Commun. math. Phys. 11, 138—167 (1968)

Algebraic Aspects of Crystallography

II. Non-primitive Translations in Space Groups

EDGAR ASCHER
Battelle Institute, Advanced Studies Center, Geneva
and
ALOYSIO JANNER
Instituut voor Theoretische Fysica, Katholieke Universiteit, Nijmegen

Received May 28, 1968

Abstract. Taking into account the fact that space groups are groups of transformations of Euclidean n-dimensional space, non-equivalent systems of non-primitive translations are defined. They can be brought into one-to-one correspondence with the elements of the group $H^1(K, R^n/Z^n)$ or with those of the group $H^1(K, Z^n/kZ^n)/H^1(K, Z^n)$. ($K$ is a point group of order k.) The consistency of these findings with the results of Part I is given by the isomorphisms

$$H^2(K, Z^n) \cong H^1(K, R^n/Z^n) \cong H^1(K, Z^n/kZ^n)/H^1(K, Z^n) .$$

Theorems are proved giving the conditions for cohomology groups $H^q(K, A)$ to be zero. These conditions are fulfilled in particular if $A = R^n$ and K is a subgroup of $GL(n, R)$ that either is compact (then $q > 0$) or has a finite normal subgroup leaving no element of R^n invariant (then $q \geqq 0$). This implies that the affine, the Euclidean and the inhomogeneous Lorentz groups are the only extensions of R^n by the corresponding homogeneous groups. By way of illustration, the theory of this paper is applied to two 2-dimensional space groups.

1. Introduction

In a previous paper [1], referred to hereafter as Part I, space groups were presented as group extensions, and several possible ways of continuing the investigation in question were mentioned.

One of these ways concerned the application of the theory of group extension and of the cohomology of groups to generalizations of space groups. A first generalization is obtained when time inversion is added to the spatial symmetry elements. The groups thus obtained are called Shubnikov groups or magnetic groups. These groups have been discussed in [2] from the point of view of group extensions. However, the generalization principally aimed at is the study of the crystallographic groups of space-time. Several papers concerning the general aspects of the problem, the discussion of special four-dimensional cases and of the two-dimensional case are being prepared.

Here we continue our investigation of the ordinary (crystallographic) space groups. This is interesting by itself, since space groups, although at the very basis of solid-state physics, are not yet fully exploited in that context. Furthermore, some of the problems one meets when dealing with the above-mentioned generalizations are already encountered – in their simplest form – in the study of space groups.

Going as far as we do in the algebraisation of the study of space groups is meaningful for physics. Let us not forget the impulse that the publication of Seitz's paper [3] has given to solid-state physics at a time – 1934 – when space groups were – in principle – perfectly known. FEDOROV and SCHOENFLIES had determined all three-dimensional space groups not later than 1891. (For a discussion of the history of this discovery, see [4].) In 1919 already, P. NIGGLI [5] had published "the most thorough investigation alloted so far to a special domain of group theory [6]". And yet in 1934 Seitz thought that "in applying the consequences of the theories of crystal symmetry to mathematical-physical problems the need is felt for a derivation and expression of these consequences in terms of a matrix-algebraic scheme". The subsequent development of solid-state physics showed that he was right.

The advantage of the algebraic methods used in this paper lies not in its possible elegance (with Boltzmann we leave that to the taylors) but in the possibility of giving conceptual proofs of theorems, proofs that involve, for instance, mappings between sets of elements and not the elements themselves. This way of thinking should also permit to bring out more clearly the general features of a physical situation without resorting to the special features of a specific model.

Placed in historical perspective, this series of papers is but a further step, after the numerous steps that have preceded, in the direction of an algebraisation of crystal physics.

In Part I it was shown that all space groups G may be presented as extensions of U by K

$$0 \to U \to G \to K \to 1$$

where U is free abelian of rank n and maximal abelian in G, and K is finite. To find all space groups amounts thus to finding all extensions of U by K. After the choice of an isomorphism $\lambda\colon U \rightarrowtail\!\!\!\twoheadrightarrow Z^n$ (i.e. after the choice of a free set of generators for U) one has thus to calculate the second cohomology group $H^2_\varphi(K, Z^n)$ of K with coefficients in Z^n, where φ is a monomorphism $\varphi\colon K \rightarrowtail GL(n, Z)$. It turned out that, in order to obtain all non-equivalent space groups, it is sufficient to take one representative $\varphi(K)$ of each conjugate class (and there is only a finite number of them) of finite subgroups of $GL(n, Z)$.

The algebraic structure of space groups as it emerged in the historical development seems at first sight to be different. Stated in modern language it appears that to each equivalence class of space groups there corresponds an element of a first cohomology group $H^1_\varphi(K, R^n/Z^n)$ and not an element of a second cohomology group as above. One arrives quite naturally at this result if one studies the structure of space groups as groups of transformations of Euclidean n-space. Then it becomes clear that some of these transformations consist of an orthogonal transformation followed by a translation that does not belong to U. Such translations are called non-primitive in contradistinction to the elements of U that are called primitive translations. The elements of the first cohomology groups $H^1_\varphi(K, R^n/Z^n)$ can be brought into a one-to-one correspondence with the non-equivalent systems of non-primitive translations.

Using the cohomology theory of groups it may be shown that

$$H^2_\varphi(K, Z^n) \cong H^1_\varphi(K, R^n/Z^n)$$

so that for a given group $\varphi(K)$ the determination of all non-equivalent systems of non-primitive translations and the determination of all non-equivalent extensions yield the same result.

Other properties of space groups can be deduced by means of cohomology. Thus we shall prove a generalization of a theorem of Speiser (appearing in [6] without proof) and several similar propositions.

The idea that proves fruitful in most demonstrations is that (introduced by I. SCHUR [7] in his proof of Maschke's theorem) of averaging over the elements of a group.

2. Mathematical Background

It will be helpful to recall or introduce here briefly some of the mathematical notions and notations used in this paper.

Let K be a group and A a left K-module. Consider then the following 0-sequence ($\delta_{q+1}\delta_q = 0$) or cochain-complex of abelian groups

$$0 \longrightarrow C^0(K,A) \xrightarrow{\delta_0} C^1(K,A) \xrightarrow{\delta_1} C^2(K,A) \xrightarrow{\delta_2} C^3(K,A) \longrightarrow \qquad (2.1)$$

The elements f^q of the abelian groups $C^q(K, A)$ are mappings

$$f^q : \underbrace{K \times \cdots \times K}_{q\text{-times}} \to A \qquad q > 0 \qquad (2.2)$$

and $C^0(K, A) = A$. The coboundary homomorphisms δ_q are defined in the following way [8][1]

$$(\delta_q f^q)(\alpha_0, \ldots, \alpha_q) = f^q(\alpha_0, \ldots, \alpha_{q-1}) + (-1)^{q+1}\alpha_0 f^q(\alpha_1, \ldots, \alpha_q) + (-1)^{q+1} \sum_{t=1}^{q} (-1)^t f^q(\alpha_0, \ldots, \alpha_{t-1}\alpha_t, \ldots, \alpha_q) \,. \qquad (2.3)$$

[1] With respect to [9] and to Part I (p. 566) there is a slight change of the definition insofar as the coboundary $\delta_q f^q$ defined here is $(-1)^{q+1}$-times the coboundary defined in Part I. This simplifies some of the subsequent formulas.

The elements of $\operatorname{Im}\delta_{q-1} = B^q(K, A)$ are called q-coboundaries for $q > 0$, those of $\operatorname{Ker}\delta_q = Z^q(K, A)$ are called q-cocycles, whereas the elements of the q-cohomology groups

$$H^q(K, A) = \operatorname{Ker}\delta_q/\operatorname{Im}\delta_{q-1} \tag{2.4}$$

are called q-cohomology classes. For $q = 0$, one sets $B^0(K, A) = 0$ so that

$$H^0(K, A) = Z^0(K, A) = \{a \in A \mid \alpha a = a\,, \quad \forall\, \alpha \in K\}\,. \tag{2.5}$$

A shorter notation that we shall use is $H^0(K, A) = A^K$.

Let now K be a finite group of order k. To prove some theorems about the order of cohomology groups, we shall introduce a homomorphism $s_q : C^q(K, A) \to C^{q-1}(K, A)$ by setting

$$(s_q f^q)\,(\alpha_0, \ldots, \alpha_{q-2}) = \sum_{\alpha \in K} f^q(\alpha_0, \ldots, \alpha_{q-2}, \alpha)\,. \tag{2.6}$$

Although the proofs may be found in the literature, e.g. [8] and [10], we want to give them here for three reasons. These results constitute the mathematical core of the paper. The mathematical device used, the averaging over the elements of a finite group, is already used in Frobenius' paper on space groups [11] and in all investigations inspired by it, e.g. [12] and [13] (the idea goes back to Schur's proof of Maschke's theorem [7]). We shall be interested in generalization of the mappings s and these generalizations, although not new, are probably not easily accessible to physicists.

Proposition 2.1. *Given definitions* (2.3) *and* (2.6), *we have*

$$s_{q+1}\delta_q + \delta_{q-1}s_q = kI \qquad q > 0\,, \tag{2.7}$$

where I is the identity mapping on $C^q(K, A)$.

Proof. We find on one hand

$$\begin{aligned}[\delta_{q-1}(s_q f^q)](\alpha_0, \ldots, \alpha_{q-1}) &= (s_q f^q)\,(\alpha_0, \ldots, \alpha_{q-2}) \\ &\quad + (-1)^q\,\alpha_0(s_q f^q)(\alpha_1, \ldots, \alpha_{q-1}) \\ &\quad + (-1)^q \sum_{t=1}^{q-1}(-1)^t (s_q f^q)\,(\alpha_0, \ldots, \alpha_{t-1}\,\alpha_t, \ldots, \alpha_{q-1})\end{aligned}$$

and on the other hand

$$\begin{aligned}[s_{q+1}(\delta_q f^q)](\alpha_0, \ldots, \alpha_{q-1}) &= \sum_{\alpha_q} (\delta_q f^q)(\alpha_0, \ldots, \alpha_q) \\ = k f^q(\alpha_0, \ldots, \alpha_{q-1}) &- (-1)^q\,\alpha_0(s_q f^q)(\alpha_1, \ldots, \alpha_{q-1}) \\ &- (-1)^q \sum_{t=1}^{q-1}(-1)^t (s_q f^q)(\alpha_0, \ldots, \alpha_{t-1}\,\alpha_t, \ldots, \alpha_{q-1}) \\ &- (s_q f^q)(\alpha_0, \ldots, \alpha_{q-2})\,.\end{aligned}$$

Here the obvious linearity and left invariance of the sum over the finite group have been used. Thus

$$[s_{q+1}(\delta_q f^q) + \delta_{q-1}(s_q f^q)](\alpha_0, \ldots, \alpha_{q-1}) = k f^q(\alpha_0, \ldots, \alpha_{q-1})$$

or

$$\forall\, f^q \in C^q(K, A)\,, \quad s_{q+1}(\delta_q f^q) + \delta_{q-1}(s_q f^q) = k f^q \quad q > 0 \qquad (2.8)$$

or also

$$s_{q+1}\delta_q + \delta_{q-1} s_q = kI\,.$$

If $f^q \in Z^q(K, A)$, then, according to (2.7)

$$k f^q = \delta_{q-1}(s_q f^q) \in B^q(K, A) \quad q > 0\,. \qquad (2.9)$$

Thus we have proved the following result:

