

1.4. THE MATHEMATICAL BACKGROUND OF THE SUBGROUP TABLES

maximal $(\mathbb{Z}/p\mathbb{Z})\overline{\mathcal{R}}$ -submodules of $\mathbf{L}(\mathcal{R})/p\mathbf{L}(\mathcal{R})$. This gives an algorithm for calculating these normal subgroups, which is implemented in the package [CARAT].

The group $\mathcal{G} := T/T^p$ is an Abelian group, with the additional property that for all $g \in \mathcal{G}$ one has $g^p = e$. Such a group is called an *elementary Abelian p-group*.

From the reasoning above we find the following lemma.

Lemma 1.4.4.2.6. Let \mathcal{M} be a maximal k -subgroup of the space group \mathcal{R} . Then $T/T(\mathcal{M})$ is an elementary Abelian p -group for some prime p . The order of $T/T(\mathcal{M})$ is p^r with $r \leq n$. \square

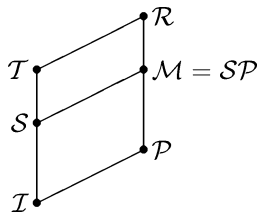
Corollary 1.4.4.2.7. Maximal subgroups of space groups are again space groups and of finite index in the supergroup. \square

Hence the first step is the determination of subgroups of \mathcal{R} that are maximal in T and normal in \mathcal{R} , and is solved by linear-algebra algorithms. These subgroups are the candidates for the translation subgroups $T(\mathcal{M})$ for maximal k -subgroups \mathcal{M} . But even if one knows the isomorphism type of $\mathcal{M}/T(\mathcal{M})$, the group $T(\mathcal{M})$ does not in general determine $\mathcal{M} \leq \mathcal{R}$. Given such a normal subgroup $\mathcal{S} \trianglelefteq \mathcal{R}$ that is contained in T , one now has to find all maximal k -subgroups $\mathcal{M} \leq \mathcal{R}$ with $\mathcal{S} = T \cap \mathcal{M}$ and $T\mathcal{M} = \mathcal{R}$. It might happen that there is no such group \mathcal{M} . This case does not occur if \mathcal{R} is a symmorphic space group in the sense of the following definition:

Definition 1.4.4.2.8. A space group \mathcal{R} is called *symmorphic* if there is a subgroup $\mathcal{P} \leq \mathcal{R}$ such that $\mathcal{P} \cap T(\mathcal{R}) = \mathcal{I}$ and $\mathcal{P}T(\mathcal{R}) = \mathcal{R}$. The subgroup \mathcal{P} is called a *complement* of the translation subgroup $T(\mathcal{R})$. \square

Note that the group \mathcal{P} in the definition is isomorphic to $\mathcal{R}/T(\mathcal{R})$ and hence a finite group.

If \mathcal{R} is symmorphic and $\mathcal{P} \leq \mathcal{R}$ is a complement of T , then one may take $\mathcal{M} := \mathcal{S}\mathcal{P}$.



This shows the following:

Lemma 1.4.4.2.9. Let \mathcal{R} be a symmorphic space group with translation subgroup T and $T_1 \leq T$ an \mathcal{R} -invariant subgroup of T (i.e. $T_1 \trianglelefteq \mathcal{R}$). Then there is at least one k -subgroup $\mathcal{U} \leq \mathcal{R}$ with translation subgroup T_1 . \square

In any case, the maximal k -subgroups, \mathcal{M} , of \mathcal{R} satisfy

$$\begin{aligned} \mathcal{M}T &= \mathcal{R} \text{ and} \\ \mathcal{M} \cap T &= \mathcal{S} \text{ is a maximal } \mathcal{R}\text{-invariant subgroup of } T. \end{aligned}$$

