Algebraic Aspects of Crystallography
Space Groups as Extensions

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N-dimensional space groups G^n are obtained from extensions of a finitely generated free abelian group U^n by a finite group K, with $\varphi : K \to \mathrm{Aut}(U^n)$ a monomorphism. Conversely, any group G^n appearing in an extension $O \to U^n \to G^n \to K \to 1$ with φ as above is a n-dimensional space group. To determine all space groups of a given dimension, one has to calculate the second cohomology group $H^2_\varphi(K, Z^n)$, taking for the pair (K, φ) one representative from each arithmetic crystal class. Isomorphic space groups belong to the same second cohomology group; they are related by automorphisms χ of Z^n that belong to the normalizer of $\varphi(K)$ in $G\,L(n, Z)$. If, furthermore, $\chi \in S\,L(n, Z)$, the space groups are identified, otherwise they form enantiomorphic pairs. The elements of the theory of group extensions as far as needed in this paper are outlined in an appendix, and morphisms of group extensions are discussed in some detail.

Introduction

Space groups are at the basis of our understanding of the physical properties of crystals. Well-known since the work of FEDOROV and SCHÖNFLIES, of BIEBERBACH[1] and FROBENIUS[2], they have been the subject of several detailed studies (we cite only those that have been particularly useful to us[3][4][5]) and still continue to occupy an important place in present-day research. Although everything about these groups is implicitly known since the beginning of this century, an explicit and detailed knowledge of their algebraic structure is valuable for a theory of physical phenomena in crystals.

There are 230 space groups in three dimensions. None is a direct product of rotations and translations (contrary to what may be read in some recent publications), but 73 of them are semi-direct products of their rotational and translational parts. The structure of the remaining 157 space groups may be given a precise algebraic characterization through the concept of group extension, of which the semi-direct product is but a special case.

It is well known that the translations (the free abelian group with three generators) form a normal and maximal abelian subgroup T of a space group G and that the quotient G/T is isomorphic to a so-called abstract crystallographic point group K. Now every group G with the property $G/T \cong K$ is an extension of the group T by a group K[6])[7])[8]). Thus every space group is an extension of the group of translations T by an abstract crystallographic point group K. The remarkable feature, however, is that the converse is also true, namely that any such extension is a space group[10]). Furthermore it turns out that all inequivalent space groups belonging to a given arithmetic crystal class form an abelian group, denoted $H_\varphi^2(K, T)$ and called the second cohomology group[11])[12]). Here φ is an one-to-one homomorphism (monomorphism) from K into the group $GL(3,Z)$ of three-dimensional integer matrices with determinant ± 1 and $\varphi(K)$ is a representative of the given arithmetic crystal class. Consequently one finds exactly all inequivalent space groups by calculating the second cohomology group for each arithmetic crystal class.

It thus becomes manifest that the theory of group extensions, together with the pertinent part of homological algebra, is a natural framework for the theory of space groups and their representations[9]). This program will be carried out in a series of papers, for which this first one should lay the foundation.

In subsequent publications it will be shown that non-primitive translations, a characteristic feature of space groups, arise quite naturally when the latter are presented as group extensions. The determination of the possible translations associated with the elements of an abstract crystallographic point group K leads to the usual method of constructing space groups by solving "Frobenius congruences"[2]). This method will be shown to be equivalent to that given here, viz. the determination of all inequivalent extensions[19]). It will also be demonstrated that taking explicitely into account the structure of space groups as extensions gives the theory of their representations greater transparency.

Lately an interest has arisen in generalisations of space groups among which the magnetic (or black and white) space groups[23]) are the simplest ones. It will be shown that the theory of group extensions is a reliable guide for all these cases.

Finally it should be mentioned that in the research on the symmetries underlying elementary particle physics, group extensions play an important role[24])[25]). The study undertaken in this and subsequent papers should prove instructive also in this field, where the problems are less accessible to intuition than is the case for crystal physics.

1. Space Groups as Extensions

In this section, we want to show that n-dimensional space groups appear in extensions of a finitely generated free abelian group U^n by a finite group K, with $\varphi : K \to \text{Aut}(U^n)$ a monomorphism, and that any such extension gives n-dimensional space groups only. The following proposition shows that the fact of φ being a monomorphism is equivalent to U^n being maximal abelian in the extension.

Proposition 1. Let $0 \to A \xrightarrow{\varkappa} G \xrightarrow{\sigma} B \to 1$ be an extension with A abelian. The homomorphism $\varphi : B \to \text{Aut}(A)$ is a monomorphism if and only if the image $\varkappa A$ is a maximal abelian subgroup of G.

Proof: Let $\varkappa A$ be maximal abelian in G. Take $g \in G$. If $g(\varkappa a) = (\varkappa a)g$, for any $a \in A$, then $g \in \varkappa A$ (since the group generated by $\varkappa A$ and g is abelian, and thus

contained in $\varkappa A$). Let α be an element of Ker φ. By definition (see A7):

$$\varkappa\,(\varphi\,\alpha\,o\,a) = r(\alpha) \cdot \varkappa\,a \cdot r(\alpha)^{-1}\,. \tag{1.1}$$

Consequently, $r(\alpha) \cdot \varkappa\,a \cdot r(\alpha)^{-1} = \varkappa\,a$, since $\varphi\,\alpha$ is the identity automorphism. Then $r(\alpha) \in \varkappa\,A$ and $\alpha = \varepsilon \in B$; in other words: φ is a monomorphism.

Suppose now φ is a monomorphism, and let $g \in G$ commute with any $\varkappa\,a$, $(a \in A)$. Then $\varkappa\,a = g(\varkappa\,a)\,g^{-1} = \varkappa\,(\varphi\,\sigma\,g\,o\,a)$, i.e. $\varphi\,\sigma\,g$ is the identity monomorphism. Thus, $\sigma\,g = \varepsilon \in B$; consequently, $g \in \varkappa\,A$, showing that $\varkappa\,A$ is maximal abelian in G.

There is another property related to normal, maximal abelian subgroups that we shall use.

Proposition 2. If, in a commutative diagram with exact rows:

$$
\begin{array}{ccccccccc}
Q & \to & A & \xrightarrow{\varkappa} & G & \xrightarrow{\sigma} & B & \to & 1 \\
 & & {\scriptstyle\lambda}\downarrow & & {\scriptstyle\mu}\downarrow & & \downarrow{\scriptstyle\nu} & & \\
O & \to & A' & \underset{\varkappa'}{\to} & G' & \underset{\sigma'}{\to} & B' & \to & 1\,.
\end{array}
$$

A' is abelian, $\varkappa\,A$ is maximal abelian in G and μ is a monomorphism, then ν is a monomorphism.

Proof: Let r be a choice of representatives for the cosets of $\varkappa\,A$ in G, and let $\alpha \in B$. Then, unless $\alpha = \varepsilon$, $\mu\,r(\alpha)$ does not belong to Im $\varkappa'$. Indeed, if $b' \in A'$, then $\mu\,r(\alpha) = \varkappa'\,b'$ leads to

$$\mu\left[\varkappa\,a \cdot r(\alpha)\right] = \varkappa'\,\lambda\,a \cdot \varkappa'\,b' = \varkappa'(\lambda\,a \cdot b') = \varkappa'(b' \cdot \lambda\,a) = \mu\left[r(\alpha) \cdot \varkappa\,a\right],$$

which is in contradiction with $\varkappa\,A$ being maximal abelian in G. Therefore, $\sigma'\,\mu\,r(\alpha) = \varepsilon'$ entails $\alpha = \varepsilon$. Now $\sigma'\,\mu\,r(\alpha) = \nu\,\sigma\,r(\alpha) = \nu\,\alpha$. Thus, $\nu\,\alpha = \varepsilon'$ entails $\alpha = \varepsilon$, i.e. ν is a monomorphism.

Definition 1. The euclidean group, the group of rigid motions of n-dimensional euclidean space, i.e. the group that leaves the euclidean metric invariant, is the semi-direct product given by the extension:

$$O \to R^n \xrightarrow{\varkappa'} E^n \xrightarrow{\sigma'} O(n,\,R) \to 1 \quad (\varphi')\,. \tag{1.2}$$

For the mapping φ' of the extension, we take the natural monomorphism (i.e. the injection of a subgroup) of $O(n,\,R)$ into $\mathrm{Aut}(R^n)$, the group of automorphisms of the abelian group $R^n = R \times R \times \ldots \times R$ (n factors). By $O(n,\,R)$, we mean the orthogonal group of the quadratic form $\overset{n}{\underset{i=1}{\Sigma}}\,r_i^2$ with $r_i \in R$. The abelian group R^n may also be given, in a natural way, the structure of a n-dimensional real vector space. Let $G\,L(n,\,R)$ be the group of automorphisms of the real vector space R^n. Then generally $G\,L(n,\,R) \subset \mathrm{Aut}(R^n)$. In our case, however, since φ' is the natural monomorphism, we have $\varphi'\,[O(n,\,R)] \subset G\,L(n,\,R)$.

An infinite crystal admits, by definition, only discrete translations; therefore, the group of rigid motions of an infinite crystal, the space group, is a subgroup of the euclidean group that contains only discrete translations. More precisely, we have:

Definition 2. A n-dimensional space group G^n is a subgroup of E^n satisfying the following conditions:

(α) $U^n \overset{\text{Def.}}{=} R^n \cap G^n \cong Z^n$ (group isomorphism),

(β) the elements of U^n generate R^n considered as real vector space.

Proposition 3. The subgroup $U^n \subset G^n$ of Definition 2 has the following properties:

  (i) U^n is free abelian (of rank n)

  (ii) U^n is normal in G^n

  (iii) U^n is maximal abelian in G^n

  (iv) G^n/U^n is finite.

Proof:

a) Property (i) is part of the definition.

b) Proof of (ii). For any $g \in G^n$:

$$g \, U^n \, g^{-1} = g \, (R^n \cap G^n) \, g^{-1} = g \, R^n \, g^{-1} \cap g \, G^n \, g^{-1} = R^n \cap G^n = U^n .$$

c) Construction of a commutative diagram. We define

$$\varkappa : U^n \to G^n; \; \varkappa' : R^n \to E^n \quad \text{and} \quad \mu : G^n \to E^n$$

as natural monomorphisms;

$$\sigma : G^n \to G^n/U^n \text{ and } \sigma' : E^n \to O(n, R)$$

as canonical epimorphisms. Furthermore, we introduce a monomorphism $\lambda : U^n \to R^n$ by $\mu \, \varkappa = \varkappa' \, \lambda$. This is possible by virtue of condition (α). Utilizing the monomorphisms we have just introduced, this condition takes the following precise form:

$(\bar{\alpha})$ $(\varkappa' \, R^n) \cap (\mu \, G^n) = \mu \, \varkappa \, U^n = \varkappa' \, \lambda \, U^n.$

One arrives at the form given in Definition 2 after the identification of a group with its monomorphic image. (To simplify the notation, we shall sometimes make such identifications.)