Corollary 2.1.1. *If K is a finite group of order k, then*

$$k H^q(K, A) = 0 \quad q > 0\,. \qquad (2.10)$$

Corollary 2.1.2. *If K is a finite group and A as an abelian group is divisible and torsion-free, then*

$$H^q(K, A) = 0 \quad q > 0\,. \qquad (2.11)$$

Put now $f^q = s_{q+1} f^{q+1}$ and apply (2.8). The result is

$$s_{q+1}\, s_{q+2}\, \delta_{q+1} = \delta_{q-1}\, s_q s_{q+1} \quad q > 0\,. \qquad (2.12)$$

For $q = 0$, direct calculation gives

$$s_1 \delta_0 + N = kI \qquad (2.13)$$

and

$$s_1 s_2 \delta_1 = N s_1 \qquad (2.14)$$

where the K-module homomorphism $N: A \to A$ is defined by

$$\forall\, a \in A\,, \quad Na = \sum_{\alpha \in K} \alpha a\,. \qquad (2.15)$$

The homomorphism N is called the norm homomorphism and has the property

$$\forall\, \alpha \in K\,, \quad \alpha N = N \alpha = N \qquad (2.16)$$

so that

$$\forall\, a \in A\,, \quad Na \in H^0(K, A)\,. \qquad (2.17)$$

Let now K be a compact topological group and T a finite-dimensional real vector space and a left K-module subject to the additional condition

$$\forall\, \alpha \in K\,, \quad \forall\, r \in R\,, \quad \forall\, t \in T\,, \quad \alpha(rt) = r(\alpha t)\,.$$

Then the elements of K are linear transformations of the finite dimensional vector space T and hence continuous. Let now $f_c^q: K \times \cdots \times K \to T$ be continuous q-cochains. Define $\tilde{s}^q: C_c^q(K, T) \to C_c^{q-1}(K, T)$ by the Haar integral

$$(\tilde{s}_q f_c^q)(\alpha_0, \ldots, \alpha_{q-2}) = \int f_c^q(\alpha_0, \ldots, \alpha_{q-2}, \alpha)\, d\alpha\,. \qquad (2.18)$$

(The integral is of course calculated componentwise after the choice of a basis for T.) Define the coboundary homomorphism δ_q by (2.3). Note that $\delta_q f_c^q$ is again a continuous function. Then proceeding exactly as in the proof of Proposition 2.1 and using the linearity and left invariance of the Haar integral, one proves the following proposition:

Proposition 2.2

$$\bar{s}_{q+1}\delta_q + \delta_{q-1}\bar{s}_q = I . \tag{2.19}$$

The above relation is valid for any $f_c^q \in C_c^q(K, T)$. If we now specialize to $f_c^q \in Z_c^q(K, T)$, then we obtain

$$\forall\, f_c^q \in Z_c^q(K, T) , \quad \delta_{q-1} s_q f_c^q = f_c^q$$

showing that $f_c^q \in B_c^q(K, T)$, i.e. that

$$H_c^q(K, T) = 0 \quad q > 0 . \tag{2.20}$$

It is not astonishing that we obtain a result similar to (2.11), for T as abelian group is torsion-free (since T as R-module is free) and divisible (since T is also a vector space over the rationals).

Let now K be any group. We shall utilize later the fact that all K-modules A can be imbedded into K-modules $\bar{A}$ such that $K^q(K, \bar{A}) = 0$ for $q > 0$.

Given a K-module A we construct a K-module $\bar{A}$, called the co-induced K-module. The elements of $\bar{A}$ are the set theoretical mappings $h : K \rightarrowtail A$ from K to A. Utilizing the group structure of A, the set $\bar{A}$ may be given the structure of an abelian group by

$$\forall\, h, h' \in \bar{A} , \quad \forall\, \alpha \in K , \quad (h + h')(\alpha) = h\alpha + h'\alpha . \tag{2.21}$$

By defining the operation of K on $\bar{A}$ through

$$\forall\, h \in \bar{A} , \quad \forall\, \alpha, \beta \in K , \quad (\beta h)(\alpha) = h(\alpha\beta) . \tag{2.22}$$

$\bar{A}$ is made a K-module since, as is easily verified,

$$[\beta(h + h')](\alpha) = (\beta h + \beta h')(\alpha)$$

and

$$[(\beta\gamma) h](\alpha) = [\beta(\gamma h)](\alpha) .$$

Proposition 2.3. *Any K-module A is isomorphic to a submodule of the co-induced K-module $\bar{A}$.*

Proof. Consider the mapping $\chi : A \rightarrowtail \bar{A}$ defined by

$$\forall\, a \in A , \quad \forall\, \alpha \in K , \quad (\chi a)(\alpha) = \alpha a . \tag{2.23}$$

It is a homomorphism of abelian groups:

$$[\chi(a + b)](\alpha) = \alpha(a + b) = \alpha a + \alpha b = (\chi a + \chi b)(\alpha) .$$

It is also a monomorphism since $\chi(a) = 0$ implies for the identity ε of K

$$[\chi(a)](\varepsilon) = a = 0 .$$

But χ is even a K-module homomorphism:

$$[\chi(\beta a)](\alpha) = \alpha\beta a = [\chi(a)](\alpha\beta) = [\beta\chi(a)](\alpha) .$$

Proposition 2.4. *Let $\bar{A}$ be a co-induced K-module. Then*

$$H^q(K, \bar{A}) = 0 \quad q > 0 . \tag{2.24}$$

Proof. Consider the q-cochains $f^q \in C^q(K, \bar{A})$. They are mappings

$$f^q: \underbrace{K \times \cdots \times K}_{q\text{-times}} \to \bar{A} .$$

Since the elements of $\bar{A}$ are mappings from K to A, f^q may be considered also as a mapping

$$f^q: \underbrace{K \times K \times \cdots \times K}_{(q+1)\text{-times}} \to A \tag{2.25}$$

and we shall write

$$[f^q(\alpha_1, \ldots, \alpha_q)](\alpha_0) = f^q(\alpha_0, \alpha_1, \ldots, \alpha_q) . \tag{2.26}$$

Owing to this new way of writing, the coboundary operators

$$\delta_q: C^q(K, \bar{A}) \to C^{q+1}(K, \bar{A})$$

become very simple. Indeed

$$[(\delta_q f^q)(\alpha_1, \ldots, \alpha_{q+1})](\alpha_0) = [(-1)^{q+1} f^q(\alpha_1, \ldots, \alpha_q) + \alpha_1 f^q(\alpha_2, \ldots, \alpha_{q+1}) + \sum_{t=1}^{q} (-1)^t f^q(\alpha_1, \ldots, \alpha_t\alpha_{t+1}, \ldots, \alpha_{q+1})](\alpha_0)$$

becomes by relation (2.22)

$$(\delta_q f^q)(\alpha_0, \alpha_1, \ldots, \alpha_{q+1}) = \sum_{t=0}^{q} (-1)^t f^q(\alpha_0, \alpha_1, \ldots, \alpha_t \alpha_{t+1}, \ldots, \alpha_{q+1}) + (-1)^{q+1} f^q(\alpha_0, \alpha_1, \ldots, \alpha_q) . \tag{2.27}$$

Now we introduce mappings $\bar{s}_q: C^q(K, \bar{A}) \to C^{q-1}(K, \bar{A})$ that (in contradistinction to the mappings s and $\bar{s}$ previously introduced) do not rely on an average over the group K. The definition of $\bar{s}$ is the following:

$$(\bar{s}_q f^q)(\alpha_0, \alpha_1, \ldots, \alpha_{q-1}) = f^q(\varepsilon, \alpha_0, \alpha_1, \ldots, \alpha_{q-1}) , \quad q > 0 . \tag{2.28}$$

Then on one hand

$$\begin{aligned}[\bar{s}_{q+1}(\delta_q f^q)](\alpha_0, \alpha_1, \ldots, \alpha_q) &= (\delta_q f^q)(\varepsilon, \alpha_0, \alpha_1, \ldots, \alpha_q) = f^q(\alpha_0, \alpha_1, \ldots, \alpha_q) \\ &\quad - f^q(\varepsilon, \alpha_0\alpha_1, \ldots, \alpha_q) + \cdots + (-1)^q f^q(\varepsilon, \alpha_0, \alpha_1, \ldots, \alpha_{q-1}\alpha_q) \\ &\quad + (-1)^{q+1} f^q(\varepsilon, \alpha_0, \alpha_1, \ldots, \alpha_{q-1}) .\end{aligned}$$

On the other hand

$$
\begin{aligned}
&[\delta_{q-1}(\bar{s}_q f^q)](\alpha_0, \alpha_1, \ldots, \alpha_q) \\
&\quad = (\bar{s}_q f^q)(\alpha_0\alpha_1, \ldots, \alpha_q) + \cdots + (-1)^{q-1}(\bar{s}_q f^q)(\alpha_0, \alpha_1, \ldots, \alpha_{q-1}\alpha_q) \\
&\qquad + (-1)^q(\bar{s}_q f^q)(\alpha_0, \alpha_1, \ldots, \alpha_{q-1}) \\
&\quad = f^q(\varepsilon, \alpha_0\alpha_1, \ldots, \alpha_q) + \cdots + (-1)^{q-1} f^q(\varepsilon, \alpha_0, \alpha_1, \ldots, \alpha_{q-1}\alpha_q) \\
&\qquad + (-1)^q f^q(\varepsilon, \alpha_0, \alpha_1, \ldots, \alpha_{q-1})
\end{aligned}
$$

so that

$$[\bar{s}_{q+1}(\delta_q f^q) + \delta_{q-1}(\bar{s}_q f^q)](\alpha_0, \ldots, \alpha_q) = f^q(\alpha_0, \ldots, \alpha_q) \tag{2.29}$$

or

$$\bar{s}_{q+1}\delta_q + \delta_{q-1}\bar{s}_q = I \tag{2.30}$$

where I is the identity mapping on $C^q(K, \bar{A})$. If now we suppose that f^q is a q-cocycle $f^q \in Z^q(K, \bar{A})$, the above relation shows that it is also a q-coboundary

$$\delta_{q-1}(\bar{s}_q f^q) = f^q .$$

Hence

$$H^q(K, \bar{A}) = 0 \qquad q > 0$$

as announced.