To find these maximal subgroups, \mathcal{M} , one first chooses such a subgroup \mathcal{S} . It then suffices to compute in the finite group $\mathcal{R}/\mathcal{S} =: \overline{\mathcal{R}}$. If there is a complement $\overline{\mathcal{M}}$ of $\overline{T} = T/\mathcal{S}$ in $\overline{\mathcal{R}}$, then every element $x \in \overline{\mathcal{R}}$ may be written uniquely as $x = mt$ with $m \in \overline{\mathcal{M}}$, $t \in \overline{T}$. In particular, any other complement $\overline{\mathcal{M}'}$ of \overline{T} in $\overline{\mathcal{R}}$ is of the form $\overline{\mathcal{M}'} = \{mt_m \mid m \in \overline{\mathcal{M}}, t_m \in \overline{T}\}$. One computes $m_1 t_{m_1} m_2 t_{m_2} = m_1 m_2 (m_2^{-1} t_{m_1} m_2) t_{m_2}$. Since $\overline{\mathcal{M}'}$ is a subgroup of $\overline{\mathcal{R}}$, it holds that $t_{m_1 m_2} = (m_2^{-1} t_{m_1} m_2) t_{m_2}$. Moreover, every mapping

$\overline{\mathcal{M}} \rightarrow \overline{\mathcal{T}}; m \mapsto t_m$ with this property defines some maximal subgroup \mathcal{M}' as above. Since $\overline{\mathcal{M}}$ and $\overline{\mathcal{T}}$ are finite, it is a finite problem to find all such mappings.

If there is no such complement $\overline{\mathcal{M}}$, this means that there is no (maximal) k -subgroup \mathcal{M} of \mathcal{R} with $\mathcal{M} \cap T = \mathcal{S}$.

1.4.5. Maximal subgroups

1.4.5.1. Maximal subgroups and primitive \mathcal{G} -sets

To determine the maximal t -subgroups of a space group \mathcal{R} , essentially one has to calculate the maximal subgroups of the finite group $\mathcal{R}/T(\mathcal{R})$. There are fast algorithms to calculate these maximal subgroups if this finite group is soluble (see Definition 1.4.5.2.1), which is the case for three-dimensional space groups. To explain this method and obtain theoretical consequences for the index of maximal subgroups in soluble space groups, we consider abstract groups again in this section.

For an arbitrary group \mathcal{G} , one has a fast method of checking whether a given subgroup $\mathcal{U} \leq \mathcal{G}$ of finite index $[\mathcal{G} : \mathcal{U}]$ is maximal by inspection of the \mathcal{G} -set \mathcal{G}/\mathcal{U} of left cosets of \mathcal{U} in \mathcal{G} . Assume that $\mathcal{U} \leq \mathcal{M} \leq \mathcal{G}$ and let $\mathcal{M}/\mathcal{U} := \{m_1\mathcal{U}, \dots, m_k\mathcal{U}\}$ with $m_i \in \mathcal{M}$, $m_1 = e$ and $\mathcal{G}/\mathcal{M} := \{g_1\mathcal{M}, \dots, g_l\mathcal{M}\}$ with $g_i \in \mathcal{G}$, $g_1 = e$. Then the set \mathcal{G}/\mathcal{U} may be written as

$$\begin{array}{ccccccc} \mathcal{G}/\mathcal{U} = & \{g_1 m_1 \mathcal{U}, & \dots, & g_1 m_k \mathcal{U}, & & & \\ & g_2 m_1 \mathcal{U}, & \dots, & g_2 m_k \mathcal{U}, & & & \\ & \vdots, & \dots, & \vdots, & & & \\ & g_l m_1 \mathcal{U}, & \dots, & g_l m_k \mathcal{U} \end{array}$$

Then \mathcal{G} permutes the lines of the rectangle above: For all $g \in \mathcal{G}$ and all $j \in \{1, \dots, l\}$, the left coset $gg_j\mathcal{M}$ is equal to some $g_a\mathcal{M}$ for an $a \in \{1, \dots, l\}$. Hence the j th line is mapped onto the set

$$\{gg_j m_1 \mathcal{U}, \dots, gg_j m_k \mathcal{U}\} = \{g_a m_1 \mathcal{U}, \dots, g_a m_k \mathcal{U}\}.$$

Definition 1.4.5.1.1. Let \mathcal{G} be a group and X a \mathcal{G} -set.

- (i) A *congruence* $\{S_1, \dots, S_l\}$ on X is a partition of X into non-empty subsets $X = \bigcup_{i=1}^l S_i$ such that for all $x_1, x_2 \in S_i$, $g \in \mathcal{G}$, $gx_1 \in S_j$ implies $gx_2 \in S_j$.
- (ii) The congruences $\{X\}$ and $\{\{x\} \mid x \in X\}$ are called the *trivial congruences*.
- (iii) X is called a *primitive \mathcal{G} -set* if \mathcal{G} is transitive on X , $|X| > 1$ and X has only the trivial congruences. \square

Hence the considerations above have proven the following lemma.