Now we show that there are homomorphisms $\nu : G^n/U^n \to O(n, R)$ and $\Lambda : \mathrm{Aut}(U^n) \to G\,L(n, R)$ such that the diagram (1.3) is commutative:

$$
\begin{array}{ccccccccc}
O & \to & U^n & \overset{\varkappa}{\to} & G^n & \overset{\sigma}{\to} & G^n/U^n & \to & 1 \\
 & & \downarrow\lambda & & \downarrow\mu & & \downarrow\nu & \searrow^{\varphi} & \mathrm{Aut}(U^n) \\
 & & & & & & & & \downarrow\Lambda \\
 & & & & & & & \overset{\varphi'}{\to} & G\,L(n, R) \\
O & \to & R^n & \underset{\varkappa'}{\to} & E^n & \underset{\sigma'}{\to} & O(n, R) & \to & 1 .
\end{array}
\qquad (1.3)
$$

The lower extension is that of Definition 1.

We are in the situation of diagram (A44), and, in the manner shown there, we define a homomorphism $\nu : G^n/U^n \to O(n, R)$ having the property:

$$\sigma' \, \mu = \nu \, \sigma \, . \qquad (1.4)$$

We have now constructed a commutative diagram of the type (A33). Formula (A62) applies, and we have

$$V \, \alpha \in G^n/U^n, \, V \, a \in U^n : \quad \lambda \, (\varphi \, \alpha \, o \, a) = \varphi' \, \nu \, \alpha \, o \, \lambda \, a \, . \qquad (1.5)$$

We construct a monomorphism Λ from $\mathrm{Aut}(U^n)$ onto $\mathrm{Aut}(\lambda \, U^n)$ according to (A41): if $\chi \in \mathrm{Aut}(U^n)$, then $\Lambda \, \chi(\lambda \, a) = \lambda(\chi \, a)$ for any $a \in U^n$. Owing to condition (β) of Definition 2, the definition of $\Lambda \, \chi$ may be extended by linearity from $\lambda \, U^n$ to R^n (as real vector space) so that we have $\Lambda : \mathrm{Aut}(U^n) \to G \, L(n, R)$. If now $\chi = \varphi \, \alpha$, then, according to (1.5):

$$\Lambda \, \varphi = \varphi' \, \nu \, , \qquad (1.6)$$

and G^n/U^n operates on R^n.

d) Proof of (iii). Let g be an element of G^n that commutes with any element of $\varkappa \, U^n$. Then $\sigma \, g \in \mathrm{Ker} \, \varphi$. Utilizing condition (β) of Definition 2 one finds that $\nu \, \sigma \, g = \mathrm{Ker} \, \varphi'$. This leads to $\sigma' \, \mu \, g = \nu \, \sigma \, g = \epsilon$, and therefore $\nu \, \sigma \, g \in \mathrm{Ker} \, \varphi' = \mathrm{Im} \, \varkappa'$. But this means, by $(\bar{\alpha})$, that $g \in \varkappa \, U^n$. Thus $\varkappa \, U^n$ is maximal abelian in G^n. Note that now by Propositions 1 and 2, φ and ν are monomorphisms.

e) Proof of (iv). We have shown that the group $\varphi(G^n/U^n) \subset \mathrm{Aut}(U^n)$ has the following properties:

– it leaves an element of U^n fixed, since $\varphi(G^n/U^n)$ is a group of automorphisms of U^n;

– by Definition 1, the group $\varphi'[O(n, R)]$ leaves the metric of R^n invariant. Let X be a subgroup of $\varphi'[O(n, R)]$ and Y a subgroup of R^n that the elements of X map onto itself. Then X leaves the metric of Y invariant. Therefore, $\varphi(G^n/U^n)$ leaves the metric of $U^n \cong Z^n$ invariant.

A group with the above two properties is finite [13]. Hence $\varphi(G^n/U^n)$ is finite, and so is also $G^n/U^n \overset{\text{Def.}}{=} K$. Thus, K is a finite group that is isomorphic to a subgroup of $G \, L(n, Z) \cong \mathrm{Aut}(U^n)$.

Proposition 4. Any normal and free abelian subgroup of a group G^n with a subgroup U^n satisfying (ii) to (iv) is contained in U^n.

Proof: Let V be a free abelian and normal subgroup of G^n, and $v \in V$. Since K is finite, there exists an integer $p > 0$, such that $v^p \in U^n$. For p one may take k, the order of the group K. Indeed, let $\sigma \, v = \alpha$, then $(\sigma \, v)^k = \sigma \, v^k = \varepsilon$, which shows that $v^k \in U^n$. Take $u \in U^n$ and consider the commutator $w = v^{-1} \, u^{-1} \, v \, u$. Then $v \, w = u^{-1} \, v \, u \in V$, and $(v \, w)^k = (u^{-1} \, v \, u)^k = u^{-1} \, v^k \, u = v^k$. Since V is free abelian, this entails $v \, w = v$ and $w = e$. Thus, $u \, v = v \, u$, and therefore $V \subset U^n$.

Corollary 4. A subgroup U^n of G^n with properties (i) to (iv) is unique.

Proof: Let U^n and V^n be two such subgroups. Then V^n fulfils the conditions of the preceding proposition; therefore, $V^n \subset U^n$. The same is also true for U^n, whence $U^n \subset V^n$.

So far we have shown:

– that a space group G^n is a group containing a uniquely determined subgroup U^n with properties (i) to (iv), or equivalently,

– that a space group G^n appears in an extension of the group $U^n \cong Z^n$ by a finite group K, with $\varphi : K \twoheadrightarrow \mathrm{Aut}(U^n) \cong G L(n, Z)$ being a monomorphism.

We now show that, conversely, any such extension gives space groups only.

Proposition 5. Let E^n be the euclidean group with the subgroup R^n $(\varkappa' : R^n \rightarrowtail E^n)$; let G^n be a group with a subgroup U^n $(\varkappa : U^n \rightarrowtail G^n)$ satisfying conditions (i) to (iv) of Proposition 3. Then there is a monomorphism $\mu : G^n \to E^n$ such

(α_1) that μ maps the subgroup $\varkappa U^n$ into the subgroup $\varkappa' R^n$,

(α_2) that, λ being the restriction of μ to U^n, one has

$$\mu \varkappa U^n = \varkappa' \lambda U^n = (\varkappa' R^n) \cap (\mu G^n) , \text{ and}$$

(β_1) that λU^n generates the real vector space R^n.

Proof: We shall first of all construct a subgroup $\overline{\lambda} U^n \subset R^n$ generating the real vector space R^n, a monomorphism $\overline{\mu}$, and a commutative diagram (1.7) with exact rows:

$$O \to U^n \xrightarrow{\varkappa} G^n \xrightarrow{\sigma} K \to 1$$

(1.7)

Let $\overline{\lambda} : U^n \twoheadrightarrow R^n$ be a monomorphism such that $\overline{\lambda} U^n$ generates R^n considered as real vector space. In the same way as is done in part c of the proof of Proposition 3, we construct a monomorphism $\overline{\Lambda} : \mathrm{Aut}(U^n) \twoheadrightarrow G L(n, R) \subset \mathrm{Aut}(R^n)$. We now put $\overline{\varphi} = \overline{\Lambda} \varphi$. The mapping $\overline{\varphi}$ then is a monomorphism that operates on the vector space R^n in such a way that (see 1.5):

$$\forall a \in U^n, \ \forall \alpha \in K : \overline{\lambda} \, (\varphi \, \alpha \, o \, a) = \overline{\varphi} \, \alpha \, o \, \overline{\lambda} \, a . \tag{1.8}$$

We now fix a mapping $r : K \twoheadrightarrow G^n$ and consequently also a factor set $m : K \times K \twoheadrightarrow U^n$ fulfilling the conditions (A4) and (A14). Putting

$$\forall \alpha, \beta \in K : \overline{m}(\alpha, \beta) = \overline{\lambda} \, m(\alpha, \beta) , \tag{1.9}$$

we fix a factor set $K \times K \twoheadrightarrow R^n$. The mappings $\overline{\varphi}$ and $\overline{m}$ determine an extension of R^n by K:

$$O \to R^n \xrightarrow{\overline{\varkappa}} M^n \xrightarrow{\overline{\sigma}} K \to 1 , \quad (\overline{\varphi}) .$$

Since $\overline{\varphi}$ is a monomorphism, $\overline{\varkappa} R^n$ is maximal abelian in M^n. Since K is finite and since R^n is divisible and does not contain elements of finite order, the extension of R^n by K splits (A32). We are in the situation of diagram (A46). Since conditions (1.8) and (1.9) hold, the mapping $\overline{\mu} : G^n \twoheadrightarrow M^n$ defined by $\overline{\mu}(a, \alpha) = (\overline{\lambda} \, a, \alpha)$ is a homomorphism that makes the diagram (1.7) commutative. By (A34, iii), $\overline{\mu}$ then is a monomorphism.

The next step is to construct a commutative diagram with a monomorphism $\tilde{\mu} : M^n \twoheadrightarrow E^n$, with an automorphism $\tilde{\lambda}$ of R^n and with the extension of R^n by $O(n, R)$, as considered in Definition 1, giving the n-dimensional euclidean group E^n.

$$
\begin{array}{ccccccc}
O \to & R^n & \xrightarrow{\bar{\varkappa}} & M^n & \xrightarrow{\bar{\sigma}} & K & \to 1 \\
& \downarrow{\lambda} & & \downarrow{\tilde{\mu}} & & \downarrow{\nu} & \searrow^{\bar{\varphi}} \; G\,L(n, R) \\
& & & & & & \downarrow{\tilde{\Lambda}} \\
& & & & & \varphi' \searrow & G\,L(n, R) \\
O \to & R^n & \xrightarrow[\varkappa']{} & E^n & \xrightarrow[\sigma']{} & O(n, R) & \to 1
\end{array}
\tag{1.10}
$$

$\bar{\varphi}(K)$ is a finite subgroup of $G\,L(n, R)$; any such group is R-equivalent to a subgroup of $O(n, R)$[14]. This means that there is an automorphism $\tilde{\lambda}$ of R^n inducing an automorphism $\tilde{\Lambda}$ of $G\,L(n, R)$:

$$
\tilde{\Lambda}\,\bar{\varphi}(K) = \tilde{\lambda}\,\bar{\varphi}\,(K)\,\tilde{\lambda}^{-1}
\tag{1.11}
$$

such that $\tilde{\Lambda}\,\bar{\varphi}(K)$ is contained in $\varphi'[O(n, R)]$. We define ν by $\varphi'\,\nu = \tilde{\Lambda}\,\bar{\varphi}$. Clearly, ν is a monomorphism and

$$
\tilde{\Lambda}\,\bar{\varphi}\,\alpha \; o \; \tilde{\lambda}\,a = \varphi'\,\nu\,\alpha \; o \; \tilde{\lambda}\,a = \tilde{\lambda}(\bar{\varphi}\,\alpha \; o \; a)\;.
\tag{1.12}
$$

We now have a diagram of type (A46) with $\tilde{\lambda}$ an automorphism and ν a monomorphism. Since both extensions are split – otherwise not, see (A60) – we may define a homomorphism $\tilde{\mu} : M^n \twoheadrightarrow E^n$ that makes the diagram (1.10) commutative. The homomorphism $\tilde{\mu}$ will then be a monomorphism. The explicit definition of $\tilde{\mu}$ is as follows. In M^n and in E^n, we choose representatives in such a way as to have trivial factor sets in both cases. Then we define $\tilde{\mu}$ by

$$
\tilde{\mu}(a, \alpha) = (\tilde{\lambda}\,\alpha, \nu\,\alpha)\;.
\tag{1.13}
$$

Putting now $\tilde{\lambda}\,\bar{\lambda} = \lambda$, $\tilde{\mu}\,\bar{\mu} = \mu$, and $\tilde{\Lambda}\,\bar{\Lambda} = \Lambda$, we arrive at the commutative diagram (1.3).

