

Chapter 4

The Split Three-Dimensional Crystallographic Groups

Definition 4.1. An n -dimensional crystallographic group Γ is a discrete, cocompact subgroup of the group of isometries of Euclidean n -space. Each $\gamma \in \Gamma$ can be written in the form $v_\gamma + A_\gamma$, where $v_\gamma \in \mathbb{R}^n$ is a translation and $A_\gamma \in O(n)$. There is a natural map $\pi : \Gamma \rightarrow O(n)$ sending $v_\gamma + A_\gamma$ to A_γ , and this map is easily seen to be a homomorphism. We get a short exact sequence as follows:

$$L \twoheadrightarrow \Gamma \twoheadrightarrow H,$$

where $H = \pi(\Gamma) \leq O(n)$ and L is the kernel. (By [Ra94, Theorem 7.4.2], L is a lattice in \mathbb{R}^n , and so necessarily isomorphic to \mathbb{Z}^n .) We note that H acts naturally on L , which makes H a point group in the sense of Definition 2.1. We say that H is the *point group* of Γ . The group Γ is a *split n -dimensional crystallographic group* if the above sequence splits, i.e., if there is a homomorphism $s : H \rightarrow \Gamma$ such that $\pi s = \text{id}_H$.

From now on, all of our crystallographic groups will be three-dimensional.

Definition 4.2. Suppose that L is a lattice in \mathbb{R}^3 and $H \leq O(3)$ satisfies $H \cdot L = L$. We let $\Gamma(L, H)$ denote the group $\langle L, H \rangle$.

Remark 4.1. It is straightforward to verify that every $\Gamma(L, H)$ is a split crystallographic group.

Theorem 4.1. Any split crystallographic group $\hat{\Gamma}$ is isomorphic to $\Gamma(L, H)$, for some lattice $L \leq \mathbb{R}^3$ and $H \leq O(3)$ satisfying $H \cdot L = L$. The groups $\Gamma(L, H)$ and $\Gamma(L', H')$ are isomorphic if and only if the pairs (L, H) and (L', H') are arithmetically equivalent.

Proof. We prove the first statement. Let $\hat{\Gamma}$ be a split crystallographic group, \hat{L} denote the lattice of $\hat{\Gamma}$, and \hat{H} denote the point group of $\hat{\Gamma}$. Since $\hat{\Gamma}$ is split, it follows that there is a finite subgroup J of $\hat{\Gamma}$ such that $\pi : \hat{\Gamma} \rightarrow \hat{H}$ satisfies $\pi(J) = \hat{H}$. It is routine to check that $\pi|_J : J \rightarrow \hat{H}$ must also be injective. Since J

is a finite group of isometries of \mathbb{R}^3 , it must be that the entire group J fixes a point $v \in \mathbb{R}^3$. We consider the isometry $T_v \in \text{Isom}(\mathbb{R}^3)$, which is simply translation by the vector v . It follows that $T_v^{-1}JT_v$ fixes the origin, so the map $\pi : T_v^{-1}JT_v \rightarrow \hat{H}$ is the identity. We can therefore write

$$1 \rightarrow \hat{L} \rightarrow T_v^{-1}\hat{F}T_v \rightarrow \hat{H} \rightarrow 1,$$

where $\hat{H} \leq T_v^{-1}\hat{F}T_v$. It follows directly that $\hat{F} \cong T_v^{-1}\hat{F}T_v = \langle \hat{L}, \hat{H} \rangle$, proving the first statement.

Now we prove the second statement. Assume that $\Gamma(L, H)$ and $\Gamma(L', H')$ are isomorphic. Ratcliffe [Ra94, Theorem 7.4.4] says that there is an affine bijection α of \mathbb{R}^3 such that $\alpha\Gamma(L, H)\alpha^{-1} = \Gamma(L', H')$. We write $\alpha = v_\alpha + A_\alpha$, where $v_\alpha \in \mathbb{R}^3$ and $A_\alpha \in GL_3(\mathbb{R})$. We note:

$$\alpha L \alpha^{-1} = A_\alpha \cdot L;$$

$$\alpha H \alpha^{-1} = (v_\alpha - A_\alpha H A_\alpha^{-1}(v_\alpha)) + A_\alpha H A_\alpha^{-1}.$$

Now $\alpha\Gamma(L, H)\alpha^{-1}$ and $\Gamma(L', H')$ must have the same kernel and image under the canonical projection $\pi : \text{Isom}(\mathbb{R}^3) \rightarrow O(3)$, so $A_\alpha \cdot L = L'$ and $A_\alpha H A_\alpha^{-1} = H'$. (These last two equations are between kernels and images, respectively.) It follows that (L, H) and (L', H') are arithmetically equivalent.

If two pairs (L, H) and (L', H') are arithmetically equivalent, then there is $\lambda \in GL_3(\mathbb{R})$ such that $\lambda L = L'$ and $\lambda H \lambda^{-1} = H'$. It follows easily that $\lambda\Gamma(L, H)\lambda^{-1} = \Gamma(L', H')$, so $\Gamma(L, H)$ and $\Gamma(L', H')$ are isomorphic.

