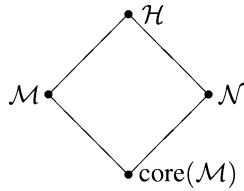


1.4. THE MATHEMATICAL BACKGROUND OF THE SUBGROUP TABLES

$$\mathcal{N}' := \mathcal{N} \text{ core}(\mathcal{M})$$

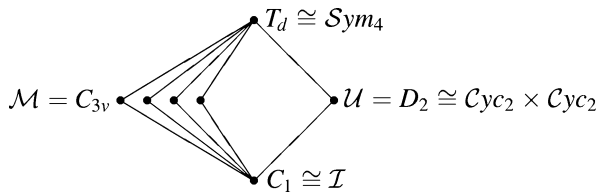
of \mathcal{N} in \mathcal{G} , then one has $\mathcal{G} = \mathcal{N}'\mathcal{M}$ and $\mathcal{M} \cap \mathcal{N}' = \text{core}(\mathcal{M})$. Hence we have seen the first part of the following theorem:

Theorem 1.4.5.3.2. Let $\mathcal{M} \leq \mathcal{G}$ be a maximal subgroup of the soluble group \mathcal{G} . Then the factor group $\mathcal{H} := \mathcal{G}/\text{core}(\mathcal{M})$ acts primitively and faithfully on $X := \mathcal{G}/\mathcal{M}$, and there is a normal subgroup $\mathcal{N}' \trianglelefteq \mathcal{G}$ with $\mathcal{M}\mathcal{N}' = \mathcal{G}$ and $\mathcal{M} \cap \mathcal{N}' = \text{core}(\mathcal{M})$. Moreover, if \mathcal{M}' is another subgroup of \mathcal{G} , with $\mathcal{M}'\mathcal{N}' = \mathcal{G}$ and $\mathcal{M}' \cap \mathcal{N}' = \text{core}(\mathcal{M})$, then \mathcal{M}' is conjugate to \mathcal{M} .

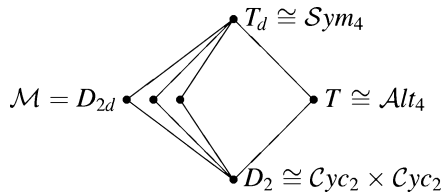


Example 1.4.5.3.3

$\mathcal{G} = \text{Sym}_4 \cong T_d$ is the tetrahedral group from Section 1.4.3.2 and $\text{Sym}_3 \cong \mathcal{M} = C_{3v} \leq \mathcal{G}$ is the stabilizer of one of the four apices in the tetrahedron. Then $\text{core}(\mathcal{M}) = \{e\}$ and \mathcal{G}/\mathcal{M} is a faithful \mathcal{G} -set which can be identified with the set of apices of the tetrahedron. The normal subgroup $\mathcal{N} = \mathcal{N}'$ is the normal subgroup \mathcal{U} of Section 1.4.3.2.



Now let $\mathcal{G} = \text{Sym}_4 \cong T_d$ be as above, and take $D_{2d} \cong \mathcal{M} \leq \mathcal{G}$ a Sylow 2-subgroup of \mathcal{G} . Then $\text{core}(\mathcal{M}) = D_2 \cong \text{Cyc}_2 \times \text{Cyc}_2$ is the normal subgroup \mathcal{U} from Section 1.4.3.2 and $\mathcal{H} = \mathcal{G}/\text{core}(\mathcal{M}) \cong \text{Sym}_3$.



These observations result in an algorithm for computing maximal subgroups of soluble groups \mathcal{G} :

- (1) compute normal subgroups \mathcal{C} [candidates for $\text{core}(\mathcal{M})$];
- (2) compute a minimal normal subgroup \mathcal{N}/\mathcal{C} of \mathcal{G}/\mathcal{C} ;
- (3) find \mathcal{M}/\mathcal{C} as a complement of \mathcal{N}/\mathcal{C} in \mathcal{G}/\mathcal{C} .

1.4.6. Quantitative results

This section gives estimates for the number of maximal subgroups of a given index in space groups.