2. Identifications

In the previous section, we have shown that a space group G^n appears in an extension

$$
O \to U^n \xrightarrow{\varkappa} G^n \xrightarrow{\sigma} K \to 1 \quad (\varphi)
\tag{2.1}
$$

with U^n free abelian, K finite and $\varphi : K \twoheadrightarrow \text{Aut}(U^n) \cong G\,L(n, Z)$ a monomorphism. The crucial point of the theory is that, in accordance with corollary 4, the subgroup $\varkappa\,U^n$ of a given G^n is uniquely determined. This enables us to give the extension a canonical form: we put $K = G^n/\varkappa\,Z^n$ and take for σ the natural epimorphism. Owing to the uniqueness of $\varkappa\,Z^n$, K, and σ depend only on G^n and not on the monomorphism $\varkappa$. The isomorphism $U^n \cong Z^n$, however, is determined only up to an automorphism χ of Z^n (χ relates a choice of generators of U^n to another one). Thus, only the injective

part of (2.1) is variable, and it is necessary to investigate only the possible monomorphisms $\varkappa : Z^n \to G^n$ and to see how they give rise to monomorphisms $\varphi : K \to G L(n, Z)$.

If the same space group G^n appears in two extensions

$$O \to Z^n \xrightarrow{\varkappa} G^n \xrightarrow{\sigma} K \to 1 \ \text{ and } \ O \to Z^n \xrightarrow{\bar{\varkappa}} G^n \xrightarrow{\bar{\sigma}} K \to 1 \,,$$

it is clear that $\varkappa$ and $\bar{\varkappa}$ differ by an automorphism χ of Z^n ($\varkappa = \bar{\varkappa}\,\chi$). From the morphism:

$$
\begin{array}{ccccccc}
O \to & Z^n & \xrightarrow{\varkappa} & G^n & \xrightarrow{\sigma} & K \to 1 & (\varphi) \\
 & \chi\downarrow & & \| & & \| & \\
O \to & Z^n & \xrightarrow[\bar{\varkappa}]{} & G^n & \xrightarrow[\bar{\sigma}]{} & K \to 1 & (\bar{\varphi})
\end{array}
$$

one finds, referring to (A62):

$$V\,\alpha \in K : \overline{\varphi}\,\alpha = \chi(\varphi\,\alpha)\chi^{-1} \,,$$

i.e. the subgroup $\varphi(K) \subset G L(n, Z)$ is defined only up to an inner automorphism of $G L(n, Z)$. A given space group G^n therefore determines a class of conjugate finite subgroups of $G L(n, Z)$.

A slightly more general situation is obtained if instead of identical space groups one considers isomorphic ones. Again, owing to corollary 4, we are able to construct, as in (A44), a morphism of group extensions (2.2), where, by virtue of (A34, vii) ω is in fact an isomorphism.

$$
\begin{array}{ccccccc}
O \to & Z^n & \xrightarrow{\varkappa} & G^n & \xrightarrow{\sigma} & K \to 1 & (\varphi) \\
 & \chi\downarrow & & \psi\downarrow & & \downarrow\omega & \\
O \to & Z^n & \xrightarrow[\bar{\varkappa}]{} & \overline{G}^n & \xrightarrow[\bar{\sigma}]{} & \overline{K} \to 1 & (\overline{\varphi}) \,.
\end{array}
\qquad (2.2)
$$

From (A62), we find

$$V\,\alpha \in K : \overline{\varphi}\,\omega\,\alpha = \chi(\varphi\,\alpha)\,\chi^{-1} \,. \qquad (2.3)$$

Thus, K and $\overline{K}$ determine the same class of conjugate finite subgroups of $G L(n, Z)$. Such a class is called an arithmetic crystal class[15]. Two pairs (K, φ) and $(\overline{K}, \overline{\varphi})$ are equivalent and belong to the same arithmetic crystal class if there exist an isomorphism $\omega : K \to \overline{K}$ and an automorphism χ of Z^n such that (2.3) holds. We have thereby proved the following proposition:

Proposition 6. A given space group determines an arithmetic crystal class. Isomorphic space groups determine the same arithmetic crystal class.

JORDAN's theorem[16] implies that the number of classes of conjugate finite subgroups of $G L(n, Z)$ is finite. Hence, the number of arithmetic crystal classes is finite. (For $n = 2$, there are 13; for $n = 3$, there are 73 arithmetic crystal classes.)

Taking one representative from each arithmetic crystal class, one obtains a finite family of non-conjugate finite subgroups of $G L(n, Z)$, called the arithmetic crystallographic point groups.

Some of these latter, say $\varphi_1(K_1)$ and $\varphi_2(K_2)$, may still be isomorphic without being conjugate. If the quotient group $K = G^n/\varkappa Z^n$ is considered as abstract group, i.e. if isomorphic groups are identified, one obtains a family of finite groups, called the abstract crystallographic point groups. Their number is at most equal to the number of arithmetic crystal classes. (For $n = 2$, there are 9; for $n = 3$, there are 18 abstract crystallographic point groups.) Now we may characterize a n-dimensional arithmetic crystal class as a class of Z-equivalent n-dimensional faithful integral representations of an abstract crystallographic point group K.

Up to now we have considered a given space group (or two isomorphic space groups) and we have determined the possible $\varphi(K)$ that may arise. Now we want to find all possible space groups G^n appearing in an extension $O \to Z^n \to G^n \to K \to 1$, taking for K an abstract crystallographic point group. The question is whether we must consider all possible monomorphisms $\varphi : K \to G\,L(n, Z)$. From the preceding discussion, it follows that we need to take only one representative of each arithmetic crystal class; for each group G^n arising from one representative of a given arithmetic crystal class, there is an isomorphic group $\overline{G^n}$ arising from another representative. Thus, to determine all space groups of a given dimension, one has to calculate the second cohomology groups $H^2_\varphi(K, Z^n)$, taking for the pair (K, φ) the arithmetic crystallographic point groups. This means that one admits only those automorphisms χ of Z^n that lead to:

$$\overline{\varphi}(K) = \varphi(K) = \chi[\varphi(K)]\,\chi^{-1}\,. \tag{2.4}$$

In other words, only automorphisms of Z^n that belong to the normalizer $N \overset{\text{Def.}}{=} N\,[\varphi(K) \subset G\,L(n, Z)]$ of $\varphi(K)$ in $G\,L(n, Z)$ are admitted.

The preceding discussion may be summarized as follows:

Corollary 6.
Let

$$O \to Z^n \overset{\varkappa}{\to} G^n \overset{\sigma}{\to} K \to 1 \quad (\varphi)$$

and

$$O \to Z^n \overset{\overline{\varkappa}}{\to} \overline{G^n} \overset{\overline{\sigma}}{\to} K \to 1 \quad (\varphi)$$

be two extensions (with the same monomorphism φ !) and $\psi : G^n \to \overline{G^n}$ an isomorphism. Then (owing to corollary 4)

$$\psi\,\varkappa\,Z^n = \overline{\varkappa}\,Z^n\,;$$

furthermore, if λ is the isomorphism defined by $\lambda = \overline{\varkappa}^{-1}\,\psi\,\varkappa$, then λ is an element of $N\,[\varphi(K) \subset G\,L(n, Z)]$.

Note that isomorphic groups may always be made to appear in the same extension.

The automorphism χ still play a rôle in our theory because we are interested in isomorphic space groups and not in equivalent extensions. Indeed, non-equivalent extensions – i.e. different elements of $H^2_\varphi(K, Z^n)$ – may give isomorphic space groups. The following proposition shows how to recognize the case of non-equivalent but isomorphic space groups.

Proposition 7. Two extensions of the same type give isomorphic space groups G^n and $\overline{G^n}$ ($\psi : G^n \to \overline{G^n}$) if and only if it is possible to choose a representative $m : K \times K \to Z^n$ of the equivalence class of G^n, a representative $\overline{m} : K \times K \to Z^n$ of the equivalence

class of $\overline{G}^n$, an automorphism ω of K, and an automorphism $\chi \in N$ of Z^n, such that:

$$\mathcal{V} \; \alpha, \beta \in K : \overline{m}(\omega \, \alpha, \omega \, \beta) = \chi \, m(\alpha, \beta) \tag{2.5}$$

and

$$\mathcal{V} \; \alpha \in K, \; \mathcal{V} \; a \in Z^n : \chi(\varphi \, \alpha \, o \, a) = \varphi \, \omega \, \alpha \, o \, \chi \, a \, . \tag{2.6}$$

Note that χ determines ω.

Proof: We shall first prove the necessity of the conditions. If G^n and $\overline{G}^n$ are isomorphic, (owing to corollary 4), we are able to construct the following commutative diagram with $\chi \in N$:

$$
\begin{array}{ccccccccc}
O & \to & Z^n & \xrightarrow{\varkappa} & G^n & \xrightarrow{\sigma} & K & \to & 1 \quad (\varphi) \\
 & & \chi \downarrow & & \psi \downarrow & & \downarrow \omega & & \\
O & \to & Z^n & \xrightarrow[\overline{\varkappa}]{} & \overline{G}^n & \xrightarrow[\overline{\sigma}]{} & K & \to & 1 \quad (\varphi) \, .
\end{array}
\tag{2.7}
$$

Let r be a choice of representatives of the cosets of $Z^n \subset G^n$. Then the factor set m given by $\varkappa \, m(\alpha, \beta) = r(\alpha) \, r(\beta) \, r(\alpha \, \beta)^{-1}$ is a representative of the equivalence class of the extension G^n. Equally, let $\overline{r}$ be a choice of representatives for the cosets of $Z^n \subset \overline{G}^n$. Then the factor set $\overline{m}$ – given by $\overline{\varkappa} \, \overline{m}(\alpha, \beta) = \overline{r}(\alpha) \, \overline{r}(\beta) \, \overline{r}(\alpha \, \beta)^{-1}$ – is a representative of the equivalence class of the extension $\overline{G}^n$. For a given choice of r, a possible choice of $\overline{r}$ is given by (see A47):

$$\overline{r} \, \omega = \psi \, r \, . \tag{2.8}$$

Then, according to (A49) and (A50):

$$\chi(\varphi \, \alpha \, o \, a) = \varphi \, \omega \, \alpha \, o \, \chi \, a \quad \text{and} \quad \chi \, m(\alpha, \beta) = \overline{m} \, (\omega \, \alpha, \omega \, \beta) \, .$$

This shows that the condition is necessary.