To a given short exact sequence of K-modules

$$0 \longrightarrow A \xrightarrow[\iota]{} B \xrightarrow[\pi]{} C \longrightarrow 0 \tag{2.31}$$

there corresponds an exact sequence of cochain complexes (i.e. the following commutative diagram):

$$
\begin{array}{ccccccccc}
 & & \downarrow & & \downarrow & & \downarrow & & \\
0 & \longrightarrow & C^{q-1}(K, A) & \xrightarrow{\iota_*} & C^{q-1}(K, B) & \xrightarrow{\pi_*} & C^{q-1}(K, C) & \longrightarrow & 0 \\
 & & \delta\downarrow & & \delta\downarrow & & \delta\downarrow & & \\
0 & \longrightarrow & C^{q}(K, A) & \xrightarrow{\iota_*} & C^{q}(K, B) & \xrightarrow{\pi_*} & C^{q}(K, C) & \longrightarrow & 0 \\
 & & \delta\downarrow & & \delta\downarrow & & \delta\downarrow & & \\
0 & \longrightarrow & C^{q+1}(K, A) & \xrightarrow{\iota_*} & C^{q+1}(K, B) & \xrightarrow{\pi_*} & C^{q+1}(K, C) & \longrightarrow & 0 \\
 & & \downarrow & & \downarrow & & \downarrow & &
\end{array}
\tag{2.32}
$$

The mappings ι_* and π_* are the K-module homomorphisms defined for any occurring q-cochain by

$$
\left.
\begin{aligned}
(\iota_* f)(\alpha_1, \ldots, \alpha_q) &= \iota[f(\alpha_1, \ldots, \alpha_q)] \\
(\pi_* f)(\alpha_1, \ldots, \alpha_q) &= \pi[f(\alpha_1, \ldots, \alpha_q)]
\end{aligned}
\right\}
\tag{2.33}
$$

respectively. Each of the occurring coboundary homomorphism is designated by one and the same symbol δ.

To the short exact sequence (2.27) there corresponds a long exact sequence of cohomology groups (see e.g. [8, p. 116]):

$$\xrightarrow{\partial_*} H^q(K, A) \xrightarrow{[\iota_*]} H^q(K, B) \xrightarrow{[\pi_*]} H^q(K, C) \xrightarrow{\partial_*} H^{q+1}(K, A) \xrightarrow{[\iota_*]} \tag{2.34}$$

with ∂_* the so-called connecting homomorphism, and $[\iota_*]$ and $[\pi_*]$ the homomorphisms induced by ι_* and π_* respectively. If f is q-cocycle, it cohomology class will be denoted by $[f]$ and the following relations hold

$$[\iota_* f] = [\iota_*]\,[f]\,, \qquad [\pi_* f] = [\pi_*]\,[f]\,. \tag{2.35}$$

Since later we shall need to know how the homomorphism ∂_* is constructed, we recall that construction here.

Let $c \in Z^q(K, C)$. Then there is an element $b \in C^q(K, B)$ such that $\pi_* b = c$. Then $\pi_* \delta b = \delta \pi_* b = \delta c = 0$ so that there exists $a \in C^{q+1}(K, A)$ with the property that $\delta b = \iota_* a$. Since $\iota_* \delta a = \delta \iota_* a = \delta b = 0$ we find that $a \in Z^{q+1}(K, A)$.

If instead of b we choose an element $b_1 \in C^q(K, A)$ such that $\pi_* b_1 = a$, then $\pi_* (b_1 - b) = 0$ so that there is an element $d \in C^q(K, A)$ with the property $b_1 = b + \iota_* d$. Then $\delta b_1 = \delta b + \delta \iota_* d = \iota_* (a + \delta d) = \iota_* a_1$, with $a_1 = a + \delta d$. Thus only the cohomology class of a is uniquely determined.

If instead of a we choose $\bar{a} \in C^{q+1}(K, A)$ such that $\delta b = \iota_* \bar{a}$, then $\iota_* (\bar{a} - a) = 0$ and $\bar{a} = a$.

Since only the cohomology class of a is determined, we want to see what happens to an element $\bar{c} \in Z^q(K, C)$ which is cohomologous to c. Then there is a $g \in C^{q-1}(K, C)$ such that $\bar{c} = c + \delta g$. Furthermore, an element $f \in C^{q-1}(K, B)$ exists such that $\pi_* f = g$. Then $\bar{c} = \pi_* (b + \delta f)$ $= \pi_* \bar{b}$ with $\bar{b} = b + \delta f$. Therefore $\delta \bar{b} = \delta b = \iota_* a$.

Thus the cohomology class $[c]$ of $\bar{c}$ determines uniquely the cohomology class $[a]$ of a. The mapping

$$\partial_* : H^q(K, C) \to H^{q+1}(K, A) \qquad q > 0$$

defined by

$$\partial_* [c] = [a] \quad \text{if} \quad c = \pi_* b \quad \text{and} \quad \delta b = \iota_* a \tag{2.36}$$

is a homomorphism.

Note that the commutative diagram

$$\begin{array}{ccccccccc}
 & & 0 & & 0 & & 0 & & \\
 & & \downarrow & & \downarrow & & \downarrow & & \\
0 & \longrightarrow & C^q(K, A) & \xrightarrow{\iota_*} & C^q(K, B) & \xrightarrow{\pi_*} & C^q(K, C) & \longrightarrow & 0 \\
 & & \downarrow{\scriptstyle\delta} & & \downarrow{\scriptstyle\delta} & & \downarrow{\scriptstyle\delta} & & \\
0 & \longrightarrow & C^{q+1}(K, A) & \xrightarrow{\iota_*} & C^{q+1}(K, B) & \xrightarrow{\pi_*} & C^{q+1}(K, C) & \longrightarrow & 0 \\
 & & \downarrow & & \downarrow & & \downarrow & &
\end{array} \tag{2.37}$$

is another exact sequence of cochain complexes that may be deduced from (2.31). The exact sequence of cohomology groups that follows is

$$0 \longrightarrow Z^q(K,A) \xrightarrow{[\iota_*]} Z^q(K,B) \xrightarrow{[\pi_*]} Z^q(K,C) \xrightarrow{\partial_*} H^{q+1}(K,A) \longrightarrow \cdots . \tag{2.38}$$

Let now $\omega : K \to \overline{K}$ be a group homomorphism and A an abelian group. Then, given $\overline{\varphi} : \overline{K} \to \operatorname{Aut} A$, A becomes a $\overline{K}$-module and is also, in a natural way, a K-module on account of $\overline{\varphi}\omega : K \to \operatorname{Aut} A$. Then ω induces a group homomorphism

$$\omega^* : C^q_{\overline{\varphi}}(\overline{K}, A) \to C^q_{\overline{\varphi}\omega}(K, A) \tag{2.39}$$

defined by

$$(\omega^* \overline{f})(\alpha_1, \ldots, \alpha_q) = \overline{f}(\omega\alpha_1, \ldots, \omega\alpha_q) \tag{2.40}$$

with $\overline{f} \in C^q_{\overline{\varphi}}(\overline{K}, A)$. The group homomorphism ω also induces a homomorphism of cochain complexes

$$\begin{array}{ccccccc} \longrightarrow C^{q-1}(\overline{K}, A) & \xrightarrow{\delta} & C^q(\overline{K}, A) & \xrightarrow{\delta} & C^{q+1}(\overline{K}, A) \longrightarrow \\ \downarrow{\scriptstyle \omega^*} & & \downarrow{\scriptstyle \omega^*} & & \downarrow{\scriptstyle \omega^*} \\ \longrightarrow C^{q-1}(K, A) & \xrightarrow{\delta} & C^q(K, A) & \xrightarrow{\delta} & C^{q+1}(K, A) \longrightarrow \end{array} \tag{2.41}$$

and a homomorphism of cohomology groups

$$[\omega^*] : H^q(\overline{K}, A) \to H^q(K, A) \tag{2.42}$$

which has the property

$$[\omega^* \overline{f}] = [\omega^*]\,[\overline{f}] . \tag{2.43}$$

Consider an extension of an abelian group A by a group K (determining a homomorphism $\varphi : K \to \operatorname{Aut} A$ and a cohomology class $[m] \in H^2_\varphi(K,A)$) and another extension of an abelian group $\overline{A}$ by a group $\overline{K}$ (determining a homomorphism $\overline{\varphi} : \overline{K} \to \operatorname{Aut} \overline{A}$ and a cohomology class $[\overline{m}] \in H^2_{\overline{\varphi}}(\overline{K}, \overline{A})$). In Part I (p. 572) it was shown that the existence of a morphism of extensions

$$\begin{array}{ccccccccl} 0 \longrightarrow & A & \longrightarrow & G & \longrightarrow & K & \longrightarrow 1 & & \varphi, [m] \\ & \downarrow{\scriptstyle \lambda} & & \downarrow{\scriptstyle \mu} & & \downarrow{\scriptstyle \nu} & & & \\ 0 \longrightarrow & \overline{A} & \longrightarrow & \overline{G} & \longrightarrow & \overline{K} & \longrightarrow 1 & & \overline{\varphi}, [\overline{m}] \end{array} \tag{2.44}$$

implies the following two relations:

$$\forall\, a \in A , \quad \lambda((\varphi\alpha)\, a) = (\overline{\varphi}\nu\alpha)\,(a) \tag{2.45}$$

and

$$[\lambda_*]\,[m] = [\nu^*]\,[\overline{m}] . \tag{2.46}$$

Given representatives of the cosets of A in G and of $\overline{A}$ in $\overline{G}$, respectively, the homomorphism μ is then characterized by

$$\forall\, a \in A , \quad \forall\, \alpha \in K , \quad \mu(a, \alpha) = (\lambda a + u(\alpha), \nu\alpha) . \tag{2.47}$$

Thus there is a one-to-one correspondence between homomorphisms $\mu : G \to \overline{G}$ and elements u of $C^1_{\overline{\varphi}\nu}(K, \overline{A})$. Conversely, if (2.45) and (2.46) are fulfilled, then a diagram (p. 570)

$$\begin{array}{ccccccccc} 0 & \longrightarrow & A & \longrightarrow & G & \longrightarrow & K & \longrightarrow & 1 \quad \varphi, [m] \\ & & \downarrow{\scriptstyle\lambda} & & & & \downarrow{\scriptstyle\nu} & & \\ 0 & \longrightarrow & \overline{A} & \longrightarrow & \overline{G} & \longrightarrow & \overline{K} & \longrightarrow & 1 \quad \overline{\varphi}, [\overline{m}] \end{array} \tag{2.48}$$

may be completed into a morphism (2.44) by defining μ through (2.47).

3. Space Groups as Groups of Operators

A space groups G operates on Euclidean n-space $\mathscr{E}$ as a subgroup of the Euclidean group E. Later on we shall be compelled to utilize more economic imbeddings of G (into subgroups of E). But everything is based (implicitly sometimes) on the properties of the Euclidean group. We therefore list here some of its properties in an order that is convenient for their demonstration.

Let T be a n-dimensional real vector space and $F : T \rightarrowtail R$ a definite quadratic form on T. A space $\mathscr{E}$ on which the abelian group T operates faithfully and transitively is called a Euclidean n-space.

The elements of T are called translations, and we shall write

$$t(x) = x + t \in \mathscr{E} \quad x \in \mathscr{E}, \quad t \in T. \tag{3.1}$$

Note that a non-zero translation has no fixed point.

To the quadratic form F on T we associate a distance d on $\mathscr{E}$ by defining

$$d(x, y) = F(x - y). \tag{3.2}$$

The group $O(T)$ of automorphisms of T that leave the quadratic form F invariant is called the orthogonal group of T.

The affine bijections g of $\mathscr{E}$ that leave the distance on $\mathscr{E}$ invariant:

$$d(gx, gy) = d(x, y) \tag{3.3}$$

are called isometries of $\mathscr{E}$. They form a group E, called the Euclidean group.

The abelian group T is of course a subgroup of E.