1.4.6.1. General results

The first very easy but useful remark applies to general groups \mathcal{G} :

Remark. Let $\mathcal{M} \leq \mathcal{G}$ be a maximal subgroup of \mathcal{G} of finite index $i := [\mathcal{G} : \mathcal{M}] < \infty$. Then $\mathcal{M} \leq \mathcal{N}_{\mathcal{G}}(\mathcal{M}) \leq \mathcal{G}$. Hence the maxim-

ality of \mathcal{M} implies that either $\mathcal{N}_{\mathcal{G}}(\mathcal{M}) = \mathcal{G}$ and \mathcal{M} is a normal subgroup of \mathcal{G} or $\mathcal{N}_{\mathcal{G}}(\mathcal{M}) = \mathcal{M}$ and \mathcal{G} has i maximal subgroups that are conjugate to \mathcal{M} .

The smallest possible index of a proper subgroup is 2. It is well known and easy to see that subgroups of index 2 are normal subgroups:

Proposition 1.4.6.1.1. Let \mathcal{G} be a group and $\mathcal{M} \leq \mathcal{G}$ a subgroup of index 2 = $|\mathcal{G}/\mathcal{M}|$. Then \mathcal{M} is a normal subgroup of \mathcal{G} . □

Proof. Choose an element $g \in \mathcal{G}$, $g \notin \mathcal{M}$. Then $\mathcal{G} = \mathcal{M} \cup g\mathcal{M} = \mathcal{M} \cup \mathcal{M}g$. Hence $g\mathcal{M} = \mathcal{M}g$ and therefore $g\mathcal{M}g^{-1} = \mathcal{M}$. Since this is also true if $g \in \mathcal{M}$, the proposition follows. QED

Let \mathcal{M} be a subgroup of a group \mathcal{G} of index 2. Then $\mathcal{M} \trianglelefteq \mathcal{G}$ is a normal subgroup and the factor group \mathcal{G}/\mathcal{M} is a group of order 2. Since groups of order 2 are Abelian, it follows that the derived subgroup \mathcal{G}_1 of \mathcal{G} (cf. Definition 1.4.5.2.1) (which is the smallest normal subgroup of \mathcal{G} such that the factor group is Abelian) is contained in \mathcal{M} . Hence all maximal subgroups of index 2 in \mathcal{G} contain \mathcal{G}_1 . If one defines $\mathcal{N} := \cap\{\mathcal{M} \leq \mathcal{G} \mid [\mathcal{G} : \mathcal{M}] = 2\}$, then \mathcal{G}/\mathcal{N} is an elementary Abelian 2-group and hence a vector space over the field with two elements. The maximal subgroups of \mathcal{G}/\mathcal{N} are the maximal subspaces of this vector space, hence their number is $2^a - 1$, where $a := \dim_{\mathbb{Z}/2\mathbb{Z}}(\mathcal{G}/\mathcal{N})$.

This shows the following:

Corollary 1.4.6.1.2. The number of subgroups of \mathcal{G} of index 2 is of the form $2^a - 1$ for some $a \geq 0$. □

Dealing with subgroups of index 3, one has the following:

Proposition 1.4.6.1.3. Let \mathcal{U} be a subgroup of the group \mathcal{G} with $[\mathcal{G} : \mathcal{U}] = 3$. Then \mathcal{U} is either a normal subgroup of \mathcal{G} or $\mathcal{G}/\text{core}(\mathcal{U}) \cong \text{S}_3$ and there are three subgroups of \mathcal{G} conjugate to \mathcal{U} . □

Proof. $\mathcal{G}/\text{core}(\mathcal{U})$ is isomorphic to a subgroup of Sym_3 that acts primitively on $\{1, 2, 3\}$. Hence either $\mathcal{G}/\text{core}(\mathcal{U}) \cong \text{Cyc}_3$ and $\mathcal{U} = \text{core}(\mathcal{U})$ is a normal subgroup of \mathcal{G} or $\mathcal{G}/\text{core}(\mathcal{U}) \cong \text{Sym}_3$, $\mathcal{U}/\text{core}(\mathcal{U}) \cong \text{Cyc}_2$ and there are three subgroups of \mathcal{G} conjugate to \mathcal{U} . QED