To show that the condition is sufficient, we start with the diagram

$$
\begin{array}{ccccccccc}
O & \to & Z^n & \xrightarrow{\varkappa} & G^n & \xrightarrow{\sigma} & K & \to & 1 \quad (\varphi) \\
 & & \chi \downarrow & & & & \downarrow \omega & & \\
O & \to & Z^n & \xrightarrow[\overline{\varkappa}]{} & \overline{G}^n & \xrightarrow[\overline{\sigma}]{} & K & \to & 1 \quad (\varphi) \, ,
\end{array}
\tag{2.9}
$$

where $\chi \in N$ and (2.5) as well as (2.6) are fulfilled. We then show that (2.9) determines a monomorphism $\psi : G^n \to \overline{G}^n$ such that the diagram is commutative.

Let r be a choice of representatives for the cosets $Z^n \subset G^n$, and $\overline{r}$ such a choice in $\overline{G}^n$; these choices being such that (2.5) and (2.6) are fulfilled.

We are now in a situation analogous to that of diagram (A46). Therefore, a mapping $\psi : G^n \to \overline{G}^n$ defined by $\psi(a, \alpha) = (\chi \, a, \omega \, \alpha)$ is a homomorphism.

On account of the Short Five Lemma (A34, vi), it then is an isomorphism, and Proposition 7 is proved.

Consider the abelian group of m-cochains $C_\varphi^m(K, Z^n) = \{f^m\}$ and the automorphisms χ of Z^n and ω of K related by (2.6).

The mapping $\chi^*: C^m \to C^m$ defined by $\chi^* f^m(\alpha_1, \ldots, \alpha_m) = f^m(\omega \alpha_1, \ldots, \omega \alpha_m)$ – formula (2.5) is a particular case of this mapping – is an automorphism of $C^m(K, Z^n)$ that maps cocycles onto cocycles and coboundaries onto coboundaries, and thus induces (for every m) an automorphism of $H^m_\varphi(K, Z^n)$.

Returning now to the case $m = 2$, we say that two elements belong to the same orbit of $H^2_\varphi(K, Z^n)$ relative to $N = N[\varphi(K) \subset G\,L(n, Z)]$ if it is possible to choose representatives m and $\overline{m}$ of their respective cohomology classes and a $\chi \in N$ such that there is a $\omega \in \text{Aut}(K)$ fulfilling (2.5) and (2.6). Since 2-cohomologous 2-cocycles belong to the same orbit, this definition does not depend on the choice of representatives. The orbits constitute a partition of $H^2_\varphi(K, Z^n)$ into disjoint classes, and there is a one-to-one correspondence between the non-isomorphic space groups associated with the arithmetic crystallographic point group (K, φ) and the set of orbits of $H^2_\varphi(K, Z^n)$ relative to N. This set generally has no group structure.

In crystallography, it is customary to identify not all isomorphic space groups appearing in extensions $O \to Z^n \to G^n \to K \to 1$ but only those having the "same orientation".

$G\,L(n, Z)$ has a subgroup $S\,L(n, Z)$ of index two consisting of the automorphisms of Z^n with determinant $+1$. The orbits of $H^2_\varphi(K, Z^n)$ relative to $N^+ = N[\varphi(K) \subset G\,L(n, Z)] \cap S\,L(n, Z)$ constitute another partition of $H^2_\varphi(K, Z^n)$ into disjoint classes. There is a one-to-one correspondence between this set of orbits and the non-isomorphic space groups of same orientation associated with the arithmetic crystallographic point group (K, φ). An orbit of $H^2_\varphi(K, Z^n)$ relative to N is also an orbit relative to N^+ if for each pair of elements in the orbit relative to N there is at least one element χ^+ of N^+ and a $\omega \in \text{Aut}(K)$ fulfilling (2.5) and (2.6). If this is not the case, the orbit relative to N is split into two orbits relative to N^+, called an enantiomorphic pair.

If in $G\,L(n, Z)$, instead of the subgroup $\varphi(K)$, one considers a conjugate subgroup $\overline{\varphi}(K)$, then, in the induced isomorphism between $H^2_\varphi(K, Z^n)$ and $H^2_{\overline{\varphi}}(K, Z^n)$, the partition into orbits relative to N^+ is left unchanged. Thus, by restricting oneself to one representative of each arithmetic crystal class, no oriented space group has been lost.

Eleven enantiomorphic pairs are known in three dimensions; there is no such pair in two dimensions. According to BUERGER[18], the members of any of these pairs cannot be distinguished by any known experimental means.

We have seen that the arithmetic crystal classes play a fundamental rôle in crystallography. Nevertheless, the notion of geometric crystal class[3] is more customary. The geometric crystal classes arise from the circumstance that the euclidean group E^n determines a class of conjugate subgroups of $G\,L(n, R)$ that are isomorphic to $O(n, R)$. In Definition 1, we choose one fixed representative of that conjugation class. Subgroups of $G\,L(n, R)$, e.g. $\varphi'[O(n, R)]$, are also determined only up to conjugation in $G\,L(n, R)$. A n-dimensional geometric crystal class then is a class of R-equivalent n-dimensional faithful real representations of a finite group K. In other words, if $\Lambda: \text{Aut}(Z^n) \to G\,L(n, R)$ is the monomorphism resulting from a monomorphism $\lambda: Z^n \to R^n$ such that λZ^n generates the real vector space R^n and if furthermore φ and $\overline{\varphi}$ are two monomorphisms from K into $G\,L(n, Z)$, then $\varphi(K)$ and $\overline{\varphi}(K)$ are geometrically equivalent if there exists a $\gamma \in G\,L(n, R)$ such that:

$$\forall\, \alpha \in K: \Lambda \overline{\varphi}\, \omega\, \alpha = \gamma (\Lambda \varphi \alpha)\, \gamma^{-1} \tag{2.10}$$

where ω is an automorphism of K.

Z-equivalence implies R-equivalence. The converse is not true. Hence, a geometric crystal class may give rise, in general, to several arithmetic crystal classes. Again, some of the non-conjugate finite subgroups of $\Lambda\,[G\,L(n,Z)]$ may still be isomorphic. Thus, an abstract crystallographic point group may give rise to several geometric crystal classes. (For $n = 2$, there are 10; for $n = 3$, there are 32 geometric crystal classes.) Furthermore, a finite subgroup of $G\,L(n, Z)$ – and also an abstract crystallographic point group – is isomorphic to a (finite) subgroup of $O(n, R)$, but the converse is not true.

Taking one representative from each geometric crystal class, one obtains a finite family of groups called the geometric crystallographic point groups (usually, these groups are simply called crystallographic point groups).

Acknowledgements

Appendix

1. *Extensions of Groups*

A group G is called an extension of a group $A = (e, a, b, \ldots)$ by a group $B = (\varepsilon, \alpha, \beta, \ldots)$, (i) if G contains a normal subgroup $A'(A' \lhd G)$ that is isomorphic to A $(A' \cong A)$, and (ii) if $G/A' \cong B$. We thus have a sequence

$$A \overset{\varkappa}{\rightarrowtail} G \overset{\sigma}{\twoheadrightarrow} B \qquad\qquad (\text{A1})$$

of a monomorphism $\varkappa : A \rightarrowtail G$ $(\varkappa\,A = A')$ and an epimorphism $\sigma : G \twoheadrightarrow B$.

A sequence of groups and group homomorphisms, $P \overset{\varkappa}{\rightarrow} Q \overset{\sigma}{\rightarrow} R$, such as sequence (A1) for instance, is called a 0-sequence (or a differential sequence) if $\text{Im}\,\varkappa \subset \text{Ker}\,\sigma$; it is called an exact sequence if $\text{Im}\,\varkappa = \text{Ker}\,\sigma$. A longer sequence

$$\ldots A^{n-1} \rightarrow A^{n} \rightarrow A^{n+1} \rightarrow \ldots$$

is called a 0-sequence (or an exact sequence) if every triplet $A^{n-1} \rightarrow A^{n} \rightarrow A^{n+1}$ is a 0-sequence (or an exact sequence, respectively). The fact that in (A1) $\varkappa$ is a monomorphism and σ is an epimorphism may be expressed by saying that the sequence

$$1 \rightarrow A \overset{\varkappa}{\rightarrow} G \overset{\sigma}{\rightarrow} B \rightarrow 1 \qquad\qquad (\text{A2})$$

is exact. An exact sequence of five groups with the two outside groups equal to unity is called a short exact sequence. A short exact sequence $1 \rightarrow A \rightarrow G \rightarrow B \rightarrow 1$ is but another name for an extension of a group A by a group B. More generally, if

$$\ldots X^{n-1} \overset{\delta_{n-1}}{\longrightarrow} X^{n} \overset{\delta_{n}}{\rightarrow} X^{n+1} \overset{\delta_{n+1}}{\longrightarrow} \ldots$$

is part of an exact sequence, the relation

$$\mathrm{Ker}\ \delta_{n+1} = X^n / \mathrm{Im}\ \delta_{n-1} \tag{A3}$$

holds.

If G is an extension of A by B, the group G can be partitioned into cosets $A\,g$ of A, $(g \in G)$. By denoting $r(\alpha)$ a representative of the coset corresponding to $\alpha \in B$, we choose a one-to-one mapping $r : B \to G$ with the property that $\sigma\,r$ is the identity mapping of B onto itself; consequently, $r\,\sigma$ maps every element of a coset on a fixed element of that coset, the representative. For a fixed r, the elements of G can be uniquely represented as $g = \varkappa\,a \cdot r(\alpha)$. The product $r(\alpha)\,r(\beta)$ lies in the coset with representative $r(\alpha\,\beta)$; thus, there are unique elements $m(\alpha, \beta) \in A$ such that

$$r(\alpha)\,r(\beta) = \varkappa\,m(\alpha,\,\beta) \cdot r(\alpha\,\beta) \ . \tag{A4}$$

It is convenient to choose $r(\varepsilon) = e$. This choice leads to

$$\bigvee \alpha \in B : m(\varepsilon,\,\varepsilon) = m(\alpha,\,\varepsilon) = m(\varepsilon,\,\alpha) = e \ . \tag{A5}$$

There is no loss of generality by assuming these conditions fulfilled, and we shall do so henceforth. The mapping $m : B \times B \to A$ is called factor set of the extension G. A factor set satisfying the conditions (A5) is called normalized. Since $\varkappa\,A$ is a normal subgroup of G, conjugation in G (say with an element $g \in G$) yields an automorphism $\Phi\,g$ of A according to

$$\varkappa\,[\Phi\,g \circ a] = g(\varkappa\,a)\,g^{-1} \ . \tag{A6}$$

The mapping $\Phi : G \to \mathrm{Aut}(A)$ of G into the group of all automorphisms of A is a homomorphism. More particularly, conjugation by an element $r(\alpha) \in G$ yields also an automorphism $\varphi\,\alpha$ of A:

$$\varkappa\,[\varphi\,\alpha \circ a] = r(\alpha) \cdot \varkappa\,a \cdot r(\alpha)^{-1} \ . \tag{A7}$$

If $r(\varepsilon) = e$, then $\varphi\,\varepsilon$ is the identity mapping i.