For any $p \in \mathscr{E}$, the set

$$E_p = \{g \in E \mid gp = p\}$$

is also a subgroup of E, called the isotropy subgroup of E at p. These two subgroups have the following property

$$\forall\, p \in \mathscr{E}, \quad T \cap E_p = 1 \in E.$$

Furthermore, for any $p \in \mathscr{E}$ and $g \in E$, there are unique elements $t \in T$ and $\alpha_p \in E_p$ such that

$$g = t\alpha_p. \tag{3.4}$$

The conjugate tE_pt^{-1} of any isotropy subgroup E_p is an isotropy subgroup:

$$tE_pt^{-1} = E_{t(p)} \tag{3.5}$$

whereas the abelian subgroup T is a normal subgroup of E:

$$gTg^{-1} = T .$$

To each $g \in E$ there corresponds a unique automorphism $\sigma' g \in GL(T)$ of T such that

$$\forall\, t \in T , \quad \forall\, x \in \mathscr{E} , \quad g(x + t) = g(x) + (\sigma' g)\, t . \tag{3.6}$$

Then

$$(\sigma' g)\, t = gtg^{-1} . \tag{3.6'}$$

From this it is easily deduced that the isometries of $\mathscr{E}$ and the automorphisms of T are related in the following manner

$$gx - gy = (\sigma' g)(x - y) . \tag{3.7}$$

Hence

$$\sigma' g \in O(T) \subset GL(T) .$$

The mapping $\sigma' : E \to O(T)$ is a homomorphism and

$$\ker \sigma' = T .$$

We thus have an exact sequence

$$0 \longrightarrow T \xrightarrow{(\varkappa')} E \xrightarrow{\sigma'} O(T) \longrightarrow 1 \tag{3.8}$$

where $\varkappa'$ is the injection of the subgroup T into E. Mappings denoting injections of subgroups will be placed between parentheses, when appearing in a diagram; in formulas they will generally be omitted. The mapping $\varphi' : O(T) \to GL(T)$ too is an injection of a subgroup. The group $O(T)$ operates, by definition, faithfully on T; thus T is a maximal abelian subgroup of E.

For $p \in \mathscr{E}$, the mapping $\Phi_p : \mathscr{E} \rightarrowtail T$ defined by

$$\Phi_p x = x - p \tag{3.9}$$

is a bijection that associates to each point $x \in \mathscr{E}$ the vector $t = x - p \in T$. (t is uniquely defined by $x = p + t = t(p)$.) Then

$$\Phi_p^{-1}(t) = p + t = t(p) . \tag{3.10}$$

This bijection permits to identify T and $\mathscr{E}$ and to give $\mathscr{E}$ (in a non-canonical way) the structure of a vector space by choice of the point p as origin in $\mathscr{E}$. The bijection Φ_p induces an isomorphism $\varphi_p : E_p \to O(T)$ defined by

$$\forall\, a_p \in E_p , \quad \forall\, x \in \mathscr{E} , \quad (\varphi_p \alpha_p)\,(\Phi_p x) = \Phi_p(\alpha_p x) . \tag{3.11}$$

It can be seen that φ_p is the restriction of σ' to $E_p \subset E$. We thus have the following diagram

$$\begin{array}{ccccccccc} & & & & E_p & & & & \\ & & & {\scriptstyle (\iota_p)} \swarrow & & \searrow {\scriptstyle \varphi_p} & & & \\ 0 & \longrightarrow & T & \xrightarrow[(\varkappa')]{} & E & \xrightarrow[\sigma']{} & O(T) & \longrightarrow & 1 \end{array} \tag{3.12}$$

with ι_p the injection of the subgroup E_p into E. The mapping $r_p : O(T) \to E$ defined by

$$r_p = \iota_p \varphi_p^{-1} \tag{3.13}$$

then is a monomorphism having the following property

$$\sigma' r_p = 1_{O(T)} . \tag{3.14}$$

A mapping r_p satisfying relation (3.14) is called a section. We have just seen that each choice of an origin gives rise to a monomorphic section r_p. This shows also that the extension (3.12) splits.

The image of the section r_p – which is a set of representatives of the cosets of T in E – is the isotropy subgroup E_p of E. Thus there exists, for any $\alpha_p \in E_p$, a unique $\alpha \in O(T)$ such that

$$\alpha_p = r_p \alpha . \tag{3.15}$$

By means of the section r_p the group E is presented as semidirect product of T by $O(T)$. We shall show, for the case of a definite quadratic form F, that these sections realise exactly all presentations of E as semidirect product of T by $O(T)$.

To do this, we shall apply here (2.20) and thus need the notion of continuity. We choose in E a topology such that $O(T)$ is compact in the quotient topology. Then σ' is an open and continuous epimorphism. The isomorphism φ_p then is a homeomorphism, and r_p is by construction continuous. (In corollary 5.5.1 we shall see that the continuity requirement may be replaced by other, often more convenient ones.)

Proposition 3.1. *A continuous section r is a monomorphism if and only if* $\operatorname{Im} r$ *is an isotropy subgroup of E.*

Proof. The sufficiency has already been proved; we now prove the necessity. Let then r be a monomorphism $O(T) \to E$. According to (3.4) there exists a unique $f(\alpha) \in T$ such that

$$r\alpha = f(\alpha)\, \alpha_p$$

and according to (3.15) we have then

$$r\alpha = f(\alpha)\, r_p \alpha$$

where r_p is a monomorphism. Two continuous sections, r and r_p, which are monomorphisms, differ by a continuous 1-cocycle. But the orthogonal group of a definite quadratic form is compact so that relation (2.20) holds. Thus $H_c^1(O(T), T) = 0$ and a continuous 1-cocycle is a continuous 1-coboundary. This means that there is an element $t \in T$ such that for any $\alpha \in O(T)$

$$f(\alpha) = (\delta t)\,\alpha = t(\alpha t)^{-1}\,.$$

(Here it proves convenient to use the multiplicative notation for the elements of T.) Then using (3.5), we find

$$\begin{aligned} r\alpha = f(\alpha)\, r_p\alpha = t(\alpha t)^{-1}\, r_p\alpha &= t(r_p\alpha)^{-1}\, t^{-1}(r_p\alpha)(r_p\alpha)^{-1} \\ &= t(r_p\alpha)\, t^{-1} = r_{t(p)}\alpha \in E_{t(p)}\,. \end{aligned}$$

Thus in all presentations of E as semi-direct product $r\alpha$ is an operation that has fixed point (for all $\alpha \in O(T)$).

We are now prepared to investigate the operation of a space group G on Euclidean n-space $\mathscr{E}$. Let $g \in G$. As element of an extension of the free abelian group U of rank n by the point group K the element g may be written (after the choice of a fixed section $r: K \rightarrowtail G$) uniquely as

$$\forall\, a \in U\,, \quad \forall\, \alpha \in K\,, \quad g = a r\alpha = (a, \alpha)\,. \tag{3.16}$$

Let μ' be an imbedding of G into the Euclidean groups E. (The existence of the imbedding is ensured by the Zassenhaus imbedding theorem [13] or by Proposition 5 of Part I.) Then we have, for a suitably chosen quadratic map $F: T \to R$, the following diagram

$$\begin{array}{ccccccccc} 0 & \longrightarrow & U & \xrightarrow{(\varkappa)} & G & \xrightarrow{\sigma} & K & \longrightarrow & 1 \\ & & \downarrow{\scriptstyle(\lambda)} & & \downarrow{\scriptstyle(\mu')} & & \downarrow{\scriptstyle(\nu)} & & \\ 0 & \longrightarrow & T & \xrightarrow[(\varkappa')]{} & E & \xrightarrow[\sigma']{} & O(T) & \longrightarrow & 1 \end{array} \tag{3.17}$$

and according to (2.47)

$$\mu'(a, \alpha) = \mu'(a \cdot r\alpha) = a \cdot u(\alpha) \cdot r_p\alpha = (a + u(\alpha), \alpha)\,. \tag{3.18}$$

By definition, the element $g = a \cdot r\alpha \in G$ operates on the Euclidean space $\mathscr{E}$ as element $\mu' g$ of the Euclidean group E. Thus $\forall\, x \in \mathscr{E}$:

$$g \circ x = (\mu' g)\, x = (a \cdot u(\alpha) \cdot r_p\alpha)\, x = (r_p\alpha)\, x + u(\alpha) + a \in \mathscr{E}\,. \tag{3.19}$$

We recall that here $r_p\alpha$ is a (finite) orthogonal transformation with fixed point $p \in \mathscr{E}$ and $a + u(\alpha) = t(\alpha)$ is a real translation, called non-primitive translation in contradistinction to the elements of $\operatorname{Im}\lambda$ which are called primitive translations. Applying the mapping Φ_p to (3.19) we get according to (3.11)

$$\begin{aligned} \Phi_p(g \circ x) &= \Phi_p[(r_p\alpha)\, x] + u(\alpha) + a = (\varphi_p r_p\alpha)\,(\Phi_p x) + u(\alpha) + a \\ &= (\alpha)\,(\Phi_p x) + u(\alpha) + a \in E\,. \end{aligned} \tag{3.19'}$$

The traditional notation ([11], [3]) for the element g is:

$$g \circ x = \{\alpha \,|\, t(\alpha)\} \circ x\,. \tag{3.20}$$

Thus α is an orthogonal transformation — $r_p \alpha$ — and $t(\alpha)$ is a non-primitive translation. When g is presented as element (a, α) of an extension of U by K, then (o, α) is generally not an orthogonal transformation, but denotes (after imbedding into the Euclidean group E) an orthogonal transformation $r_p \alpha$ followed by a non-primitive translation $u(\alpha)$. The element (a, ε) corresponds of course to a primitive translation.

Obviously it is sufficient to study the non-primitive translations $u(K)$ associated with the (abstract crystallographic) point group K. The cochain $u \in C^1(K, T)$ will be called a system of non-primitive translations for the space group G.

The study of space groups as group of transformations of Euclidean n-space is the study of the different non-equivalent ways in which systems of non-primitive translations can be associated with the elements of a point group K.

Let us remark that, after having clarified the situation of G as subgroup $\mu' G$ of the Euclidean group E, it will be sufficient to imbed G into subgroup X of E that is a semi-direct product and contains the image of μ':

$$\mathrm{Im}\mu' \subset X \subset E \,, \quad X \text{ semi-direct} \,. \tag{3.21}$$

We shall discuss two subgroups of E that fulfill these conditions.

4. Systems of Non-Primitive Translations

Henceforth we choose the same fixed basis in the free abelian group U and the real vector space T, and thus deal with the isomorphic images Z^n, R^n, $O(n, R)$, $GL(n, R)$ of U, T, $O(T)$ and $GL(T)$ respectively. Note that here $O(n, R)$ is not necessarily a group of orthogonal matrices. We imbed Z^n into R^n always by the natural injection $\iota : Z^n \to R^n$ that applies Z^n onto the integer n-tuples of R^n; thus ιZ^n generates the real vector space R^n.