1.4.6.2. Three-dimensional space groups

We now come to space groups. By Lemma 1.4.5.2.3, all three-dimensional space groups are soluble. Theorem 1.4.5.3.1 says that the index of a maximal subgroup of a soluble group is a prime power (or infinite). Since the index of a maximal subgroup of a space group is always finite (see Corollary 1.4.4.2.7), we get:

Corollary 1.4.6.2.1. Let \mathcal{G} be a three-dimensional space group and $\mathcal{M} \leq \mathcal{G}$ a maximal subgroup. Then $[\mathcal{G} : \mathcal{M}]$ is a prime power. □

Let \mathcal{R} be a three-dimensional space group and $\mathcal{P} = \mathcal{R}/\mathcal{I}(\mathcal{R})$ its point group. It is well known that the order of \mathcal{P} is of the form $2^a 3^b$ with $a = 0, 1, 2, 3$ or 4 and $b = 0, 1$. By Corollary 1.4.4.2.4, the t -subgroups of \mathcal{R} are in one-to-one correspondence with the subgroups of \mathcal{P} . Let us look at the t -subgroups of \mathcal{R} of index 3. It is clear that \mathcal{P} has no subgroup of index 3 if $b = 0$, since the index of a subgroup divides the order of the finite group \mathcal{P} by the theorem of Lagrange. If $b = 1$, then any subgroup \mathcal{S} of \mathcal{P} of index 3 has order $|\mathcal{P}|/3 = 2^a$ and hence is a Sylow 2-subgroup of \mathcal{P} . Therefore there is such a subgroup \mathcal{S} of index 3 in \mathcal{P} by the first theorem of Sylow, Theorem 1.4.3.3.1. By the second theorem of Sylow, Theorem 1.4.3.3.2, all these Sylow 2-subgroups of \mathcal{P} are

1. SPACE GROUPS AND THEIR SUBGROUPS

conjugate in \mathcal{P} . Therefore, by Proposition 1.4.6.1.3, the number of these groups is either 1 or 3:

Corollary 1.4.6.2.2. Let \mathcal{R} be a three-dimensional space group.

If the order of the point group of \mathcal{R} is not divisible by 3 then \mathcal{R} has no t -subgroups of index 3.

If 3 is a factor of the order of the point group of \mathcal{R} , then \mathcal{R} has either one t -subgroup of index 3 (which is then normal in \mathcal{R}) or three conjugate t -subgroups of index 3. \square

1.4.7. Qualitative results

1.4.7.1. General theory

In this section, we want to comment on the very subtle question of deciding whether two space groups \mathcal{R}_1 and \mathcal{R}_2 are isomorphic.

This problem can be treated in several stages:

Let \mathcal{R}_1 and \mathcal{R}_2 be space groups. Since the translation subgroups $\mathcal{T}(\mathcal{R}_i)$ are characteristic subgroups of \mathcal{R}_i (the maximal Abelian normal subgroup of finite index), each isomorphism $\varphi: \mathcal{R}_1 \rightarrow \mathcal{R}_2$ induces isomorphisms of the corresponding translation subgroups

$$\varphi': \mathcal{T}(\mathcal{R}_1) \rightarrow \mathcal{T}(\mathcal{R}_2)$$

(by restriction) as well as of the point groups

$$\bar{\varphi}: \mathcal{P}_1 := \mathcal{R}_1/\mathcal{T}(\mathcal{R}_1) \rightarrow \mathcal{R}_2/\mathcal{T}(\mathcal{R}_2) =: \mathcal{P}_2.$$

It is convenient to view $\mathcal{T}(\mathcal{R}_i)$ as a lattice on which the point group \mathcal{P}_i acts as group of linear mappings (*cf.* the start of Section 1.4.4). Then the isomorphism φ' is an isomorphism of \mathcal{P}_1 -sets, where \mathcal{P}_1 acts on $\mathcal{T}(\mathcal{R}_1)$ *via* conjugation and on $\mathcal{T}(\mathcal{R}_2)$ *via*

$$g\mathcal{T}(\mathcal{R}_1) \cdot t := \varphi(g)t\varphi(g)^{-1} \text{ for all } g\mathcal{T}(\mathcal{R}_1) \in \mathcal{P}_1, t \in \mathcal{T}(\mathcal{R}_2).$$

Since $\varphi(\mathcal{T}(\mathcal{R}_1)) = \mathcal{T}(\mathcal{R}_2)$ and $\mathcal{T}(\mathcal{R}_2)$ centralizes itself, this action is well defined, *i.e.* independent of the choice of the coset representative g .

