups which are extensions of P by T are affine equivalent if and only if their cohomology classes in $H^2(P,T)$ belong to the same orbit in the action of $N_{GL(T)}(P)$.*

We now express this in a fashion which is compatible with our previous description of $H^2(P,T)$ in terms of the relation module. Let $1 \to R \to F \to P \to 1$ be a presentation of P and suppose the extension $\mathcal{E}$ is represented by a homomorphism $f : R/R' \to T$, continuing with the previous notation. Lift β^{-1} to give a homomorphism γ as shown:

$$\begin{array}{ccccc} R & \longrightarrow & F & \longrightarrow & P \\ \Big\downarrow{\scriptstyle\gamma} & & \Big\downarrow & & \Big\downarrow{\scriptstyle\beta^{-1}} \\ R & \longrightarrow & F & \longrightarrow & P. \end{array}$$

Define ${}^{\alpha}f : R/R' \to T$ by ${}^{\alpha}f(rR') = \alpha f(\gamma(r)R')$. Then we have

(5.14) PROPOSITION. *If $\mathcal{E}$ is an extension represented by f then the extension $\alpha\mathcal{E}$ is represented by ${}^{\alpha}f$.*

This last result enables us to determine the action of $N_{GL(T)}(P)$ on $H^2(P,T)$ by computer. This completes the description of the method of determining the equivalence classes of space groups in a given dimension n which is known as the Zassenhaus algorithm. In summary, its steps are:

(i) Determine the isomorphism classes of finite subgroups P of $GL_n(\mathbb{Z})$ and obtain presentations for them.

(ii) For each such P determine all $\mathbb{Z}P$-lattices T of rank n up to $\mathbb{Z}P$-isomorphism. For each T determine $N_{GL(T)}(P)$.

(iii) Compute $H^2(P,T)$.

(iv) Compute the orbits of $N_{GL(T)}(P)$ on $H^2(P,T)$.

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