Let now a n-dimensional space group G be given by a short exact sequence (4.1). Let $\varphi : K \to GL(n, Z)$ be a monomorphism, $r : K \to G$ a section and $m \in Z^2_\varphi(K, Z^n)$ the corresponding factor set:

$$0 \longrightarrow Z^n \xrightarrow[\varkappa]{} G \xrightarrow[\sigma]{} K \longrightarrow 1 \qquad \varphi, m, r \,. \tag{4.1}$$

We shall imbed G into a group M satisfying conditions (3.21). This group is exactly the group that we called M^n in the proof of Proposition 5 of Part I. First we define the action $(\bar\varphi : K \to GL(n, R))$ of K on R^n by putting

$$\forall a \in Z^n \,, \quad \forall\, \alpha \in K \,, \quad \iota[(\varphi\alpha)\, a] = (\bar\varphi\alpha)\,(\iota a) \tag{4.2}$$

and extend this definition from ιZ^n to R^n by linearity. The relation (4.2) means now that ι is a K-module homomorphism. We shall, for simplicity, often omit φ and $\bar\varphi$ and thus write, instead of (4.2):

$$\iota(\alpha a) = \alpha(\iota a) \,. \tag{4.3}$$

Now, by (2.11), $H^q(K, R^n) = 0$ for $q > 0$, so that any extension M of R^n by K splits. We choose to present M as semi-direct product, by which we mean that the section $\bar{r} : K \to M$ is a monomorphism and that the corresponding factor system $\bar{m}$ is the trivial one:

$$\bar{m} = 0 \in Z^2(K, R^n) .$$

To construct a morphism between the two extensions, we have to impose the following relation (according to (2.46))

$$\iota_* m = \delta u \tag{4.4}$$

or

$$\iota m(\alpha, \beta) = u(\alpha) + \alpha u(\beta) - u(\alpha\beta) \tag{4.5}$$

with $u \in C^1(K, R^n)$. Then there exists a homomorphism $\mu : G \to M$ such that the following diagram is commutative

$$\begin{array}{ccccccccc} 0 & \longrightarrow & Z^n & \xrightarrow{\varkappa} & G & \xrightarrow{\sigma} & K & \longrightarrow & 1 \qquad \varphi, m, r \\ & & {\scriptstyle(\iota)}\downarrow & & {\scriptstyle(\mu)}\downarrow & & \| & & \\ 0 & \longrightarrow & R^n & \xrightarrow[\bar{\varkappa}]{} & M & \xrightarrow[\bar{\sigma}]{} & K & \longrightarrow & 1 \qquad \bar{\varphi}, 0, \bar{r} . \end{array} \tag{4.6}$$

The homomorphism μ is given by

$$\forall\ \alpha \in K , \quad \mu r \alpha = \bar{\varkappa} u(\alpha) \cdot \bar{r} \alpha . \tag{4.7}$$

Owing to the Short Five Lemma ([8], p. 13), μ is in fact a monomorphism.

The group M is a subgroup of the Euclidean group E (cf. Proposition 5 of Part I) because the following morphism of extensions can be constructed

$$\begin{array}{ccccccccc} 0 & \longrightarrow & R^n & \xrightarrow{\bar{\varkappa}'} & M & \xrightarrow{\bar{\sigma}'} & K & \longrightarrow & 1 \qquad (\bar{\varphi}, 0, \bar{r}) \\ & & \| & & {\scriptstyle\bar{\mu}}\downarrow & & \downarrow{\scriptstyle\nu} & & \\ 0 & \longrightarrow & R^n & \xrightarrow[\varkappa']{} & E & \xrightarrow[\sigma']{} & O(n, R) & \longrightarrow & 1 \qquad (\varphi', 0, r_p) \end{array} \tag{4.8}$$

and the following two relations hold

$$\forall\ \alpha \in K , \quad \forall\ \bar{a} \in R^n , \quad (\bar{\varphi} \alpha)\, \bar{a} = \varphi'(\nu \alpha)\, \bar{a} , \tag{4.9}$$

$$\bar{\mu} \bar{r} = r_p \nu \tag{4.10}$$

i.e. $\bar{r}$ is a restriction of the monomorphic section $r_p : O(n, R) \to E$ to $K \subset O(n, R)$. Then, putting $\mu' = \bar{\mu}\mu$,

$$\mu' r \alpha = \varkappa' u(\alpha) \cdot r_p \nu \alpha$$

and $u(\alpha)$ is clearly a non-primitive translation. We may now define the action of an element $g \in G$ on a point $x \in \mathscr{E}$ by

$$g \circ x = (\mu' g)\, x . \tag{4.11}$$

As defined by (4.4) or equivalently by (4.7), a system of non-primitive translations is not uniquely determined, since no fewer than three arbitrary choices occur. In the latter formula these are the choices of the cochain u that determines the imbedding μ and the choices of the sections r and $\bar{r}$ (which latter however we want to remain a monomorphism). We shall now eliminate the arbitrariness introduced by these choices. Our discussion will be based on the following short exact sequence of cochain complexes

$$\begin{array}{ccccccccc} & & 0 & & 0 & & 0 & & \\ & & \downarrow & & \downarrow & & \downarrow & & \\ 0 & \longrightarrow & Z^n & \xrightarrow{\iota} & R^n & \xrightarrow{\pi} & R^n/Z^n & \longrightarrow & 0 \\ & & \delta\downarrow & & \delta\downarrow & & \delta\downarrow & & \\ 0 & \longrightarrow & C^1(K, Z^n) & \xrightarrow{\iota_*} & C^1(K, R^n) & \xrightarrow{\pi_*} & C^1(K, R^n/Z^n) & \longrightarrow & 0 \\ & & \delta\downarrow & & \delta\downarrow & & \delta\downarrow & & \\ 0 & \longrightarrow & C^2(K, Z^n) & \xrightarrow{\iota_*} & C^2(K, R^n) & \xrightarrow{\pi_*} & C^2(K, R^n/Z^n) & \longrightarrow & 0 \\ & & \delta\downarrow & & \delta\downarrow & & \delta\downarrow & & \end{array} \quad (4.12)$$

Here π is the canonical projection $\pi: R^n \to R^n/Z^n$ and K operates on R^n/Z^n according to

$$\forall\, \bar{a} \in R^n\,, \quad \forall\, \alpha \in K\,, \quad \pi[(\bar{\varphi}\alpha)\,\bar{a}] = (\hat{\varphi}\alpha)\,(\pi\bar{a})\,. \qquad (4.13)$$

Again $\hat{\varphi}$ (and $\bar{\varphi}$) will be omitted frequently so that, instead of (4.13) we write

$$\pi(\alpha\bar{a}) = \alpha(\pi\bar{a})\,.$$

Thus π is a K-module homomorphism.

According to (4.4) the 1-cochain u is characterized by

$$\iota_* m = \delta u\,, \quad m \in Z^2(K, Z^n)\,, \quad u \in C^1(K, R^n)\,. \qquad (4.14)$$

Any other choice of a 1-cochain u' is permitted provided that

$$\iota_* m = \delta u'\,.$$

Hence

$$\delta(u' - u) = 0\,.$$

As a consequence of (2.11)

$$u' - u \in Z^1(K, R^n) = B^1(K, R^n)$$

so that $\exists\, d' \in R^n$:

$$u' = u + \delta d'\,.$$

Let us now choose another section $r_1: K \rightarrowtail G$. This leads to another choice of a 2-cocycle $m' \in Z^2(K, Z^n)$ such that

$$m' - m \in B^2(K, Z^n)\,.$$

Hence $\exists\, c \in C^1(K, Z^n)$

$$m' = m + \delta c\,.$$

Then

$$\iota_* m' = \iota_*(m + \delta c) = \delta u' + \delta \iota_* c = \delta(u + \delta d' + \iota_* c) = \delta u'' .$$

Finally let us choose a new monomorphic section $\bar{r}_1 : K \to M$. Such a choice leaves the factor sets $K \times K \to R^n$ unchanged, viz. identically equal to zero. Since $H^1(K, R^n) = 0$ any two monomorphic sections differ by a 1-coboundary so that $\exists\, d'' \in R^n$

$$\forall\, \alpha \in K \quad \bar{r}_1 \alpha = [(\delta d'')(\alpha)]\, \bar{r} \alpha$$

and this change introduces but another zero, $\delta\delta d''$, into the expression of $\iota_* m'$:

$$\iota_* m' = \delta(u + \delta d' + \delta d'' + \iota_* c) = \delta \bar{u} . \tag{4.15}$$

Thus the most general system $\bar{u}$ of non-primitive translations differs from an arbitrary one by a 1-coboundary $\delta(d' + d'') \in B^1(K, R^n)$ (a "non-primitive coboundary") and a 1-cochain $\iota_* c$ (a "primitive cochain"):

$$\bar{u} = u + \delta d + \iota_* c . \tag{4.16}$$

Note that both the change from u to u' and the change from $\bar{r}$ to $\bar{r}_1$ correspond to a change of origin for the group M (and the group E). To get rid of the primitive cochains we project by the induced epimorphism $\pi_* : C^1(K, R^n) \to C^1(K, R^n/Z^n)$ and find

$$\pi_* \bar{u} = \pi_* u + \pi_* \delta d , \tag{4.17}$$

or

$$\pi_* \bar{u} \equiv \pi_* u \quad (\text{mod } B^1(K, R^n/Z^n)) \tag{4.18}$$

where from (4.14) one finds

$$\pi_* u \in Z^1(K, R^n/Z^n) . \tag{4.19}$$

Thus the 1-cohomology class

$$\sigma = [\pi_* \bar{u}] = [\pi_* u] \in H^1(K, R^n/Z^n) \tag{4.20}$$

of an arbitrary system u of non-primitive translations does not depend on the choice of an origin for M (and is also free from the arbitrariness of the choice of $r : K \rightarrowtail G$).

Let us summarize what we have found so far.

Proposition 4.1. *The element $u \in C^1(K, R^n)$ is a system of non-primitive translations for a space group if and only if*

$$\pi_* u \in Z^1(K, R^n/Z^n) . \tag{4.21}$$

Proof. The necessity has been proved (cf. 4.19). The sufficiency is easily verified. Relation (4.21) gives indeed

$$0 = \delta(\pi_* u) = \pi_*(\delta u) .$$

Hence $\exists\, m \in Z^2(K, Z^n)$:

$$\delta u = \iota_* m .$$

Since furthermore (4.3) remains true, the conditions are fulfilled for the construction of a monomorphism $\mu : G \to M$ such that (4.7) holds.

Note that (4.21) is nothing but a form of the Frobenius congruences:

$$\forall\, \alpha, \beta \in K\,, \quad u(\alpha\beta) \equiv u(\alpha) + \alpha u(\beta) \quad (\mathrm{mod}\, Z^n)\,. \tag{4.22}$$

ZASSENHAUS [13] calls systems $u(K)$ that satisfy (4.21) „zulässige Vektorsysteme". Our systems of non-primitive translations are then „zulässige Vektorsysteme".

Proposition 4.2. *Any system of non-primitive translations for a space group $G = (K, Z^n, \varphi, m)$ determines the same element of the first cohomology group $H^1(K, R^n/Z^n)$.*

Such systems are called equivalent systems. Thus two systems u and $\overline{u}$ are equivalent

$$u \sim \overline{u} \quad \text{if} \quad [\pi_* u] = [\pi_* \overline{u}]\,. \tag{4.23}$$

Condition (4.23) means $\exists\, f \in R^n$:

$$\overline{u} \equiv u + \delta f \quad (\mathrm{mod}\, C^1(K, Z^n))$$

or

$$\forall\, \alpha \in K\,, \quad \overline{u}(\alpha) \equiv u(\alpha) + (\varepsilon - \alpha) f \quad (\mathrm{mod}\, Z^n)\,. \tag{4.24}$$

Systems u fulfilling condition (4.24) are called „stark äquivalent" in reference [13].