The following theorem will show that the isomorphism of sufficiently large factor groups of \mathcal{R}_1 and \mathcal{R}_2 implies a ‘near’ isomorphism of the space groups themselves. To give a precise formulation we need one further definition.

Definition 1.4.7.1.1. For $d \in \mathbb{N}$ define

$$O_d := \left\{ \frac{a}{b} \mid a, b \in \mathbb{Z}, b \neq 0, \gcd(b, d) = 1 \right\} \leq \mathbb{Q},$$

which is the set of all rational numbers for which the denominator is prime to d . For the space group $\mathcal{R} \leq \mathcal{E}_n$ let $\mathcal{R} \leq \mathcal{R}_{(d)} \leq \mathcal{E}_n$ be the group $\mathcal{R}_{(d)} := \langle \mathcal{T}(\mathcal{R})_{(d)}, \mathcal{R} \rangle$, where

$$\mathcal{T}(\mathcal{R})_{(d)} = \{at \mid a \in O_{(d)}, t \in \mathcal{T}(\mathcal{R})\} \leq \mathcal{T}_n,$$

i.e. one allows denominators that are prime to d in the translation subgroup. \square

One has the following:

Theorem 1.4.7.1.2. Let \mathcal{R}_1 and \mathcal{R}_2 be two space groups with point groups of order $d_i := |\mathcal{R}_i/\mathcal{T}(\mathcal{R}_i)|$. Let $\mathbf{N}(\mathcal{R}_i)$ denote the set of normal subgroups of \mathcal{R}_i having finite index in \mathcal{R}_i . Then the following three conditions are equivalent:

- (i) There are normal subgroups $\mathcal{S}_i \trianglelefteq \mathcal{R}_i$ with $\mathcal{R}_1/\mathcal{S}_1 \cong \mathcal{R}_2/\mathcal{S}_2$ and with $\mathcal{S}_i \subseteq d_i^2\mathcal{T}(\mathcal{R}_i)$ if $d_i \neq 2$ and $\mathcal{S}_i \subseteq 16\mathcal{T}(\mathcal{R}_i)$ if $d_i = 2$ ($i = 1, 2$).
- (ii) $(\mathcal{R}_1)_{(d_1)} \cong (\mathcal{R}_2)_{(d_2)}$.
- (iii) There is a bijection $\mu: \mathbf{N}(\mathcal{R}_1) \rightarrow \mathbf{N}(\mathcal{R}_2)$ such that $\mathcal{R}_1/\mathcal{N} \cong \mathcal{R}_2/\mu(\mathcal{N})$ for all $\mathcal{N} \in \mathbf{N}(\mathcal{R}_1)$. \square

For a proof of this theorem, see Finken *et al.* (1980).

Remark. If \mathcal{R}_i are three- or four-dimensional space groups, the isomorphism in (ii) already implies the isomorphism of \mathcal{R}_1 and \mathcal{R}_2 , but there are counterexamples for dimension 5.

1.4.7.2. Three-dimensional space groups

Corollary 1.4.7.2.1. Let \mathcal{R} be a three-dimensional space group with translation subgroup \mathcal{T} and p be a prime not dividing the order of the point group \mathcal{R}/\mathcal{T} . Let \mathcal{U} be a subgroup of \mathcal{R} of index p^α for some $\alpha \in \mathbb{Z}_{>0}$. Then

- (a) \mathcal{U} is a k -subgroup.
- (b) \mathcal{U} is isomorphic to \mathcal{R} . \square

Proof.

- (a) $\mathcal{U} \leq \mathcal{UT} \leq \mathcal{R}$ implies that $[\mathcal{R} : \mathcal{UT}]$ divides $[\mathcal{R} : \mathcal{U}] = p^\alpha$. Since $\mathcal{T} \leq \mathcal{UT} \leq \mathcal{R}$, one obtains $[\mathcal{R} : \mathcal{UT}]$ as a factor of $[\mathcal{R} : \mathcal{T}]$. But p is not a factor of $[\mathcal{R} : \mathcal{T}]$, hence $[\mathcal{R} : \mathcal{UT}] = 1$ and $\mathcal{R} = \mathcal{UT}$. According to the remark following Definition 1.4.4.2.2, \mathcal{U} is a k -subgroup.