Lemma 1.4.5.1.2. Let $\mathcal{M} \leq \mathcal{G}$ be a subgroup of the group \mathcal{G} . Then \mathcal{M} is a maximal subgroup if and only if the \mathcal{G} -set \mathcal{G}/\mathcal{M} is primitive. \square

The advantage of this point of view is that the groups \mathcal{G} having a faithful, primitive, finite \mathcal{G} -set have a special structure. It will turn out that this structure is very similar to the structure of space groups.

If X is a \mathcal{G} -set and $\mathcal{N} \trianglelefteq \mathcal{G}$ is a normal subgroup of \mathcal{G} , then \mathcal{G} acts on the set of \mathcal{N} -orbits on X , hence $\{\mathcal{N}x \mid x \in X\}$ is a congruence on X . If X is a primitive \mathcal{G} -set, then this congruence is trivial, hence $\mathcal{N}x = \{x\}$ or $\mathcal{N}x = X$ for all $x \in X$. This means that \mathcal{N} either acts trivially or transitively on X .

1. SPACE GROUPS AND THEIR SUBGROUPS

One obtains the following:

Theorem 1.4.5.1.3. [Theorem of Galois (ca 1830).] Let \mathcal{H} be a finite group and let X be a faithful, primitive \mathcal{H} -set. Assume that $\{e\} \neq \mathcal{N} \trianglelefteq \mathcal{H}$ is an Abelian normal subgroup. Then

- (a) \mathcal{N} is a minimal normal subgroup of \mathcal{H} (i.e. for all $\mathcal{N}_1 \trianglelefteq \mathcal{H}$, $\mathcal{N}_1 \subseteq \mathcal{N} \Leftrightarrow \mathcal{N}_1 = \mathcal{N}$ or $\mathcal{N}_1 = \{e\}$).
- (b) \mathcal{N} is an elementary Abelian p -group for some prime p and $|X| = |\mathcal{N}|$ is a prime power.
- (c) $\mathcal{C}_{\mathcal{H}}(\mathcal{N}) = \mathcal{N}$ and \mathcal{N} is the unique minimal normal subgroup of \mathcal{H} . \square

Proof. Let $\{e\} \neq \mathcal{N} \trianglelefteq \mathcal{H}$ be an Abelian normal subgroup. Then \mathcal{N} acts faithfully and transitively on X . To establish a bijection between the sets \mathcal{N} and X , choose $x \in X$ and define $\varphi : \mathcal{N} \rightarrow X; n \mapsto n \cdot x$. Since \mathcal{N} is transitive, φ is surjective. To show the injectivity of φ , let $n_1, n_2 \in \mathcal{N}$ with $\varphi(n_1) = \varphi(n_2)$. Then $n_1 \cdot x = n_2 \cdot x$, hence $n_1^{-1}n_2x = x$. But then $n_1^{-1}n_2$ acts trivially on X , because if $y \in X$ then the transitivity of \mathcal{N} implies that there is an $n \in \mathcal{N}$ with $n \cdot x = y$. Then $n_1^{-1}n_2 \cdot y = n_1^{-1}n_2n \cdot x = nn_1^{-1}n_2 \cdot x = n \cdot x = y$, since \mathcal{N} is Abelian. Since X is a faithful \mathcal{H} -set, this implies $n_1^{-1}n_2 = e$ and therefore $n_1 = n_2$. This proves $|\mathcal{N}| = |X|$. Since this equality holds for all nontrivial Abelian normal subgroups of \mathcal{H} , statement (a) follows. If p is some prime dividing $|\mathcal{N}|$, then the Sylow p -subgroup of \mathcal{N} is normal in \mathcal{N} , since \mathcal{N} is Abelian. Therefore, it is also a characteristic subgroup of \mathcal{N} and hence a normal subgroup in \mathcal{H} (see the remarks below Definition 1.4.3.5.3). Since \mathcal{N} is a minimal normal subgroup of \mathcal{H} , this implies that \mathcal{N} is equal to its Sylow p -subgroup. Therefore, the order of \mathcal{N} is a prime power $|\mathcal{N}| = p^r$ for some prime p and $r \in \mathbb{N}$. Similarly, the set $\mathcal{N}^{p^r} := \{n^{p^r} \mid n \in \mathcal{N}\}$ is a normal subgroup of \mathcal{H} properly contained in \mathcal{N} . Therefore, $\mathcal{N}^{p^r} = \{e\}$ and \mathcal{N} is elementary Abelian. This establishes (b).