With the aid of the mapping $\varphi : B \to \mathrm{Aut}(A)$, the multiplication of two elements of G can be written:

$$[\varkappa\,a \cdot r(\alpha)]\,[\varkappa\,b \cdot r(\beta)] = \varkappa\,[a(\varphi\,\alpha \circ b)\,m(\alpha,\,\beta)] \cdot r(\alpha\,\beta) \ . \tag{A8}$$

The mapping φ is generally not a homomorphism. Indeed, owing to (A4):

$$[(\varphi\,\alpha)\,(\varphi\,\beta)] \circ a = m(\alpha,\,\beta)\,[\varphi(\alpha\,\beta) \circ a]\,m(\alpha,\,\beta)^{-1} \ . \tag{A9}$$

Furthermore, the mapping φ depends on the choice of representatives r. Instead of taking $r(\alpha)$ as representative of the coset $\varkappa\,A \cdot r(\alpha)$, we may take as well any element $r'(\alpha)$ satisfying

$$r'(\alpha) = \varkappa\,c(\alpha) \cdot r(\alpha) \ , \quad c(\alpha) \in A \ . \tag{A10}$$

Then

$$r'(\alpha) \cdot \varkappa\,a \cdot r'(\alpha)^{-1} = \varkappa\,[\varphi'\,\alpha \circ a] = \varkappa\,[c(\alpha)\,(\varphi\,\alpha \circ a)\,c(\alpha)^{-1}] \ ,$$

and

$$\varphi'\,\alpha \circ a = c(\alpha)\,(\varphi\,\alpha \circ a)\,c(\alpha)^{-1} \ . \tag{A11}$$

Thus, to every element $\alpha \in B$, there corresponds in fact an automorphism of A modulo an inner automorphism of A, i.e. an element of the quotient group $\mathrm{Aut}(A)/I(A) = \mathfrak{A}(A)$. The group $\mathfrak{A}(A)$ is called group of automorphism classes, or group of outer automorphisms. According to (A9), the mapping $\Psi : B \to \mathfrak{A}(A)$ is a homomorphism,

so that we have the following diagram of three short exact sequences [$C(A)$ denotes the center of A]:

$$
\begin{array}{ccccccccc}
& & & & 1 & & & & \\
& & & & \downarrow & & & & \\
& & & & C(A) & & & & \\
& & & & \downarrow & & & & \\
1 & \rightarrow & A & \rightarrow & G & \rightarrow & B & \rightarrow & 1 \\
& & \downarrow & & \Phi\downarrow & & \downarrow\Psi & & \\
1 & \rightarrow & I(A) & \rightarrow & \mathrm{Aut}(A) & \rightarrow & \mathfrak{A}(A) & \rightarrow & 1 \ . \\
& & & & \downarrow & & & & \\
& & & & 1 & & & &
\end{array}
\qquad (A12)
$$

The diagram, furthermore, is commutative. A diagram of groups and group homomorphisms is called commutative if any two paths along directed arrows from one group to another group yield the same (composite) homomorphism.

A further consequence of (A10) is that we get a new factor set $m' : B \times B \rightarrow A$ that is related to the old one by:

$$
m'(\alpha, \beta) = c(\alpha) \, [\varphi \, \alpha \, o \, c(\beta)] \, m(\alpha, \beta) \, c(\alpha \, \beta)^{-1} \ . \qquad (A13)
$$

To preserve the normalization of the new factor set, we must choose $c(\varepsilon) = e$.

There is a further relation concerning the factor set. From the associativity of multiplication applied to the product $r(\alpha) \, r(\beta) \, r(\gamma)$, it follows that

$$
\varphi \, \alpha \, o \, m(\beta, \gamma) = m(\alpha, \beta) \, m(\alpha \, \beta, \gamma) \, m(\alpha, \beta \, \gamma)^{-1} \ . \qquad (A14)
$$

We call system of mappings (φ, m) from B to A (or simply system) the two mappings $\varphi : B \rightarrow \mathrm{Aut}(A)$ and $m : B \times B \rightarrow A$ obeying to (A9) and (A14). A system (φ, m) from B to A such that $\varphi \, \varepsilon = i$, and $m(\varepsilon, \varepsilon) = m(\alpha, \varepsilon) = m(\varepsilon, \alpha) = e$ is called normalized. A given extension of A by B determines a set of systems of mappings from B to A.

Two systems (φ, m) and (φ', m') from B to A are called equivalent if there exists a mapping $c : B \rightarrow A$ such that (A11) and (A13) are satisfied. It may be verified that the equivalence thus defined is reflexive, symmetric, and transitive. Equivalent systems from B to A determine a unique mapping $\Psi : B \rightarrow \mathfrak{A}(A)$. Any system from B to A is equivalent to a normalized one. A given extension G of A by B determines – up to equivalence – a unique system from B to A.

Two extensions, $1 \rightarrow A \rightarrow G \rightarrow B \rightarrow 1$ and $1 \rightarrow A \rightarrow G' \rightarrow B \rightarrow 1$, the first one with system (φ, m) and the second one with system (φ', m') are equivalent if the systems (φ, m) and (φ', m') are equivalent. The equivalence of extensions thus defined does not depend on the choice of (φ, m) and (φ', m').

Given two groups A and B and a system (φ, m) from B to A, the set $G[A, B, \varphi, m]$ of all pairs (a, α) with $a \in A$, $\alpha \in B$ and with the multiplication law given by

$$
(a, \alpha) \, (b, \beta) = (a \, [\varphi \, \alpha \, o \, b] \, m(\alpha, \beta), \alpha \, \beta) \qquad (A15)
$$

is a group. Furthermore, if $\varkappa : A \rightarrow G$ is defined by $\varkappa \, a = (a, \varepsilon)$ and if $\sigma : G \rightarrow B$ is defined by $\sigma(a, \alpha) = \alpha$, then $1 \rightarrow A \xrightarrow{\varkappa} G \xrightarrow{\sigma} B \rightarrow 1$ is exact (i.e. G is an extension of A

by B). Any system $(\overline{\varphi}, \overline{m})$ determined by this extension is equivalent to the system (φ, m); the particular choice $r: B \rightarrow G$ defined by $r(\alpha) = (e, \alpha)$ leads to the initial system (φ, m).

Let G be an extension of A by B and (φ', m') a system from B to A thereby determined. The extension G is said to split if (φ', m') is equivalent to a system (φ, m_0) from B to A such that $m_0(\alpha, \beta) = e \in A$ for any $\alpha, \beta \in B$. Such a system (φ, m_0) is called a split system, and m_0, a trivial factor set. From (A13) we find, by putting $m'(\alpha, \beta) = e$:

$$m(\alpha, \beta) = [\varphi \, \alpha \, o \, c(\beta)]^{-1} \, c(\alpha)^{-1} \, c(\alpha \, \beta) . \tag{A16}$$

The extension G is said to be the direct product extension if (φ', m') is equivalent to a system (i, m_0) where i is the identity automorphism of A. In a split extension, the mapping $r: B \rightarrow G$ may be chosen to be a monomorphism, a right inverse of the epimorphism $\sigma: G \rightarrow B$; the set $r(B)$ of coset representatives then is a subgroup of G that is isomorphic to B; furthermore, from (A9), $\varphi(\alpha \, \beta) = (\varphi \, \alpha) \, (\varphi \, \beta)$, i.e. the mapping $\varphi: B \rightarrow \mathrm{Aut}(A)$ then is a homomorphism. A group $G \, [A, B, \varphi, m_0]$ with multiplication law (A15) is called a semi-direct product of A by B, and is noted $A \times_{\varphi} B$. A group $G \, [A, B, i, m_0]$ with multiplication law (A15) is called the direct product $A \times B$, of A by B.

Henceforth in this paragraph, we suppose that A is an abelian group (written additively). Then the diagram (A12) collapses into

$$0 \rightarrow A \xrightarrow{\varkappa} G \xrightarrow{\sigma} B \rightarrow 1 ,$$
$$\Phi \searrow \quad \downarrow \varphi$$
$$\mathrm{Aut}(A) \tag{A17}$$

where $\varphi: B \rightarrow \mathrm{Aut}(A)$ is now a homomorphism that does not depend anymore on the choice of representatives for the cosets of $\varkappa \, A \subset G$. Through φ, the group B operates on A. Thus, B is a group of operators for A, and A is given the structure of a B-module.

If (φ, m) and (φ', m') are two systems from B to A, determined by an extension of A by B, then $\varphi = \varphi'$, as is seen from (A11). Thus, instead of equivalent systems, we may speak of equivalent factor sets, satisfying (A13). The set $\mathrm{Ext}(A, B, \varphi)$ of all equivalence classes of extensions

$$0 \rightarrow A \rightarrow G \rightarrow B \rightarrow 1 \quad (\varphi) \tag{A18}$$

of an abelian group A by a group B with fixed φ has a simple structure, as we shall see presently.

If m_1 and m_2 are factor sets for an extension of A by B, then $m_3 = m_1 + m_2$, defined by

$$\forall \, \alpha, \beta \in B: m_3(\alpha, \beta) = m_1(\alpha, \beta) + m_2(\alpha, \beta) = m_2(\alpha, \beta) + m_1(\alpha, \beta) , \tag{A19}$$

is again a factor set. By computing $\varphi \, \gamma \, o \, m_3(\alpha, \beta)$, one verifies that (A14) is indeed satisfied. The factor sets form an abelian group $F_{\varphi}(A, B)$. The mapping $f: B \times B \rightarrow A$ defined by

$$f(\alpha, \beta) = c(\alpha) + \varphi \, \alpha \, o \, c(\beta) - c(\alpha \, \beta) , \tag{A20}$$

where c is a one-to-one mapping form B into A, also is a factor set. Comparison with (A13) shows that f is the difference between two equivalent factor sets. One may also

see that f is equivalent to the factor set of a split system. The set of all f is a subgroup $T_\varphi(A, B)$ of $F_\varphi(A, B)$. The set $\text{Ext}(A, B, \varphi)$ of all equivalence classes of extensions is an abelian group, and we have:

$$\text{Ext}(A, B, \varphi) = F_\varphi(A, B)/T_\varphi(A, B). \tag{A21}$$

Extensions belonging to the same group $\text{Ext}(A, B, \varphi)$ are called extensions of the same type.

