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SPACE GROUPS OF COXETER TYPE

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Foreword

This paper is one of a series which is primarily concerned with the structure of those space groups in n-dimensional Euclidean space for which the point groups are generated by reflections, i.e., are crystallographic Coxeter groups. The determination of all possible space groups dates back to the last century for $n \leq 3$ and has been extended to $n = 4$ by Brown, Neubüser and Zassenhaus with the aid of a computer and some previous work by Dade. However, since eventually every finite group will occur as the point group of some space group, one cannot expect a reasonable solution to the problem for a general n. On the other hand, by restricting oneself to an accessible class of point groups, such as we have chosen, one can hope to obtain a satisfactory answer. The interest in Coxeter groups is also heightened by the fact that, together with their subgroups, such groups are sufficient for $n \leq 3$.

If we start with the lattice Λ as being embedded in some vectorspace V and the pointgroup $K \subseteq GL(V)$ as the two building blocks of a spacegroup S, then the various possible space groups which can be build from Λ and K consist of elements of the form (t_g,g) with $t_g \in V$ and $g \in K$. The point group element $g \in K$ determines t_g up to an additive summand from Λ. Moreover, since necessarily $(t_g,g)\cdot(t_h,h) = (t_g+gt_h,gh) = (t_{gh}+t,gh)$ with $t \in \Lambda$, the map $K \to V : g \to t_g$ is not completely arbitrary, but restricted by various compatibility conditions. Mathematically, these can be described by saying that the glue between Λ and K, which glues Λ and K together to a space group S, is an element in the first cohomology group $H^1(K,V/\Lambda)$. Thus to classify spacegroups it is helpful to get as many informations about this cohomology group as possible. Unfortunately, this leads far away from classical crystallography and deeply into the field of abstract algebra und thus might not be digestable by every reader. Still, at least for mathematically inclined people, the papers [4] and [5] constitute a good introduction into what is being done in this paper and should be consulted beforehand. It is hoped that at least for those who are interested in the structure of higher dimensional crystallographic space groups this paper presents a large variety of important and richly structured examples and a good testing ground for whatever conjectures one may have in mind.

0. Introduction.

Let V be the vector space of translations of a finite dimensional real affine space and K a crystallographic linear Coxeter group in V for which $H^1(K,V) = 0$. If Λ is a lattice in V invariant under K, the determination of space groups with point group K and lattice Λ requires the calculation of the cohomology group $H^1(K,V/\Lambda)$. In this paper, we establish some general results regarding this problem, which clarify earlier arguments in [4] and [2], extending them beyond the finite case, as well as those in [5] and [6]. We also consider the group $H^1(K^+,V/\Lambda)$, where K^+ is the rotation subgroup of K.

For a discussion of linear Coxeter groups, we refer the reader to [5]. The notation established there will be used without further explanation in this paper, with one exception: for the sake of consistency with [2] and [4], we denote $\langle \alpha_j, \check{\alpha}_i \rangle$ by n_{ji}, rather than n_{ij}.

Recall [4] that $\Lambda^{\bullet}$ denotes the group of all $v \in V$ such that $v-gv \in \Lambda$ for all $g \in K$. The <u>odd</u> Coxeter graph Γ^o of K is obtained from the ordinary graph Γ by retaining only the edges marked by 3 (and thus deleting those marked by 4,6 or ∞). If ρ is the number of connected components in Γ^o, we have

$$K/[K,K] \cong (\mathbb{Z}/2\mathbb{Z})^{\rho}. \quad (1)$$

If π is a graph automorphism of Γ and D is a diagonal matrix $\mathrm{diag}(d_1,\dots,d_m)$, with all $d_i > 0$, satisfying $D^{-1}ND = {}^{\pi}N$, where ${}^{\pi}N$ is the matrix $(n_{\pi i,\, \pi j})$, the mapping

$$\alpha_i \to d_i\, \alpha_{\pi i} \quad (2)$$

belongs to the normaliser of K in $GL(V_K)$. Conversely, when K is finite, every coset of K in this normaliser is represented by such a mapping and, furthermore, there exists a suitable matrix D for every graph automorphism π [4].

1. The group $H^1(K,V/\Lambda)$.

Suppose Λ is a lattice in V invariant under K. Then there exists [5] a 'basic system' $B = \{b_i\, \alpha_i\}$ of K in V_K such that

$Q(B) \subset \Lambda_K \subset P(B)$ and $\Lambda_K^* = P(B)$, making $\Lambda^* = V^K \oplus P(B)$. Basic systems B and B' are considered equivalent if they are related by a mapping of the form (2); it is sufficient to consider only one basic system from each equivalence class, of which there is only a finite number [5]. For convenience, we rename the elements of B to be $\alpha_1, \ldots, \alpha_m$; the matrix N is then integral. The index of Q(B) in P(B) is $|\det N|$. An important role is played by the subgroup $\Lambda + 2\Lambda^*$. If $\overline{\Lambda}_K$ denotes the projection of Λ on V_K (recall from [4] that $\overline{\Lambda}_K \subset P(B)$), we have

$$\Lambda + 2\Lambda^* = V^K \oplus (\overline{\Lambda}_K + 2P(B)) \quad . \tag{3}$$