To see that (c) holds, let $g \in \mathcal{C}_{\mathcal{H}}(\mathcal{N})$. Choose $x \in X$. Then $g \cdot x = y \in X$. Since \mathcal{N} acts transitively, there is an $n \in \mathcal{N}$ such that $n \cdot x = y$. Hence $n^{-1}g \cdot x = x$. As above, let $z \in X$ be any element of X . Then there is an element $n_1 \in \mathcal{N}$ with $z = n_1 \cdot x$. Hence $n^{-1}g \cdot z = n^{-1}gn_1 \cdot x = n_1n^{-1}g \cdot x = n_1 \cdot x = z$. Since z was arbitrary and X is faithful, this implies that $g = n \in \mathcal{N}$. Therefore, $\mathcal{C}_{\mathcal{H}}(\mathcal{N}) \subseteq \mathcal{N}$. Since \mathcal{N} is Abelian, one has $\mathcal{N} \subseteq \mathcal{C}_{\mathcal{H}}(\mathcal{N})$, hence $\mathcal{N} = \mathcal{C}_{\mathcal{H}}(\mathcal{N})$. To see that \mathcal{N} is unique, let $\mathcal{P} \neq \mathcal{N}$ be another normal subgroup of \mathcal{H} . Since \mathcal{N} is a minimal normal subgroup, one has $\mathcal{N} \cap \mathcal{P} = \{e\}$, and, therefore, for $p \in \mathcal{P}$, $n \in \mathcal{N}$: $n^{-1}p^{-1}np \in \mathcal{N} \cap \mathcal{P} = \{e\}$. Hence \mathcal{P} centralizes \mathcal{N} , $\mathcal{P} \subseteq \mathcal{C}_{\mathcal{H}}(\mathcal{N}) = \mathcal{N}$, which is a contradiction. \square

Hence the groups \mathcal{H} that satisfy the hypotheses of the theorem of Galois are certain subgroups of an affine group $\mathcal{A}_n(\mathbb{Z}/p\mathbb{Z})$ over a finite field $\mathbb{Z}/p\mathbb{Z}$. This affine group is defined in a way similar to the affine group \mathcal{A}_n over the real numbers where one has to replace the real numbers by this finite field. Then \mathcal{N} is the translation subgroup of $\mathcal{A}_n(\mathbb{Z}/p\mathbb{Z})$ isomorphic to the n -dimensional vector space

$$(\mathbb{Z}/p\mathbb{Z})^n = \left\{ \mathbf{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} \mid x_1, \dots, x_n \in \mathbb{Z}/p\mathbb{Z} \right\}$$

over $\mathbb{Z}/p\mathbb{Z}$. The set X is the corresponding affine space $\mathbb{A}_n(\mathbb{Z}/p\mathbb{Z})$. The factor group $\overline{\mathcal{H}} = \mathcal{H}/\mathcal{N}$ is isomorphic to a subgroup of the linear group of $(\mathbb{Z}/p\mathbb{Z})^n$ that does not leave invariant any nontrivial subspace of $(\mathbb{Z}/p\mathbb{Z})^n$.

1.4.5.2. Soluble groups

Definition 1.4.5.2.1. Let \mathcal{G} be a group. The *derived series* of \mathcal{G} is the series $(\mathcal{G}_0, \mathcal{G}_1, \dots)$ defined via $\mathcal{G}_0 := \mathcal{G}$, $\mathcal{G}_i := \langle g^{-1}h^{-1}gh \mid g, h \in \mathcal{G}_{i-1} \rangle$. The group \mathcal{G}_1 is called the *derived subgroup* of \mathcal{G} . The group \mathcal{G} is called *soluble* if $\mathcal{G}_n = \{e\}$ for some $n \in \mathbb{N}$. \square

Remarks

- (i) The \mathcal{G}_i are characteristic subgroups of \mathcal{G} .
- (ii) \mathcal{G} is Abelian if and only if $\mathcal{G}_1 = \{e\}$.
- (iii) \mathcal{G}_1 is characterized as the smallest normal subgroup of \mathcal{G} , such that $\mathcal{G}/\mathcal{G}_1$ is Abelian, in the sense that every normal subgroup of \mathcal{G} with an Abelian factor group contains \mathcal{G}_1 .
- (iv) Subgroups and factor groups of soluble groups are soluble.
- (v) If $\mathcal{N} \trianglelefteq \mathcal{G}$ is a normal subgroup, then \mathcal{G} is soluble if and only if \mathcal{G}/\mathcal{N} and \mathcal{N} are both soluble.