So far, we have shown that the relations

$$\sigma = [\pi_* u]\,, \qquad \delta u = \iota_* m$$

determine a mapping $\Delta : H^2(K, Z^n) \to H^1(K, R^n/Z^n)$ such that for any $[m] \in H^2(K, Z^n)$

$$\Delta[m] = [\pi_* u] = \sigma \in H^1(K, R^n/Z^n)\,. \tag{4.25}$$

To show that this mapping is an isomorphism, we first prove the following proposition.

Proposition 4.3. *Given the K-modules R^n and R^n/Z^n* we have

$$H^q(K, R^n/Z^n) \cong H^{q+1}(K, Z^n) \qquad q > 0\,. \tag{4.26}$$

Proof. Consider the exact sequence of K-modules

$$0 \longrightarrow Z^n \xrightarrow[\iota]{} R^n \xrightarrow[\pi]{} R^n/Z^n \longrightarrow 0$$

giving rise to the long exact sequence

$$\longrightarrow H^q(K, R^n) \xrightarrow{[\pi_*]} H^q(K, R^n/Z^n) \xrightarrow{\partial_*} H^{q+1}(K, Z^n) \xrightarrow{[\iota_*]} H^{q+1}(K, R^n) \longrightarrow$$

and take into account that, according to (2.11),

$$H^q(K, R^n) = 0 \quad \text{for} \quad q > 0\,.$$

Proposition 4.4. *The mapping $\Delta : H^2(K, Z^n) \to H^1(K, R^n/Z^n)$, defined by $\Delta[m] = [\pi_* u] \in H^1(K, R^n/Z^n)$ and $\delta u = \iota_* m$, is an isomorphism, and*

$$\Delta = \partial_*^{-1}\,. \tag{4.27}$$

Proof. We first show that

$$\partial_* \Delta = I \tag{4.28}$$

where I is the identity mapping on $H^2(K, Z^n)$. We have to calculate $[a]$ given by

$$\partial_* \Delta [m] = \partial_* [\pi_* u] = [a] . \tag{4.29}$$

But $[a]$ is given, according to (2.36), by the pair of relations

$$\pi_* u = \pi_* b , \quad \delta b = \iota_* a \tag{4.30}$$

and $[a]$ is independent of the particular choice of the elements b and a that fulfill these relations. Therefore we may choose $b = u$. Then

$$\delta b = \delta u = \iota_* m = \iota_* a \tag{4.31}$$

and

$$m = a . \tag{4.32}$$

Thus (4.28) is proved. The connecting homomorphism ∂_* is an isomorphism, according to the preceding Proposition. Then

$$\Delta = (\partial_*^{-1} \partial_*) \Delta = \partial_*^{-1} (\partial_* \Delta) = \partial_*^{-1}$$

and Δ is an isomorphism, the inverse of the connecting isomorphism ∂_*.

In Part I we have seen that two isomorphic n-dimensional space groups G and $\overline{G}$ determine the same arithmetic crystal class and that therefore one may assume, without any loss of generality, that they determine the same (arithmetic crystallographic) point group $\varphi(K)$. Hence G and $\overline{G}$ determine elements $[m]$ and $[\overline{m}]$ of the second cohomology group $H^2(K, Z^n)$, and generally $[m] \neq [\overline{m}]$. The necessary and sufficient condition for G and $\overline{G}$ to be isomorphic was shown to be (cf. Part I, Proposition 7) the existence of isomorphisms $\chi : Z^n \to Z^n$ and $\omega : K \to K$ such that

$$\forall\, a \in Z^n , \quad \forall\, \alpha \in K , \quad \chi[(\varphi\alpha)\, a] = (\varphi\omega\alpha)\,(\chi a) \tag{4.33}$$

and

$$[\chi_*]\,[m] = [\omega^*]\,[\overline{m}] \in H^2(K, Z^n) . \tag{4.34}$$

Note that by (4.33) χ determines ω:

$$\forall\, \alpha \in K , \quad \varphi\omega\alpha = \chi(\varphi\alpha)\,\chi^{-1} \tag{4.35}$$

and this shows that χ is an element of the normaliser N of $\varphi(K)$ in $GL(n, Z)$. Relation (4.34) may be translated into a relation between equivalence classes of non-primitive translations.

Proposition 4.5. *Two n-dimensional space groups G and $\overline{G}$ are isomorphic if and only if it possible to choose systems of non-primitive translations u and $\overline{u}$ for G and $\overline{G}$ respectively, an automorphism χ of Z^n and an automorphism ω of K such that for any $a \in Z^n$ and any $\alpha \in K$ one has*

$$\chi[(\varphi\alpha)\, a] = (\varphi\omega\alpha)\,(\chi a) , \quad \chi u(\alpha) = \overline{u}(\omega\alpha) . \tag{4.36}$$

Here the automorphism χ has been extended by linearity to R^n.

Proof. We only have to show that (4.34) is equivalent to

$$[\chi_*]\,\sigma = [\omega^*]\,\bar{\sigma} \tag{4.37}$$

where σ and $\bar{\sigma}$ are the equivalence classes of u and $\bar{u}$ respectively. The homomorphism $[\chi_*]: H^q(K, R^n/Z^n) \to H^q(K, R^n/Z^n)$ is induced by the automorphism χ of R^n/Z^n defined by

$$\begin{array}{ccccc} Z^n & \xrightarrow{\iota} & R^n & \xrightarrow{\pi} & R^n/Z^n \\ \chi\big\downarrow & & \chi\big\downarrow & & \big\downarrow\chi \\ Z^n & \xrightarrow[\iota]{} & R^n & \xrightarrow[\pi]{} & R^n/Z^n\,. \end{array} \tag{4.38}$$

The equivalence between (4.34) and (4.37) is proved by straightforward diagram chasing. To the particular choice of u and $\bar{u}$ satisfying $\chi u(\alpha) = \bar{u}(\omega\alpha)$ corresponds the particular choice of m and $\bar{m}$ of Proposition 7 of Part I satisfying $\chi m(\alpha, \beta) = \bar{m}(\omega\alpha, \omega\beta)$. Note also that condition (4.37) means the same as

$$\forall\, f \in R^n\,, \quad \forall\, \alpha \in K\,, \quad \chi u(\alpha) \equiv \bar{u}(\omega\alpha) + (\varepsilon - \omega\alpha)\, f \quad (\text{mod}\, Z^n)$$

or

$$\bar{u}(\alpha) \equiv \chi u(\omega^{-1}\alpha) + (\alpha - \varepsilon)\, f \quad (\text{mod}\, Z^n)$$

which is Zassenhaus' „gewöhnliche Aequivalenz“ [13].

5. Some Properties of Non-Primitive Translations

The properties of non-primitive translations concern mainly the limitations imposed on the order of these.

Proposition 5.1. *Let G be a space group with point group K of order k. Then it is possible to choose the origin for G in such a way that k-times a system of non-primitive translations is primitive.*

Proof. A system of non-primitive translations u obeys to (4.4): $\iota_* m = \delta_1 u$ with $u \in C^1(K, R^n)$. Furthermore, according to (2.8)

$$s_2\delta_1 u + \delta_0 s_1 u = s_2\delta_1 u + k\,\delta_0 \frac{1}{k}\, s_1 u = ku\,. \tag{5.1}$$

Since R^n is divisible, we may introduce the centre of gravity $\langle u \rangle$ of the system of non-primitive translations u by

$$\langle u \rangle = \frac{1}{k}\, s_1 u \in R^n\,. \tag{5.2}$$

Then

$$\iota_* s_2 m = s_2 \iota_* m = s_2\delta_1 u = k(u - \delta_0\,\langle u \rangle) = k\bar{u}\,. \tag{5.3}$$

Clearly $\overline{u}$ is a system of non-primitive translations and the change of origin is that from an arbitrary one to the centre of gravity $\langle u\rangle$. Note that

$$\overline{u} - \delta_0 \langle \overline{u} \rangle = \overline{u} - \frac{1}{k} \delta_0 N \langle u \rangle = \overline{u} \tag{5.4}$$

where the norm homomorphism N is defined by (2.15).

Corollary 5.1.1. *Suppose that G is a split extension of Z^n by K presented as semi-direct product. Then by a suitable change of origin it is possible to eliminate all non-primitive translations.*

Proof. By hypothesis $m = 0$ so that $k\overline{u} = 0$; hence $\overline{u} = 0$ (since R^n is torsion-free).

Corollary 5.1.2. *For a given $\alpha \in K$ with period k_α we have*

$$k_\alpha \overline{u}(\alpha) \equiv 0 \quad (\mathrm{mod}\, Z^n) . \tag{5.5}$$

Proof. Proceed as in Proposition 5.1., but introduce the centre of gravity $\langle u \rangle_\alpha$ only relative to the cyclic group $\{\alpha\}$ generated by α.

We recall that

$$H^0(K, R^n) = \{x \in R^n \,|\, \alpha x = x \,,\ \forall\, \alpha \in K\} \equiv A^K . \tag{5.6}$$

A^K is a RK-submodule of R^n and, according to Maschke's theorem ([14], [6, p. 156], [10, p. 253]) there exists a RK-submodule $A' \subset R^n$ such that

$$R^n = A^K + A' . \tag{5.7}$$

This induces a corresponding decomposition of the RK-modules $C^q(K, R^n)$

$$C^q(K, R^n) = C^q(K, A^K) + C^q(K, A') . \tag{5.8}$$

Thus any q-cochain $f \in C^q(K, A)$ may be decomposed

$$f = f^K + f' \tag{5.9}$$

with

$$f^K \in C^q(K, A^K) \qquad \alpha f^K \in C^q(K, A^K) \tag{5.10}$$

and

$$f' \in C^q(K, A') \qquad \alpha f' \in C^q(K, A') . \tag{5.11}$$

It follows that

$$N_q f' \in C^q(K, A^K) \cap C^q(K, A') = 0 \tag{5.12}$$

where $N_q : C^q(K, A) \to C^q(K, A)$ is defined by

$$(N_q f)(\alpha_1, \ldots, \alpha_q) = N[f(\alpha_1, \ldots, \alpha_q)] \tag{5.13}$$

and N is defined by (2.15). Thus

$$N_q f = N_q f^K + N_q f' = k f^K . \tag{5.14}$$

For the following it will be sufficient to limit ourselves to 1-cochains.

Proposition 5.2. Seitz' Theorem. *Let u be a system of non-primitive translations for a space group, then*

$$\forall\, \alpha \in K , \quad k u^K(\alpha) \equiv 0 \quad (\mathrm{mod}\, Z^n) . \tag{5.15}$$

Proof. According to (5.14) we have

$$ku^K(\alpha) = Nu(\alpha)\,. \tag{5.16}$$

But from $\iota_* m = \delta u$ we have

$$\sum_\beta \iota m(\beta, \alpha) = \sum_\beta [u(\beta) + \beta u(\alpha) - u(\beta\alpha)] = Nu(\alpha) \tag{5.17}$$

showing that $Nu(\alpha) \equiv 0 \pmod{Z^n}$.