Given a 0-sequence of abelian groups and group homomorphisms

$$X^0 \xrightarrow{\delta_0} X^1 \xrightarrow{\delta_1} X^2 \xrightarrow{\delta_2} \ldots \tag{A22}$$

we have, by definition, $\delta_{n+1}\,\delta_n = 0$. The δ_n are called differentiation homomorphisms (or coboundary operators). We define

$$\text{Im } \delta_{n-1} = B^n, \quad \text{Ker } \delta_n = Z^n. \tag{A23}$$

Then, $B^n \subset Z^n \subset X^n$, so that we can construct

$$H^n = Z^n/B^n. \tag{A24}$$

Consider now the mappings:

$$f^n: \underbrace{B \times B \times \cdots \times B}_{n \text{ times}} \to A. \tag{A25}$$

The f^n are called n-cochains and form an abelian group $C_\varphi^n(B, A)$. By definition, we put $C_\varphi^0 = A$. Since, through φ, B operates on A, it operates also on $C_\varphi^n(B, A)$. We subject f^n to the normalization conditions $f^n(\alpha_1, \alpha_2, \ldots, \alpha_n) = 0$ whenever, at least one of the α_i equals ε. We now define mappings $\delta_n: C_\varphi^n \to C_\varphi^{n+1}$ by:

$$(\delta_n f^n)(\alpha_0, \alpha_1, \ldots, \alpha_n) = (-1)^{n-1} f^n(\alpha_0, \alpha_1, \ldots, \alpha_{n-1}) + \alpha_0 f^n(\alpha_1, \alpha_2, \ldots, \alpha_n)$$

$$+ \sum_{t=1}^{n} (-1)^t f^n(\alpha_0, \alpha_1, \ldots, \alpha_{t-2}, \alpha_{t-1}\,\alpha_t, \alpha_{t+1}, \ldots, \alpha_n). \tag{A26}$$

For $n = 0, 1, 2$, we find:

$$(\delta_0 f^0)(\alpha) = \alpha f^0 - f^0 \in C_\varphi^1, \tag{A27}$$

$$(\delta_1 f^1)(\alpha, \beta) = f^1(\alpha) + \alpha f^1(\beta) - f^1(\alpha\,\beta) \in C_\varphi^2, \tag{A28}$$

$$(\delta_2 f^2)(\alpha, \beta, \gamma) = -f^2(\alpha, \beta) - f^2(\alpha\,\beta, \gamma) + f^2(\alpha, \beta\,\gamma) + \alpha f^2(\beta, \gamma) \in C_\varphi^3. \tag{A29}$$

It can be shown that $\delta_{n+1}\,\delta_n = 0$, so that

$$A \to C_\varphi^1(B, A) \to C_\varphi^2(B, A) \to C_\varphi^3(B, A) \to \cdots \tag{A30}$$

is a 0-sequence. We than can define $B_\varphi^n(B, A)$, $Z_\varphi^n(B, A)$, and $H_\varphi^n(B, A)$ by (A23) and (A24). The elements of $B_\varphi^n(B, A)$ are called n-coboundaries, those of $Z_\varphi^n(B, A)$ are called n-cocycles, whereas $H_\varphi^n(B, A)$ is the n-th cohomology group of the 0-sequence (A30). Two 2-cocycles that differ by a 2-coboundary are called 2-cohomologous. $H_\varphi^2(B, A)$ is the set of cohomology classes of 2-cocycles. Comparison of (A14) and (A29) shows that a factor set is a 2-cocycle; comparison of (A13) and (A28) shows that the difference between two equivalent factor sets is a 2-coboundary. To the equivalence classes of extensions, there correspond the cohomology classes of 2-cocycles. Hence, the group $\text{Ext}(A, B, \varphi)$ is isomorphic to the second cohomology group $H_\varphi^2(B, A)$ [19][20]:

$$\text{Ext}(A, B, \varphi) \cong H_\varphi^2(B, A). \tag{A31}$$

We utilize also the following properties of cohomology groups[21]:

If K is a finite group of order k, then for $n > 0$ the order of every element of $H_\varphi^n(K, A)$ divides k. If, furthermore, the abelian group A is finitely generated, the group $H_\varphi^n(K, A)$ is finite.
If K is finite and A is a divisible abelian group with no elements of finite order, then for $n > 0$, $H_\varphi^n(K, A) = 0$.
$$\left. \right\} \quad (A32)$$

2. Morphisms of Group Extensions

Consider the following commutative diagram with exact rows

$$
\begin{array}{ccccccccc}
1 & \to & A & \overset{\varkappa}{\to} & G & \overset{\sigma}{\to} & B & \to & 1 \quad (\varphi) \\
& & \lambda\downarrow & & \mu\downarrow & & \nu\downarrow & & \\
1 & \to & A' & \underset{\varkappa'}{\to} & G' & \underset{\sigma'}{\to} & B' & \to & 1 \quad (\varphi')
\end{array}
\qquad (A33)
$$

and with the mappings $\varphi : B \to \mathrm{Aut}(A)$ and $\varphi' : B' \to \mathrm{Aut}(A')$. The triplet $\Gamma(\lambda, \mu, \nu)$ of group homomorphisms is called a morphism of the upper extension to the lower one. Since diagrams such as (A33) are repeatedly encountered in our investigations, we develop here some formulas pertaining to it. (In this section, A and A' are not necessarily abelian groups.)

We have following simple rules

- (i) If μ is an epimorphism, so is ν.
- (ii) If μ is a monomorphism, so is λ.
- (iii) If λ and ν are monomorphisms, so is μ.
- (iv) If λ and ν are epimorphisms, so is μ.
- (v) If μ is an isomorphism, λ is a monomorphism and ν is an epimorphism. (Consequence of (i) and (ii).)
- (vi) If λ and ν are isomorphisms, so is μ. (Consequence of (iii) and (iv).)
- (vii) If any two of the three mappings λ, μ, and ν are isomorphisms, so is the third one.

$$\left. \right\} \quad (A34)$$

Propositions (iii), (iv), and (vi) are the content of the Short Five Lemma[22].

Let $r : B \to G$ be a choice of representatives of the cosets of $\varkappa A \lhd G$, and $r' : B' \to G'$ such a choice for the cosets of $\varkappa' A' \lhd G'$. From the commutativity: $\nu \sigma = \sigma' \mu$ we deduce:

$$\nu = \sigma' \mu r . \qquad (A35)$$

Furthermore, $\sigma' r' \nu = \sigma' \mu r$, so that

$$\forall \alpha \in B : [\sigma' \mu r(\alpha)] [\sigma' r'(\nu \alpha)]^{-1} = \varepsilon' \in B' .$$

Thus

$$\mu r(\alpha) r'(\nu \alpha)^{-1} \in \mathrm{Ker}\, \sigma' = \mathrm{Im}\, \varkappa' .$$

Consequently, there is an element of A' that may depend on α, and that we denote $u(\alpha) \in A'$, such that

$$\mu r(\alpha) r'(\nu \alpha)^{-1} = \varkappa' u(\alpha) .$$

For a fixed mapping r, the possible mappings r' are related by:

$$\forall \alpha \in B : \mu r(\alpha) = \varkappa' u(\alpha) \cdot r'(\nu \alpha) . \qquad (A36)$$

Special cases arise from special choices of $u(\alpha)$. If r' and r are normalized so that $r'(\varepsilon') = r(\varepsilon) = e$, then

$$u(\varepsilon) = e \; . \tag{A37}$$

With the help of (A36), the action of the homomorphism μ can be written more explicitly:

$$\mu(a, \alpha) = \mu \left[\varkappa \, a \cdot r(\alpha) \right] = \mu \, \varkappa \, a \cdot \mu \, r(\alpha) = \varkappa' \, \lambda \, a \cdot \varkappa' \, u(\alpha) \cdot r'(\nu \, \alpha) =$$
$$= \varkappa' \left[\lambda \, a \cdot u(\alpha) \right] \cdot r'(\nu \, \alpha) = (\lambda \, a \cdot u(\alpha), \nu \, \alpha) \; . \tag{A38}$$

We now look how φ and φ' are related.

$$\varkappa' \, \lambda(\varphi \, \alpha \, o \, a) = \mu \, \varkappa(\varphi \, \alpha \, o \, a) = \mu \left[r(\alpha) \cdot \varkappa \, a \cdot r(\alpha)^{-1} \right] =$$
$$= \mu \, r(\alpha) \cdot \mu \, \varkappa \, a \cdot \mu \, r(\alpha)^{-1} = \varkappa' \, u(\alpha) \cdot r'(\nu \, \alpha) \cdot \varkappa' \, \lambda \, a \cdot r'(\nu \, \alpha)^{-1} \cdot \varkappa \, u(\alpha)^{-1} =$$
$$= \varkappa' \, u(\alpha) \cdot \varkappa'(\varphi' \, \nu \, \alpha \, o \, \lambda \, a) \cdot \varkappa' \, u(\alpha)^{-1} =$$
$$= \varkappa' \left[u(\alpha) \, (\varphi' \, \nu \, \alpha \, o \, \lambda \, a) \, u(\alpha)^{-1} \right] \; .$$

Thus

$$\lambda(\varphi \, \alpha \, o \, a) = u(\alpha) \, (\varphi' \, \nu \, \alpha \, o \, \lambda \, a) \, u(\alpha)^{-1} \; . \tag{A39}$$

Finally, we want to establish a relation between the factor sets $m : B \times B \to A$ and $m' : B' \times B' \to A'$.

$$\mu \left[r(\alpha) \, r(\beta) \right] = \mu \left[\varkappa \, m(\alpha, \beta) \cdot r(\alpha \, \beta) \right] = \mu \, \varkappa \, m(\alpha, \beta) \cdot \mu \, r(\alpha \, \beta) =$$
$$= \varkappa' \, \lambda \, m(\alpha, \beta) \cdot \varkappa' \, u(\alpha \, \beta) \cdot r'(\nu \, \alpha \cdot \nu \, \beta) = \varkappa' \left[\lambda \, m(\alpha, \beta) \cdot u(\alpha \, \beta) \right] \cdot r'(\nu \, \alpha \cdot \nu \, \beta).$$

$$\mu \left[r(\alpha) \, r(\beta) \right] = \mu \, r(\alpha) \cdot \mu \, r(\beta) = \varkappa' \, u(\alpha) \cdot r'(\nu \, \alpha) \cdot \varkappa' \, u(\beta) \cdot r'(\nu \, \beta) =$$
$$= \varkappa' \left\{ u(\alpha) \left[\varphi' \, \nu \, \alpha \, o \, u(\beta) \right] m'(\nu \, \alpha, \nu \, \beta) \right\} \cdot r'(\nu \, \alpha \cdot \nu \, \beta) \; .$$

Comparison of the two results shows that

$$\lambda \, m(\alpha, \beta) = u(\alpha) \left[\varphi' \, \nu \, \alpha \, o \, u(\beta) \right] m'(\nu \, \alpha, \nu \, \beta) \, u(\alpha \, \beta)^{-1} \; . \tag{A40}$$

Let λ be a monomorphism. We now are able to define a mapping Λ from $\mathrm{Aut}(A)$ onto $\mathrm{Aut}(\lambda \, A)$ in the following way: Let χ be any element of $\mathrm{Aut}(A)$, and let a be any element of A. Put $\chi \, a = b$; then $\Lambda \, \chi$ maps $\lambda \, a$ onto $\lambda \, b$, i.e.

$$V \, a \in A : (\Lambda \, \chi) \, (\lambda \, a) = \lambda \, (\chi \, a) \quad \text{or} \quad (\Lambda \, \chi) \, \lambda = \lambda \, \chi \; . \tag{A41}$$

$\Lambda \, \chi$ is indeed, by definition, a mapping $\lambda \, A \to \lambda \, A$. We show that it is an automorphism:

$$\Lambda \, \chi \left[\lambda \, a \cdot \lambda \, b \right] = \Lambda \, \chi \left[\lambda(a \, b) \right] = \lambda \, \chi(a \, b) = \lambda \, \chi \, a \cdot \lambda \, \chi \, b = \Lambda \, \chi(\lambda \, a) \cdot \Lambda \, \chi(\lambda \, b) \; .$$

Furthermore, from

$$e' = (\Lambda \, \chi) \, (\lambda \, a) = \lambda(\chi \, a)$$

one concludes that $e = \chi \, a$, that $e = a$, and that $\lambda \, a = e'$.