Example 1.4.5.2.2

The derived series of $\text{Cyc}_2 \times \text{Sym}_4$ is

$$\text{Cyc}_2 \times \text{Sym}_4 \supseteq \text{Alt}_4 \supseteq \text{Cyc}_2 \times \text{Cyc}_2 \supseteq \mathcal{I}$$

(or in Hermann–Mauguin notation $m\bar{3}m \supseteq 23 \supseteq 222 \supseteq 1$) and that of $\text{Cyc}_2 \times \text{Cyc}_2 \times \text{Sym}_3$ is

$$\text{Cyc}_2 \times \text{Cyc}_2 \times \text{Sym}_3 \supseteq \text{Cyc}_3 \supseteq \mathcal{I}$$

(Hermann–Mauguin notation: $6/mmm \supseteq 3 \supseteq 1$).

Hence these two groups are soluble. (For an explanation of the groups that occur here and later, see Section 1.4.3.6.)

Now let $\mathcal{R} \leq \mathcal{E}_3$ be a three-dimensional space group. Then $\mathcal{T}(\mathcal{R})$ is an Abelian normal subgroup, hence $\mathcal{T}(\mathcal{R})$ is soluble. The factor group $\mathcal{R}/\mathcal{T}(\mathcal{R})$ is isomorphic to a subgroup of either $\text{Cyc}_2 \times \text{Sym}_4$ or $\text{Cyc}_2 \times \text{Cyc}_2 \times \text{Sym}_3$ and therefore also soluble. Using the remark above, one deduces that all three-dimensional space groups are soluble.

Lemma 1.4.5.2.3. Let \mathcal{R} be a three-dimensional space group. Then \mathcal{R} is soluble. \square

1.4.5.3. Maximal subgroups of soluble groups

Now let \mathcal{G} be a soluble group and $\mathcal{M} \leq \mathcal{G}$ a maximal subgroup of finite index in \mathcal{G} . Then the set of left cosets $X := \mathcal{G}/\mathcal{M}$ is a primitive finite \mathcal{G} -set. Let $\mathcal{K} = \text{core}(\mathcal{M})$ be the kernel of the action of \mathcal{G} on X . Then the factor group $\mathcal{H} := \mathcal{G}/\mathcal{K}$ acts faithfully on X . In particular, \mathcal{H} is a finite group and X is a primitive, faithful \mathcal{H} -set. Since \mathcal{G} is soluble, the factor group \mathcal{H} is also a soluble group. Let $\mathcal{H} \supseteq \mathcal{H}_1 \supseteq \dots \supseteq \mathcal{H}_{n-1} \supseteq \{e\}$ be the derived series of \mathcal{H} with $\mathcal{N} := \mathcal{H}_{n-1} \neq \{e\}$. Then \mathcal{N} is an Abelian normal subgroup of \mathcal{H} . The theorem of Galois (Theorem 1.4.5.1.3) states that \mathcal{N} is an elementary Abelian p -group for some prime p and $|X| = |\mathcal{N}| = p^r$ for some $r \in \mathbb{N}$. Since $X = \mathcal{G}/\mathcal{M}$, the order of X is the index $[\mathcal{G} : \mathcal{M}]$ of \mathcal{M} in \mathcal{G} . Therefore one gets the following theorem:

Theorem 1.4.5.3.1. If $\mathcal{M} \leq \mathcal{G}$ is a maximal subgroup of finite index in the soluble group \mathcal{G} , then its index $[\mathcal{G} : \mathcal{M}]$ is a prime power. \square

In the proof of Theorem 1.4.5.1.3, we have established a bijection between \mathcal{N} and the \mathcal{H} -set X , which is now $X := \mathcal{G}/\mathcal{M}$. Taking the full pre-image