Corollary 5.2.1. *For a given $\alpha \in K$ with period k_α we have*

$$k_\alpha u^K(\alpha) \equiv 0 \quad (\mathrm{mod}\, Z^n)\,. \tag{5.18}$$

The above corollary may be found in [3] with a wrong proof. (The operator $\varepsilon + \cdots + \alpha^{k_\alpha - 1}$ does not necessarily equal 0.)

Let H be a finite normal subgroup of finite order h of a (not necessarily finite) group K and A a K-module. Define the homomorphism $N_H : A \to A$ by

$$\forall\, a \in A\,, \quad N_H a = \sum_{\beta \in H} \beta a\,. \tag{5.19}$$

N_H is a K-module homomorphism since

$$N_H(\alpha a) = \sum_{\beta \in H} \beta\alpha a = \sum_{\beta \in H} \alpha\alpha^{-1}\beta\alpha a = \alpha N_H a\,. \tag{5.20}$$

Furthermore N_H induces a homomorphism $N_H^q : H^q(K, A) \to H^q(K, A)$ defined by

$$N_H^q[f^q(\alpha_1, \ldots, \alpha_q)] = [N_H f^q(\alpha_1, \ldots, \alpha^q)]\,. \tag{5.21}$$

Proposition 5.3. *With the above definitions we have*

$$N_H^q = hI \quad q \geqq 0\,, \tag{5.22}$$

I being the identity mapping on $H^q(K, A)$.

Proof. The proof will be by induction on q. For $q = 0$ the theorem is trivially true since $H^0(K, A)$ is the submodule of elements invariant under K. Suppose now that the proposition is true for $q - 1$. Let $\overline{A}$ be the co-induced K-module associated to A and $A' = \overline{A}/A$. Then the following diagram of K-modules

$$\begin{array}{ccccccccc} 0 & \longrightarrow & A & \xrightarrow{\chi} & \overline{A} & \xrightarrow{\pi} & A' & \longrightarrow & 0 \\ & & \downarrow{\scriptstyle N_H} & & \downarrow{\scriptstyle N_H} & & \downarrow{\scriptstyle N_H} & & \\ 0 & \longrightarrow & A & \xrightarrow[\chi]{} & \overline{A} & \xrightarrow[\pi]{} & A' & \longrightarrow & 0 \end{array} \tag{5.23}$$

is commutative and induces the following commutative diagram of cohomology groups:

$$\begin{array}{ccccccc} \longrightarrow & H^{q-1}(K, A') & \xrightarrow{\partial_*} & H^q(K, A) & \longrightarrow & H^q(K, \overline{A}) & \longrightarrow \\ & \downarrow{\scriptstyle N_H^{q-1}} & & \downarrow{\scriptstyle N_H^q} & & \downarrow{\scriptstyle N_H^q} & \\ \longrightarrow & H^{q-1}(K, A') & \xrightarrow[\partial_*]{} & H^q(K, A) & \longrightarrow & H^q(K, \overline{A}) & \longrightarrow\,. \end{array} \tag{5.24}$$

But $H^q(K, \overline{A}) = 0$ since $\overline{A}$ is co-induced, so that the connecting homomorphisms ∂_* are epimorphisms. Thus

$$\forall\, x \in H^q(K, A)\,, \quad \exists\, y \in H^{q-1}(K, A') : \partial_* y = x\,. \tag{5.25}$$

Then

$$N_H^q x = N_H^q \partial_* y = \partial_* N_H^{q-1} y = \partial_* h y = h \partial_* y = h x\,. \tag{5.26}$$

Corollary 5.3.1. *If $N_H a = 0$ for any $a \in A$, then*

$$h H^q(K, A) = 0 \quad q \geqq 0\,. \tag{5.27}$$

Corollary 5.3.2. *Let A be divisible and torsion-free. If $N_H A = 0$ for any $a \in A$, then*

$$H^q(K, A) = 0 \quad q \geqq 0 \tag{5.28}$$

since $H^q(K, A)$ is torsion-free.

Proposition 5.4. *(Generalization of Speiser's theorem.) Let K be a (not necessarily finite) group, Z^n a K-module, and H a finite normal subgroup of K of order h that leaves no non-zero element of Z^n invariant, then for $q \geqq 0$*

$$\left.\begin{aligned} h H^q(K, Z^n) &= 0 \\ h H^q(K, R^n/Z^n) &= 0\,. \end{aligned}\right\} \tag{5.29}$$

Proof. The hypothesis amounts to

$$H^0(H, Z^n) = 0 \tag{5.30}$$

which, since $N_H Z^n \in H^0(H, Z^n)$, implies

$$N_H Z^n = 0\,. \tag{5.31}$$

If the action of K on R^n is defined by way of the natural homomorphism $\iota : Z^n \to R^n$ according to (4.12), and the action of K on R^n/Z^n by (4.13), then we have also

$$N_H R^n/Z^n = 0 \tag{5.32}$$

and application of Corollary 5.3.1. yields the desired result.

Corollary 5.4.1. (Speiser's theorem) [6, p. 229]. *Let G be a space group with point group K. If K has a normal subgroup H of order h that leaves no non-zero vector invariant, it is possible to choose the origin for G in such a way that h-times a system of non-primitive translations is primitive.*

In particular, if K contains the inversion -1_n, then $h = 2$.

Proposition 5.5. *Let K be a group of n-dimensional real matrices containing the inversion -1_n. Then*

$$H^q(K, R^n) = 0 \quad q \geqq 0\,.$$

(The same is true in the complex case.)

Proof. Take for H the group generated by -1_n. It is a finite normal subgroup of K and $N_H R^n = 0$. Furthermore, R^n is divisible and torsion-free.

Corollary 5.5.1. *Any extension of* R^n *by* $GL(n, R)$, $O(n, R)$, *or* $O(n-1,1)$ *– the n-dimensional Lorentz group – is split.*

Note that we had already deduced from (2.20) that $H^q_c(O(n,R), R^n) = 0$ for $q > 0$. Now this result has been extended to $q = 0$ and arbitrary cochains. However, (2.20) also yields

$$H^q_c(SO(n, R), R^n) = 0 \quad q > 0\,, \tag{5.33}$$

a result that cannot be obtained from proposition 5.5. when n is odd.

6. Imbedding of a Space Group into a Symmorphic Space Group

We now choose another group, $\overline{G}$, satisfying conditions (3.21). The group $\overline{G}$ will be the split extension (symmorphic space group) belonging to the arithmetic crystal class $\varphi(K)$.

Proposition 6.1. *Any space group* G *is a subgroup of the split extension* $\overline{G}$ *belonging to the same arithmetic crystal class as* G.

Proof. Consider the diagram

$$\begin{array}{ccccccccc} 0 \to & Z^n & \to & G & \to & K & \to 1 & & \varphi, m \\ & {\scriptstyle k}\downarrow & & & & \| & & & \\ 0 \to & Z^n & \to & \overline{G} & \to & K & \to 1 & & \varphi, 0\,. \end{array} \tag{6.1}$$

The two conditions (2.45) and (2.46) are fulfilled since obviously

$$k\,[(\varphi\alpha)\,a] = (\varphi\alpha)\,(ka) \tag{6.2}$$

and since

$$k_*\,[m] = 0 \tag{6.3}$$

by Corollary 2.1.1. Thus there exists a monomorphism $\tilde{\mu}: G \to \overline{G}$ defined by

$$\tilde{\mu}(a, \alpha) = (ka + v(\alpha), \alpha)\,, \quad v \in C^1(K, Z^n) \tag{6.4}$$

that makes the diagram commutative.

Furthermore, the index of G in $\overline{G}$ is k^n.

If the group K fulfills the conditions of Proposition 5.4, then the mapping k can be replaced by a mapping h.

Since $\overline{G}$ can be presented as semi-direct product and can be imbedded into the Euclidean group E, v is clearly a system of non-primitive translations. The question now arises how this system is related to a system u determined by (4.4).

First we remark that $(1/k)_*\,\iota_*\,v \sim u$ in the sense of (4.23). Here $(1/k)_*: C^q(K, R^n) \to C^q(K, R^n)$ is the mapping induced by $1/k: R^n \to R^n$. The equivalence we want to prove is a simple consequence of $[k_*]\,H^q(K, R^n/Z^n) = 0$. Indeed

$$[k_*]\,[\pi_* u] = 0 = [\pi_*\,\iota_* v]$$

so that

$$[\pi_* u] = \left[\pi_* \left(\frac{1}{k}\right)_* \iota_* v\right] . \tag{6.5}$$

A second remark is that, according to (2.9), $k_* m = \delta_1 s_2 m$, so that $s_2 m$ is a possible choice for the system of non-primitive translations v. As in Section 4, an arbitrary system v may differ from this particular one in three ways. First, another monomorphism $\mu' : G \to \overline{G}$ may be chosen; this would add a 1-cocycle $b' \in Z^1(K, Z^n)$ to v. Second, another 2-cocycle $m' \in [m]$ may be chosen to represent G; this adds a 1-cochain $k_* c$ to v. Third, a term $b'' \in Z^1(K, Z^n)$ may be added, corresponding to the choice of a new monomorphic section $\bar{r}_1 : K \to \overline{G}$. Thus the most general system of non-primitive translations v is given by

$$v = s_2 m + b + k_* c \tag{6.6}$$

with

$$\delta v = k_* (m + \delta c) \tag{6.7}$$

where

$$m \in Z(K, Z^n) , \quad b = b' + b'' \in Z^1(K, Z^n) , \quad c \in C^1(K, Z^n) . \tag{6.8}$$

The difference with (4.16) is that b is not a coboundary. Therefore we shall construct equivalence classes in a slightly different manner from that adopted in Section 4.