Now we show that the mapping Λ is an isomorphism from $\mathrm{Aut}(A)$ onto $\mathrm{Aut}(\lambda \, A)$, i.e. if $\Lambda \, \chi$ is the identity mapping on $\lambda \, A$, then χ is the identity mapping on A. Indeed, from $\lambda \, a = (\Lambda \, \chi) \, (\lambda \, a) = \lambda(\chi \, a)$, one concludes that $a = \chi \, a$.

In the particular case of $\chi = \varphi \, \alpha$, we find

$$V \, a \in A : \Lambda \, \varphi \, \alpha \, o \, \lambda \, a = \lambda(\varphi \, \alpha \, o \, a) \quad \text{or} \quad (\Lambda \, \varphi \, \alpha) \, \lambda = \lambda(\varphi \, \alpha) \; . \tag{A42}$$

Combination of (A39) and (A42) gives

$$(\Lambda \varphi \alpha \circ \lambda a) u(\alpha) = u(\alpha) (\varphi' \nu \alpha \circ \lambda a) . \qquad (A43)$$

We now discuss three useful cases of incomplete morphisms, and how they can be completed.

First case:

$$
\begin{array}{ccccccccc}
1 & \to & A & \xrightarrow{\varkappa} & G & \xrightarrow{\sigma} & B & \to & 1 \quad (\varphi) \\
  &   & \lambda\downarrow & & \mu\downarrow & & & & \\
1 & \to & A' & \xrightarrow[\varkappa']{} & G' & \xrightarrow[\sigma']{} & B' & \to & 1 \quad (\varphi') .
\end{array}
\qquad (A44)
$$

Take two elements g and h that belong to the same coset of $\varkappa A \subset G$. Then $g\, h^{-1} \in \varkappa A$ and $\mu(g\, h^{-1}) = (\mu\, g)(\mu\, h)^{-1} \in \mu \varkappa A \subset \varkappa' A'$, thereby showing that $\mu\, g$ and $\mu\, h$ belong to the same coset of $\varkappa' A' \subset G'$. The homomorphism μ thus induces a mapping $\nu : B \to B'$ that is implicitly defined thus: if $\sigma\, g = \alpha$ and $\mu\, g = g'$, then $\sigma'\, g' = \alpha' = \nu\, \alpha$. Hence, $\sigma'\, \mu\, g = \nu\, \alpha = \nu\, \sigma\, g$ and $\sigma'\, \mu = \nu\, \sigma$. Besides $\sigma\, g = \alpha$, $\mu\, g = g'$, and $\sigma'\, g' = \nu\, \alpha$, we put also $\sigma\, h = \beta$, $\mu\, h = h'$, and $\sigma'\, h' = \nu\, \beta$. We then consider $g\, h$. Since $\sigma(g\, h) = \sigma\, g \cdot \sigma\, h = \alpha\, \beta$, we have $\sigma'\, \mu(g\, h) = \nu(\alpha\, \beta)$. But we find also $\sigma'\, \mu(g\, h) = \sigma'\, \mu\, g \cdot \sigma'\, \mu\, h = (\nu\, \alpha)(\nu\, \beta)$. Thus, $\nu(\alpha\, \beta) = (\nu\, \alpha)(\nu\, \beta)$, and ν is a homomorphism.

Second case:

$$
\begin{array}{ccccccccc}
1 & \to & A & \xrightarrow{\varkappa} & G & \xrightarrow{\sigma} & B & \to & 1 \quad (\varphi) \\
  &   &   & & \mu\downarrow & & & & \\
1 & \to & A' & \xrightarrow[\varkappa']{} & G' & \xrightarrow[\sigma']{} & B' & \to & 1 \quad (\varphi') .
\end{array}
\qquad (A45)
$$

Let μ by a homomorphism such that $\mu \varkappa A \subset \varkappa' A'$ and explicitly given by $\mu(a, \alpha) = (a'\, u(\alpha), \alpha')$. (Compare with (A38).)

We define the two mappings $\lambda : A \to A'$ and $\nu : B \to B'$ by $a' = \lambda\, a$ and $\alpha' = \nu\, \alpha$. Thus, $\mu(a, \alpha) = (\lambda\, a \cdot u(\alpha), \nu\, \alpha)$. Putting $\alpha = \varepsilon$, one finds $\mu \varkappa\, a = \varkappa' \lambda\, a$. Calculating $\sigma'\, \mu(a, \alpha) = \sigma'(\lambda\, a \cdot u(\alpha), \nu\, \alpha) = \nu\, \alpha = \nu\, \sigma(a, \alpha)$, one finds $\sigma'\, \mu = \nu\, \sigma$. We now show that λ is a homomorphism: $\mu(\varkappa\, a \cdot \varkappa\, b) = \mu \varkappa(a\, b) = \varkappa' \lambda(a\, b)$, but also $\mu(\varkappa\, a \cdot \varkappa\, b) = \mu \varkappa\, a \cdot \mu \varkappa\, b = \varkappa' \lambda\, a \cdot \varkappa' \lambda\, b = \varkappa'(\lambda\, a \cdot \lambda\, b)$. Since $\varkappa'$ is a monomorphism, this shows that $\lambda(a\, b) = \lambda\, a \cdot \lambda\, b$. The mapping ν is also a homomorphism. We calculate

$$\sigma'\, \mu\, [r(\alpha)\, r(\beta)] = \sigma'\, \mu\, [\varkappa\, m(\alpha, \beta) \cdot r(\alpha\, \beta)] = \sigma'\, \mu \varkappa\, m(\alpha, \beta) \cdot \sigma'\, \mu\, r(\alpha\, \beta) =$$

$$= \sigma'\, \varkappa'\, \lambda\, m(\alpha, \beta) \cdot \nu(\alpha\, \beta) = \nu(\alpha\, \beta);$$

but we have also

$$\sigma'\, \mu\, [r(\alpha)\, r(\beta)] = \sigma'\, \mu\, r(\alpha) \cdot \sigma'\, \mu\, r(\beta) = (\nu\, \alpha)(\nu\, \beta),$$

so that $\nu(\alpha\, \beta) = (\nu\, \alpha)(\nu\, \beta)$.

Third case:

$$
\begin{array}{ccccccccc}
1 & \to & A & \xrightarrow{\varkappa} & G & \xrightarrow{\sigma} & B & \to & 1 \quad (\varphi) \\
  &   & \lambda\downarrow & & & \nu\downarrow & & & \\
1 & \to & A' & \xrightarrow[\varkappa']{} & G' & \xrightarrow[\sigma']{} & B' & \to & 1 \quad (\varphi') .
\end{array}
\qquad (A46)
$$

We define a mapping $\mu : G \to G'$ by $\mu(a, \alpha) = (\lambda\, a \cdot u(\alpha), \nu\, \alpha)$. As in the case of the preceding diagram, one shows that $\mu\, \varkappa = \varkappa'\, \lambda$ and $\sigma'\, \mu = \nu\, \sigma$ hold. To show that μ is a homomorphism, it is necessary to suppose that the two mappings φ and φ' verify (A39), and that the two factor sets m and m' verify (A40). Under these conditions

$$\mu\, \{\varkappa\, a \cdot r(\alpha) \cdot \varkappa\, b \cdot r(\beta)\} = \mu\, \{\varkappa\, [a(\varphi\, \alpha\, o\, b)\, m(\alpha, \beta)] \cdot r(\alpha\, \beta)\} =$$

$$= \varkappa'\, \lambda[a(\varphi\, \alpha\, o\, b)\, m(\alpha, \beta)] \cdot \varkappa'\, u(\alpha\, \beta) \cdot r'\, [\nu(\alpha\, \beta)] =$$

$$= \varkappa'\, [\lambda\, a \cdot \lambda(\varphi\, \alpha\, o\, b) \cdot \lambda\, m(\alpha, \beta) \cdot u(\alpha\, \beta)] \cdot r'(\nu\, \alpha \cdot \nu\, \beta) =$$

$$= \varkappa'\, \{\lambda\, a \cdot u(\alpha)\, [\varphi'\, \nu\, \alpha\, o\, \lambda\, b]\, u(\alpha)^{-1}\, u(\alpha)\, [\varphi'\, \nu\, \alpha\, o\, u(\beta)]\, m'(\nu\, \alpha, \nu\, \beta)\, u(\alpha\, \beta)^{-1}\, u(\alpha\, \beta)\} \cdot$$

$$\cdot\, r'(\nu\, \alpha \cdot \nu\, \beta) =$$

$$= \varkappa'\, [\lambda\, a \cdot u(\alpha)] \cdot r'(\nu\, \alpha) \cdot \varkappa'\, \lambda\, b \cdot r'(\nu\, \alpha)^{-1}\, r'(\nu\, \alpha) \cdot \varkappa'\, u(\beta) \cdot r'(\alpha\, \beta)^{-1}\, \varkappa'\, m'(\nu\, \alpha, \nu\, \beta) \cdot$$

$$\cdot\, r'(\nu\, \alpha \cdot \nu\, \beta) =$$

$$= \varkappa'\, [\lambda\, a \cdot u(\alpha)] \cdot r'(\nu\, \alpha) \cdot \varkappa'\, [\lambda\, b \cdot u(\beta)] \cdot r'(\nu\, \beta) = \mu\, [\varkappa\, a \cdot r(\alpha)] \cdot \mu\, [\varkappa\, b \cdot r(\beta)]\, .$$

We now consider special cases of diagram (A33).

    a) It is always possible to choose r' (for given r) so as to obtain $u(\alpha) = e'$ for all $\alpha \in B$. Then:

$$\mu\, r(\alpha) = r'(\nu\, \alpha) \tag{A47}$$

$$\mu(a, \alpha) = (\lambda\, a, \nu\, \alpha) \tag{A48}$$

$$\lambda(\varphi\, \alpha\, o\, a) = \varphi'\, \nu\, \alpha\, o\, \lambda\, a \quad \text{or} \quad \lambda(\varphi\, \alpha) = (\varphi'\, \nu\, \alpha)\, \lambda \tag{A49}$$

$$\lambda\, m(\alpha, \beta) = m'(\nu\, \alpha, \nu\, \beta)\, . \tag{A50}$$

If λ is a monomorphism:

$$\varLambda\, \varphi = \varphi'\, \nu\, . \tag{A51}$$

    b) Let λ and ν be the identity homomorphisms:

$$\begin{array}{ccccccc}
1 & \to & A & \overset{\varkappa}{\to} & G & \overset{\sigma}{\to} & B & \to & 1 & \quad (\varphi) \\
 & & \| & & \mu\downarrow & & \| & & & \\
1 & \to & A & \underset{\varkappa'}{\to} & G' & \underset{\sigma'}{\to} & B & \to & 1 & \quad (\varphi')\, .
\end{array} \tag{A52}$$

Then, by (A34), μ is an isomorphism. Furthermore:

$$\mu\, r(\alpha) = \varkappa'\, u(\alpha) \cdot r'(\alpha) \tag{A53}$$

$$\mu(a, \alpha) = (a\, u(\alpha), \alpha) \tag{A54}$$

$$\varphi\, \alpha\, o\, a = u(\alpha)\, (\varphi'\, \alpha\, o\, a)\, u(\alpha)^{-1} \tag{A55}$$

$$m(\alpha, \beta) = u(\alpha)\, [\varphi'\, \alpha\, o\, u(\beta)]\, m'(\alpha, \beta)\, u(\alpha\, \beta)^{-1}\, . \tag{A56}$$

Comparison of (A55) and (A56) with (A11) and (A13), respectively, reveals that the diagram (A52) represents the case of two equivalent extensions. (The difference between the two sets of formulas is purely notational, the rôle of the primed and of the unprimed extension being exchanged.)