Theorem 4.2 (List of Split Three-Dimensional Crystallographic Groups). *Let \mathbf{x} , \mathbf{y} , and \mathbf{z} denote the standard coordinate vectors, and let*

$$\mathbf{v}_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad \mathbf{v}_2 = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, \quad \mathbf{v}_3 = \begin{pmatrix} 0 \\ -1 \\ 1 \end{pmatrix}.$$

A complete list of the split three-dimensional crystallographic groups $\langle L, H \rangle$ (up to isomorphism) appears in Table 4.1.

Proof. Table 4.1 lists all pairings of lattices and point groups from Theorems 3.1 and 3.3. We have already shown that no two of the pairs from Theorem 3.1 determine the same arithmetic equivalence class (Theorem 3.2). Also, no two of the pairs from Theorem 3.3 determine the same arithmetic class. If the pair (L_1, H_1) is chosen from the pairs listed in Theorem 3.1, and (L_2, H_2) is chosen from the pairs listed in Theorem 3.3, then $(L_1, H_1) \not\sim (L_2, H_2)$, since H_1 contains the inversion (-1) and H_2 does not, and containing the inversion will be preserved by arithmetic equivalence. Thus, all 73 pairs in Table 4.1 represent distinct equivalence classes.

It is clear from Theorems 3.1 and 3.3 that any pair (L, H) is equivalent to one on the list, since H must be conjugate to one of the standard point groups. It follows that there are exactly 73 classes of such pairs.

Table 4.1 The split three-dimensional crystallographic groups

L	H					
	$S_4^+ \times (-1)$	S_4^+	S'_4	$A_4^+ \times (-1)$	A_4^+	D_4''
$\langle \mathbf{x}, \mathbf{y}, \mathbf{z} \rangle$	$D_4^+ \times (-1)$	D_4^+	C'_2	$D_2^+ \times (-1)$	D_2^+	C'_4
	$C_4^+ \times (-1)$	C_4^+	D'_2	$C_2^+ \times (-1)$	C_2^+	D'_4
	$C_1^+ \times (-1)$	C_1^+	\hat{D}'_4			
	$S_4^+ \times (-1)$	S_4^+	S'_4	$A_4^+ \times (-1)$	A_4^+	D_4''
$\langle \frac{1}{2}(\mathbf{x} + \mathbf{y} + \mathbf{z}), \mathbf{y}, \mathbf{z} \rangle$	$D_4^+ \times (-1)$	D_4^+	C'_2	$D_2^+ \times (-1)$	D_2^+	C'_4
	$C_4^+ \times (-1)$	C_4^+	D'_2	$C_2^+ \times (-1)$	C_2^+	D'_4
	\hat{D}'_4					
	$S_4^+ \times (-1)$	S_4^+	S'_4	$A_4^+ \times (-1)$	A_4^+	D'_2
$\frac{1}{2} \langle (\mathbf{x} + \mathbf{y}), (\mathbf{x} + \mathbf{z}), (\mathbf{y} + \mathbf{z}) \rangle$	$D_2^+ \times (-1)$	D_2^+				
$\langle \frac{1}{2}(\mathbf{x} + \mathbf{z}), \mathbf{y}, \mathbf{z} \rangle$	$D_2^+ \times (-1)$	D_2^+	D'_2	D'_{2_2}		
	$D_6^+ \times (-1)$	D_6^+	C'_6	$C_6^+ \times (-1)$	D'_6	C_6^+
$\langle \mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3 \rangle$	$D_3^+ \times (-1)$	\hat{D}'_6	C_3^+	$C_3^+ \times (-1)$	D'_3	D_3^+
	D'_6					
$\langle \frac{1}{3}(\mathbf{v}_1 + \mathbf{v}_2 + \mathbf{v}_3), \mathbf{v}_2, \mathbf{v}_3 \rangle$	$D_3^+ \times (-1)$	D_3^+	D'_3	$C_3^+ \times (-1)$	C_3^+	
$\langle \mathbf{v}_1, \frac{1}{3}(\mathbf{v}_2 + \mathbf{v}_3), \mathbf{v}_3 \rangle$	$D_3^+ \times (-1)$	D_3^+	D'_3			

The theorem now follows from Theorem 4.1.

Remark 4.2. Let $\hat{\Gamma}$ be a point group. For the sake of brevity, we will sometimes let $\hat{\Gamma}_i$ denote the split crystallographic group $\langle L_i, \hat{\Gamma} \rangle$, where L_i denotes the i th lattice (in the order that they are listed in Table 4.1). Thus, $(D_2^+)_1$ denotes the split crystallographic group generated by the point group D_2^+ and the standard cubical lattice.

We will let Γ_i denote the i th maximal split crystallographic group; i.e., the pairing of the i th lattice with the largest point group from Table 4.1. Thus, for instance, Γ_1 denotes the group $\langle \mathbf{x}, \mathbf{y}, \mathbf{z} \rangle \rtimes (S_4^+ \times (-1))$.