Consider the short exact sequence of K-modules

$$0 \longrightarrow Z^n \xrightarrow{k} Z^n \xrightarrow{p} Z^n/kZ^n \longrightarrow 0 \tag{6.9}$$

and the corresponding exact sequence of cochain complexes

$$\begin{array}{ccccccccc}
 & & 0 & & 0 & & 0 & & \\
 & & \downarrow & & \downarrow & & \downarrow & & \\
0 & \longrightarrow & C^1(K, Z^n) & \xrightarrow{k_*} & C^1(K, Z^n) & \xrightarrow{p_*} & C^1(K, Z^n/kZ^n) & \longrightarrow & 0 \\
 & & \downarrow \delta & & \downarrow \delta & & \downarrow \delta & & \\
0 & \longrightarrow & C^2(K, Z^n) & \xrightarrow{k_*} & C^2(K, Z^n) & \xrightarrow{p_*} & C^2(K, Z^n/kZ^n) & \longrightarrow & 0 . \\
 & & \downarrow \delta & & \downarrow \delta & & \downarrow \delta & &
\end{array} \tag{6.10}$$

From (6.6) we deduce

$$p_* v = p_* s_2 m + p_* b \tag{6.11}$$

and

$$p_* \delta v = \delta p_* v = 0 = \delta p_* s_2 m = p_* (\delta_* s_2 m) . \tag{6.12}$$

Thus

$$p_* v , \quad p_* s_2 m \in Z^1(K, Z^n/kZ^n) \tag{6.13}$$

and

$$p_* v \equiv p_* s_2 m \quad (\mathrm{mod}\, p_* Z^1(K, Z^n)) . \tag{6.14}$$

Thus the particular system $s_2 m$ and the most general system v determine the same equivalence class σ modulo $p_* Z^1(K, Z^n)$:

$$\sigma = (p_* s_2 m + p_* Z^1(K, Z^n)) \in Z^1(K, Z^n/kZ^n)/p_* Z^1(K, Z^n) . \qquad (6.15)$$

We want to show that the mapping

$$\Gamma : H^2(K, Z^n) \to Z^1(K, Z^n/kZ^n)/p_* Z^1(K, Z^n) \qquad (6.16)$$

defined by

$$\Gamma[m] = p_* s_2 m + p_* Z^1(K, Z^n) \qquad (6.17)$$

is an isomorphism. We consider the exact sequence

$$Z^1(K, Z^n) \xrightarrow{k_*} Z^1(K, Z^n) \xrightarrow{p_*} Z^1(K, Z^n/kZ^n) \xrightarrow{\partial_*} H^2(K, Z^n) \xrightarrow{[k_*]} H^2(K, Z^n) \qquad (6.18)$$

obtained from (6.10). Since

$$[k_*]\, H^2(K, Z^n) = 0$$

we find that

$$Z^1(K, Z^n/kZ^n)/p_* Z^1(K, Z^n) \cong H^2(K, Z^n) . \qquad (6.19)$$

Let ψ be that isomorphism. Let $c \in Z^1(K, Z^n/kZ^n)$, then

$$\psi(c + p_* Z^1(K, Z^n)) = \partial_* c = [a] \qquad (6.20)$$

and $[a]$ is given, according to (2.36), by the two relations $c = p_* b$ and $\delta b = k_* a$, and is independent of the choice of b. We calculate

$$\psi \Gamma[m] = \psi(p_* s_2 m + p_* Z^1(K, Z^n)) = \partial_* p_* s_2 m = [a] . \qquad (6.21)$$

Now a is given by

$$p_* s_2 m = p_* b , \quad \delta b = k_* a ; \qquad (6.22)$$

choosing $b = s_2 m$ we find, using (2.9)

$$\delta s_2 m = k_* m = k_* a \qquad (6.23)$$

or

$$m = a . \qquad (6.24)$$

Thus

$$\psi \Gamma = I \qquad (6.25)$$

where I is the identity mapping on $H^2(K, Z^n)$. Thus Γ is an isomorphism:

$$\Gamma = \psi^{-1} . \qquad (6.26)$$

Since $p_* B^1(K, Z^n) = B^1(K, Z^n/kZ^n)$ it follows that

$$Z^1(K, Z^n/kZ^n)/p_* Z^1(K, Z^n) \cong H^1(K, Z^n/kZ^n)/[p_*]\, H^1(K, Z^n) .$$

Using (2.34) and the fact that $[k_*]\, H^1(K, Z^n) = 0$, one sees that $[p_*]$ is a monomorphism, so that

$$Z^1(K, Z^n/kZ^n)/p_* Z^1(K, Z^n) \cong H^1(K, Z^n/kZ^n)/H^1(K, Z^n) .$$

7. An Illustration: The two 2-Dimensional Space Groups *pm* and *pg*

(i) Definition of $\varphi(K)$. Let K be the cyclic group of order two generated by the element α. Let e_1 and e_2 constitute a basis of U. This determines an isomorphism $\lambda : U \cong Z^2$ through $\lambda e_1 = \begin{pmatrix}1\\0\end{pmatrix}$ and $\lambda e_2 = \begin{pmatrix}1\\0\end{pmatrix}$. As was done in Chapter 4, we identify λU and U. Define the monomorphism $\varphi : K \to GL(2, Z)$ by

$$(\varphi\alpha)\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}1\\0\end{pmatrix}, \quad (\varphi\alpha)\begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}0\\-1\end{pmatrix}$$

or

$$\varphi\alpha = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}.$$

Any finite subgroup $\varphi(K)$ of $GL(n, Z)$ is isomorphic to a finite subgroup of $O(n, R)$ and thus leaves a positive definite metric invariant. In our case

$$(\varphi\alpha)^T G(\varphi\alpha) = G$$

(where $(\varphi\alpha)^T$ is the transposed of the matrix $(\varphi\alpha)$) gives

$$G = \begin{pmatrix}g_{11} & 0\\0 & g_{22}\end{pmatrix} \quad \text{with } g_{11} > 0\,, \quad g_{22} > 0\,.$$

The lattice generated by e_1 and e_2 and left invariant by $\varphi(K)$ is thus rectangular. We shall write α instead of $\varphi\alpha$ and 1 for $\varphi\varepsilon$.

(ii) Non-equivalent extensions. For the normalized 2-cocycles $m \in Z^2(K, Z^n)$, we find

$$(1 - \alpha)\, m(\alpha, \alpha) = 0$$

giving

$$m(\alpha, \alpha) = \left\{\begin{pmatrix}x\\0\end{pmatrix} \middle|\, x \in Z\right\}.$$

The 2-coboundaries δc are determined by

$$(\delta c)\,(\alpha, \alpha) = c(\alpha) + \alpha c(\alpha) - c(\alpha^2)$$

giving

$$(\delta c)\,(\alpha, \alpha) = \left\{\begin{pmatrix}2y\\0\end{pmatrix} \middle|\, y \in Z\right\}.$$

Therefore we have two inequivalent cohomology classes, $[m_1]$ and $[m_2]$, defined by

$$[m_1]\,(\alpha, \alpha) = \left\{\begin{pmatrix}2z\\0\end{pmatrix} \middle|\, z \in Z\right\}, \quad [m_2]\,(\alpha, \alpha) = \left\{\begin{pmatrix}2z+1\\0\end{pmatrix} \middle|\, z \in Z\right\},$$

$H^2(K, Z^2)$ is thus the cyclic group C_2 generated by $[m_2]$. To represent the cohomology classes, we may choose the two cocycles, m_1 and m_2, defined by

$$m_1(\alpha, \alpha) = \begin{pmatrix}0\\0\end{pmatrix}, \quad m_2(\alpha, \alpha) = \begin{pmatrix}1\\0\end{pmatrix}.$$

Recall that the 2-cocycles m and the sections r are related by

$$(r\alpha)^2 = \varkappa m(\alpha, \alpha)$$

so that

$$(r_1\alpha)^2 = 0 , \quad (r_2\alpha)^2 = e_1 .$$

The corresponding space groups are generated by e_1, e_2, and $r\alpha$ according to

$$pm = \{e_1, e_2, r_1\alpha \,|\, (r_1\alpha)^2 = 1\} = (Z^2, K, \varphi, m_1)$$

$$pg = \{e_1, e_2, r_2\alpha \,|\, (r_2\alpha)^2 = e_1\} = (Z^2, K, \varphi, m_2) .$$

(iii) Non-equivalent systems of non-primitive translations. For the normalized 1-cocycles $s \in Z^1(K, R^n/Z^n)$, we find

$$(1 + \alpha)\, s(\alpha) = 0$$

giving

$$s(\alpha) = \left\{\begin{pmatrix} s_1 \\ s_2 \end{pmatrix} \middle|\, 2\, s_1 \equiv 0 \quad (\text{mod}\ R/Z) , \quad s_2 \in R/Z\right\} .$$

The 1-coboundaries δg are determined by

$$(\delta g)(\alpha) = (1 - \alpha)\, g = \left\{\begin{pmatrix} 0 \\ 2g_2 \end{pmatrix} \middle|\, g_2 \in R/Z\right\} .$$

Therefore we have two inequivalent cohomology classes, $[s_1] = [\pi_* u_1]$ and $[s_2] = [\pi_* u_2]$, defined by

$$[s_1](\alpha) = \left\{\begin{pmatrix} 0 \\ x \end{pmatrix} \middle|\, x \in R/Z\right\}, \quad [s_2](\alpha) = \left\{\begin{pmatrix} 1/2 \\ x \end{pmatrix} \middle|\, x \in R/Z\right\} .$$

$H^1(K, R^2/Z^2)$ is thus the cyclic group C_2 generated by $[s_2]$. To present the cohomology classes, we may choose the two cocycles, $s_1 = \pi_* u_1$ and $s_2 = \pi_* u_2$, defined by

$$s_1(\alpha) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad s_2(\alpha) = \begin{pmatrix} 1/2 \\ 0 \end{pmatrix}$$

so that

$$u_1(\alpha) = \left\{\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \middle|\, z_1, z_2 \in Z\right\}, \quad u_2(\alpha) = \left\{\begin{pmatrix} z_1 + 1/2 \\ z_2 \end{pmatrix} \middle|\, z_1, z_2 \in Z\right\} .$$

Again we may choose the following two inequivalent systems of non-primitive translations,

$$u_1(\alpha) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad u_2(\alpha) = \begin{pmatrix} 1/2 \\ 0 \end{pmatrix} .$$

The connecting homomorphism ∂_* acts as follows:

$$\partial_* [s_j] = [m_j] \quad j = 1, 2 .$$

The corresponding space groups are

$$pm = (Z^2, K, \varphi, u_1)$$

and

$$pg = (Z^2, K, \varphi, u_2) .$$

(iv) Action of the element $r\alpha$ on $\mathscr{E}$. According to (3.19) the action of $r\alpha$ on a point $x \in \mathscr{E}$ is given by

$$r\alpha \circ x = (\mu' r\alpha)\, x = (u(\alpha) \cdot r_p \alpha)\, x = (r_p \alpha)\, x + u(\alpha) \in \mathscr{E} .$$

Thus, by (3.19′)

$$\Phi_p(r\alpha \circ x) = \Phi_p[(r_p\alpha)\, x] + u(\alpha) = \alpha(\Phi_p x) + u(\alpha) \in T .$$

Putting

$$\Phi_p x = t_1 e_1 + t_2 e_2$$

and extending the isomorphism λ by linearity to $\lambda: T \cong R^2$, we find for pm, after identification of λT with R^2:

$$\Phi_p(r_1 \alpha \circ x) = (\alpha)\, (\Phi_p x) = \begin{pmatrix} t_1 \\ -t_2 \end{pmatrix} \in R^2 .$$

Therefore $r_1\alpha$ is a mirror "m" on the e_1-axis. For pg, we find

$$\Phi_p(r_2\alpha \circ x) = (\alpha)\, (\Phi_p x) + u_2(\alpha) = \begin{pmatrix} t_1 \\ -t_2 \end{pmatrix} + \begin{pmatrix} 1/2 \\ 0 \end{pmatrix} = \begin{pmatrix} t_1 + 1/2 \\ -t_2 \end{pmatrix} .$$

The element $r_2\alpha$ acts as a glide "g" where the mirror component is the same as in pm but is followed by non-primitive translation $\frac{1}{2} e_1$.

Acknowledgements. The authors express their gratitude to Dr. M. André for having put at their disposal his unpublished lecture notes on the cohomology of groups and for having critically discussed the present paper. The financial contribution accorded by the Curatoren of the Katholieke Universiteit Nijmegen is gratefully acknowledged.

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A. Janner
Instituut voor Theor. Fysica
Katholieke Universiteit
Nijmegen, Nederland

E. Ascher
Battelle Institute
Advanced Studies Center
7, route de Drize
CH 1227 Carouge, Geneva