Conversely, let

$$1 \to A \xrightarrow{\varkappa} G \xrightarrow{\sigma} B \to 1 \quad (\varphi)$$

and

$$1 \to A \xrightarrow{\varkappa'} G' \xrightarrow{\sigma'} B \to 1 \quad (\varphi')$$

be two equivalent extensions, i.e. there exists a mapping $c : B \to A$ such that the respective systems from B to A, (φ, m) and (φ', m'), are related by (A11) and (A13). Let $r : B \to G$ and $r' : B \to G'$ be choices of representatives that lead, by (A4) and (A7), to these systems.

We now show that the mapping μ defined by

$$\forall\, a \in A,\ \forall\, \alpha \in B : \mu\,[\varkappa\, a \cdot r(\alpha)] = \varkappa'\,[a\, c(\alpha)^{-1}] \cdot r'(\alpha) \tag{A57}$$

is an isomorphism that makes the diagram (A52) commutative. Using (A8), (A11), and (A13), we first show that μ is a homomorphism:

$$\mu\,[\varkappa\, a \cdot r(\alpha)\cdot \varkappa\, b \cdot r(\beta)] = \mu\,\{\varkappa\,[a\,(\varphi\,\alpha\, o\, b)\, m(\alpha, \beta)] \cdot r(\alpha\, \beta)\} =$$
$$= \varkappa'\,\{a\,[\varphi\,\alpha\, o\, b]\, m(\alpha, \beta)\, c(\alpha\, \beta)^{-1}\} \cdot r'(\alpha\, \beta) =$$
$$= \varkappa'\,\{a\, c(\alpha)^{-1}\,[\varphi'\,\alpha\, o\, b]\,[\varphi'\,\alpha\, o\, c(\beta)^{-1}]\, m'(\alpha, \beta)\} \cdot r'(\alpha\, \beta) =$$
$$= \varkappa'\,[a\, c(\alpha)^{-1}] \cdot r'(\alpha) \cdot \varkappa'\,[b\, c(\beta)^{-1}] \cdot r'(\beta) =$$
$$= \mu\,[\varkappa\, a \cdot r(\alpha)] \cdot \mu\,[\varkappa\, b \cdot r(\beta)]\,.$$

Putting in (A57) $\alpha = \varepsilon$, one obtains $\mu\,\varkappa\, a = \varkappa'\, a$, i.e. $\mu\,\varkappa = \varkappa'$. Furthermore:

$$\sigma'\,\mu\,[\varkappa\, a \cdot r(\alpha)] = \sigma'\,\{\varkappa'\,[a\, c(\alpha)^{-1}] \cdot r'(\alpha)\} = \alpha = \sigma\,[\varkappa\, a \cdot r(\alpha)]\,,$$

i.e. $\sigma'\,\mu = \sigma$. The diagram (A52) that we have constructed is commutative.

Diagram (A52) may thus be taken as abstract definition of the equivalence of two extensions.

c) Let G' be a split extensions of A' by B'. Then the representatives r' may be chosen in such a way that $r' : B' \to G'$ is a monomorphism and that $m'(\alpha', \beta') = e'$ for all $\alpha', \beta' \in B'$. With such a choice, (A40) becomes:

$$\lambda\, m(\alpha, \beta) = u(\alpha)\,[\varphi'\, \nu\, \alpha\, o\, u(\beta)]\, u(\alpha\, \beta)^{-1}\,. \tag{A58}$$

Concerning split extensions, we have the following rules:

If, in diagram (A33), ν is an isomorphism and if the unprimed extension splits, then so does the primed extension. (A59)

Proof: Let r be a choice of representatives for the cosets of $\varkappa\, A \lhd G$ such that $r : B \to G$ is a monomorphism. Then the mapping $r' : B' \to G'$ defined by $r' = \mu\, r\, \nu^{-1}$ is a homomorphism, and $\sigma'\, r' = \sigma'\, \mu\, r\, \nu^{-1} = \nu\, \sigma\, r\, \nu^{-1} = i$. Hence, r' is a monomorphism and a possible choice of representatives of $\varkappa'\, A' \lhd G'$. Thus, the primed extension splits.

If, in diagram (A33), λ is an isomorphism and if the primed extension splits, then so does the unprimed extension. (A60)

Proof: For G', we choose $m'(\alpha', \beta') = e'$ for any $\alpha', \beta' \in B'$. Then, by (A58):

$$\lambda\, m(\alpha, \beta) = u(\alpha)\,[\varphi'\, \nu\, \alpha\, o\, u(\beta)]\, u(\alpha\, \beta)^{-1}\,.$$

Now we define

$$\forall\, \alpha \in B : u(\alpha) = \lambda\, c(\alpha)^{-1}\,.$$

Then, using (A39), we find

$$\lambda\, m(\alpha, \beta) = \lambda\, [\varphi\, \alpha\, o\, c(\beta)]^{-1} \cdot \lambda\, c(\alpha)^{-1} \cdot \lambda\, c(\alpha\, \beta)$$

and

$$m(\alpha, \beta) = \varphi\, \alpha\, o\, c(\beta)^{-1}\, c(\alpha)^{-1}\, c(\alpha\, \beta) \; .$$

Comparison with (A16) shows that G is a split extension.

d) Let A be an additively written abelian group. Then

$$\mu(a, \alpha) = (\lambda\, a + u(\alpha),\, \nu\, \alpha) \;\; \text{from (A38)} \tag{A61}$$

$$\lambda(\varphi\, \alpha\, o\, a) = \varphi'\, \nu\, \alpha\, o\, \lambda\, a \;\; \text{or} \;\; \lambda(\varphi\, \alpha)\, \lambda^{-1} = \varphi'\, \nu\, \alpha \;\; \text{from (A39)} \tag{A62}$$

$$\lambda\, m(\alpha, \beta) = m'(\nu\, \alpha,\, \nu\, \beta) + u(\alpha) + \varphi'\, \nu\, \alpha\, o\, u(\beta) - u(\alpha\, \beta) \;\; \text{from (A40)} \; . \tag{A63}$$

If λ is a monomorphism:

$$\Lambda\, \varphi = \varphi'\, \nu \;\; \text{from (A43)} \; . \tag{A64}$$

References

[1] L. BIEBERBACH, Math. Annalen *70*, 297 (1911) and *72*, 400 (1912).

[2] G. FROBENIUS, Sitzber. preuss. Akad. Wiss., Physik.-math. Kl. 654 (1911).

[3] J. J. BURCKHARDT, *Die Bewegungsgruppen der Kristallographie* (Verlag Birkhäuser, Basel 1947).

[4] N. F. M. HENRY and K. LONSDALE, *International Tables for X-ray Crystallography*, Volume I, Symmetry Groups (The Kynoch Press, Birmingham, England, 1952).

[5] D. K. FADDEEV, *Tablicy osnovnyh unitarnyh predstavlenij fedorovskih grupp* (Izdatelstvo Akademii Nauk SSSR, 1961). English translation: Pergamon Press 1964.

[6] Extensions seem to appear for the first time in: O. HÖLDER, Math. Annalen *48*, 301 (1893). The theory of extensions has been formulated by O. SCHREIER in Monatsh. Math. und Phys. *34*, 165 (1926), and Abh. Math. Seminar Univ. Hamburg *4*, 321 (1923).

[7] A. G. KUROSH, *The Theory of Groups* (Chelsea Publishing Company, New York 1960), 2nd english ed. Vol. II.

[8] MARSHALL HALL, JR., *The Theory of Groups* (The MacMillan Company, New York 1959).

[9] K. OLBRYCHSKI, Phys. Stat. Sol. *3*, 1868 (1963).

[10] H. ZASSENHAUS, Comm. Math. Helv. *21*, 117 (1948) (see also ref. 19).

[11] The Original Treatment of the Homology of Group Extension is due to S. EILENBERG and S. MACLANE, Ann. Math. *48*, 51 (1957) and *48*, 326 (1947); B. EECKMANN, Comm. Math. Helv. *18*, 232 (1945-46).

[12] S. MACLANE, Homology (Springer-Verlag, Berlin 1963).

[13] See e.g. ref. [1], p. 406.

[14] See e.g. A. SPEISER, *Die Theorie der Gruppen von endlicher Ordnung* (Birkhäuser, Basel 1956), p. 153.

[15] J. J. BURCKHARDT, Comm. Math. Helv. *6*, 159 (1933/34).

[16] C. JORDAN, J. Ecole Polytechn. 48 (1880).

[17] Ref. [1], p. 408.

[18] M. J. BUERGER, *Elementary Crystallography* (John Wiley & Sons, Inc., New York 1956), p. 459.

[19] After the present work had been formulated, we found ZASSENHAUS' paper (Ref. [10]). In that paper, ZASSENHAUS already derives the main algebraic properties of space groups. Since the algorithm derived there is based, like Frobenius' method, essentially on non-primitive translations, we shall take due account of this work in a subsequent paper.

[20] Ref. [12], p. 112.

[21] Ref. [12], p. 117.

[22] Ref. [12], p. 13.

[23] N. V. BELOV, N. N. NERONOVA, and T. S. SMIRNOVA, Trudy Instituta Kristallografii Akademii Nauk SSSR *11* (1955); W. OPECHOWSKI and R. GUCCIONE, Magnetism vol. II A, G. T. Rado H. Suhl ed. (Academic Press 1965), p. 105.

[24] L. MICHEL, Phys. Rev. *137*, B405 (1965).

[25] F. KAMBER and N. STRAUMANN, Helv. Phys. Acta *37*, 563 (1964).