- (b) Let $d_1 := |\mathcal{R}/\mathcal{T}| = |\mathcal{U}/\mathcal{T}(\mathcal{U})|$. Let $d := d_1^2$ if $d_1 \neq 2$ and $d := 16$ otherwise, and let $\mathcal{T}' := d\mathcal{T}$. Since $\gcd([\mathcal{R} : \mathcal{U}], d) = 1$, one has $\mathcal{UT}' = \mathcal{R}$ and $\mathcal{T}' \cap \mathcal{U} = d\mathcal{T}(\mathcal{U})$. By the third isomorphism theorem, Theorem 1.4.3.5.2, it follows that

$$\mathcal{R}/\mathcal{T}' = \mathcal{UT}'/\mathcal{T}' \cong \mathcal{U}/\mathcal{T}' \cap \mathcal{U} = \mathcal{U}/d\mathcal{T}(\mathcal{U}).$$

By Theorem 1.4.7.1.2 (i) \Rightarrow (ii), one has $\mathcal{R}_{(d_1)} \cong \mathcal{U}_{(d_1)}$. By the remark above, this already implies that \mathcal{R} and \mathcal{U} are isomorphic. QED

Theorem 1.4.7.2.2. Let \mathcal{R} be a three-dimensional space group and \mathcal{U} be a maximal subgroup of \mathcal{R} of index > 4 . Then

- (a) \mathcal{U} is a k -subgroup.
- (b) \mathcal{U} is isomorphic to \mathcal{R} . \square

Proof. Since \mathcal{R} is soluble, the index $[\mathcal{R} : \mathcal{U}] = p^\alpha$ is a prime power (see Theorem 1.4.5.3.1). If p is not a factor of $|\mathcal{R}/\mathcal{T}(\mathcal{R})|$, the statement follows from Corollary 1.4.7.2.1. Hence we only have to consider the cases $p = 2, \alpha > 2$ and $p = 3, \alpha > 1$. Since 9 is not a factor of the order of any crystallographic point group in dimension 3, assertion (a) follows if the index of \mathcal{U} is divisible by 9. If \mathcal{U} is a maximal t -subgroup, then \mathcal{R}/\mathcal{U} is a primitive \mathcal{P} -set for the point group \mathcal{P} of \mathcal{R} . Since the point groups \mathcal{P} of dimension 3 have no primitive \mathcal{P} -sets of order divisible by 8, assertion (a) also follows if the index of \mathcal{U} is divisible by 8.

For all three-dimensional space groups \mathcal{R} , the module $\mathbf{L}(\mathcal{R})/2\mathbf{L}(\mathcal{R})$ [where $\mathcal{T}(\mathcal{R})$ is identified with the corresponding lattice $\mathbf{L}(\mathcal{R})$ in $\tau(\mathbb{E}_3)$ as in Section 1.4.4] is not simple as a module for the point group $\mathcal{P} = \mathcal{R}/\mathcal{T}(\mathcal{R})$. [It suffices to check this property for the two maximal point groups $\mathcal{C}_{yc_2} \times \mathcal{S}ym_4 (= m\bar{3}m)$ and $\mathcal{C}_{yc_2} \times \mathcal{C}_{yc_2} \times \mathcal{S}ym_3 (= 6/mmm)$.] This means that $2\mathbf{L}(\mathcal{R})$ is not a maximal \mathcal{R} -invariant sublattice of $\mathbf{L}(\mathcal{R})$. Since the translation subgroup $\mathcal{T}(\mathcal{U})$ of a maximal k -subgroup \mathcal{U} of index equal to a power of 2 in \mathcal{R} is a maximal \mathcal{R} -invariant subgroup of $\mathcal{T}(\mathcal{R})$ that contains $2\mathcal{T}(\mathcal{R})$, one now finds that \mathcal{R} has no maximal k -subgroup of index 8.