Elements $\alpha_i, \alpha_j \in B$ are called <u>equivalent</u> if $m_{ij} = 2$ and $(\alpha_i - \alpha_j)/2 \in P(B)$, so that $n_{ik} = n_{jk} \bmod 2\mathbb{Z}$ for all k (notation: $\alpha_i \sim \alpha_j$). If $(\alpha_i - \alpha_j)/2 \in \Lambda$, we say that they are **equivalent** mod Λ ($\alpha_i \sim_\Lambda \alpha_j$). Also call $\alpha_i \in B$ <u>null</u> if $\alpha_i/2 \in P(B)$, i.e. $n_{ik} = 0 \bmod 2\mathbb{Z}$ for all k. The lattice $P(B)^*$ is spanned by P(B) and the elements $\omega_i/2$ for null α_i (where ω_i is the fundamental weight corresponding to α_i). Therefore, if ν is the number of null elements in B, we have

$$P(B)^*/P(B) \cong (\mathbb{Z}/2\mathbb{Z})^\nu \quad . \tag{4}$$

The exact sequence $0 \to \Lambda^*/\Lambda \to V/\Lambda \to V/\Lambda^* \to 0$ induces the exact cohomology sequence

$$0 \to \Lambda^{**}/\Lambda^* \to \mathrm{Hom}(K, \Lambda^*/\Lambda) \to H^1(K, V/\Lambda) \to H^1(K, V/\Lambda^*).$$

Since $\Lambda^{**} = V^K \oplus P(B)^*$, the above sequence is the same as

$$0 \to P(B)^*/P(B) \xrightarrow{\beta} \mathrm{Hom}(K, (V^K \oplus P(B))/\Lambda) \xrightarrow{\gamma} H^1(K, V/\Lambda) \xrightarrow{\phi} H^1(K, V_K/P(B)).$$

The calculation of $H^1(K, V/\Lambda)$ is based on this sequence. The map β assigns to an element of the form $\omega_i/2 + P(B)$ the homomorphism $s_j \to \delta_{ij}\alpha_i/2 + \Lambda$, where δ_{ij} is the Kronecker delta, which is a coboundary. If μ is the dimension over $\mathbb{Z}/2\mathbb{Z}$ of the subgroup of elements annihilated by 2 in $(V^K \oplus P(B))/\Lambda$, it follows from (1) that

$$\mathrm{Hom}(K, (V^K \oplus P(B))/\Lambda) \cong (\mathbb{Z}/2\mathbb{Z})^{\rho\mu} \quad . \tag{5}$$

The image of γ is called the subgroup of <u>weightlike</u> classes in $H^1(K, V/\Lambda)$ and is easily calculated. We conclude from (4) and (5) that

$$\mathrm{Im}(\gamma) \cong (\mathbb{Z}/2\mathbb{Z})^{\rho\mu - \nu} \quad . \tag{6}$$

Note also [4] that $\mathrm{Im}(\gamma)$ is stable under the action of the normaliser $N(K, \Lambda)$ on $H^1(K, V/\Lambda)$, since an element of this normaliser must also preserve Λ^*. In many cases γ is surjective, but to complete the determination of $H^1(K, V/\Lambda)$ we need to calculate the image of ϕ.

If an element $g \in K$ is of order $n < \infty$, let $N(g): V \to V$ be the map $1 + g + \ldots + g^{n-1}$.

Lemma 1. Suppose $i \neq j$ and $m_{ij} < \infty$. Then for all $v \in V$,

$$N(s_i s_j)(v) = m_{ij}v - m_{ij}/(4-n_{ij}n_{ji})((2\langle v, \check{\alpha}_i\rangle - n_{ji}\langle v, \check{\alpha}_j\rangle)\alpha_i + (2\langle v, \check{\alpha}_j\rangle - n_{ij}\langle v, \check{\alpha}_i\rangle)\alpha_j).$$

Proof. First note that

$$s_i s_j(v) = v - \langle v, \check{\alpha}_j\rangle \alpha_j - (\langle v, \check{\alpha}_i\rangle - n_{ji}\langle v, \check{\alpha}_j\rangle)\alpha_i. \qquad (7)$$

Therefore $N(s_i s_j)(v) = m_{ij}v - x$, where $x = x_i\alpha_i + x_j\alpha_j$ for some $x_i, x_j \in \mathbb{R}$. Since $N(s_i s_j)(v)$ is invariant under $s_i s_j$, it is clear from (7) that both $\check{\alpha}_i$ and $\check{\alpha}_j$ must vanish on it, i.e. that

$$m_{ij}\langle v, \check{\alpha}_i\rangle = 2x_i + n_{ji}x_j, \quad m_{ij}\langle v, \check{\alpha}_j\rangle = n_{ij}x_i + 2x_j.$$

Solving these equations, we obtain the stated formula.

Suppose t is a function $\{s_1, \ldots, s_m\} \longrightarrow V$ and let $p_{ij} = \langle t(s_i), \check{\alpha}_j\rangle$; then t will induce a cocycle $\overline{t}: K \to V/\Lambda$ if and only if $(1+s_i)t(s_i) \in \Lambda$ for all i and

$$N(s_i s_j)(t(s_i)+s_i t(s_j)) \in \Lambda \qquad (8)$$

for all $i \neq j$ such that $m_{ij} < \infty$. The cocycle $\overline{t}$ will be a coboundary if and only if there exist $c_i \in \mathbb{R}$ such that $t(s_i) = c_i\alpha_i \mod \Lambda$ for all i. By subtracting from an arbitrary function t the coboundary inducing function $s_i \to p_{ii}\alpha_i/2$, we are able to assume from now on that

$$p_{ii} \in \mathbb{Z} \quad \text{for all } i. \qquad (9)$$

With this assumption and the aid of Lemma 1, one sees that eqns. (8) amount to the following conditions on t:

(A_1) $2t(s_i) \in \Lambda$ for all i;

(A_2) if $m_{ij} = 2$, $p_{ij}\alpha_j + p_{ji}\alpha_i \in \Lambda$;

(A_3) if $m_{ij} = 3$, $t(s_i) + t(s_j) = p_{ij}\alpha_i + p_{ji}\alpha_j \mod \Lambda$.

It follows from (A_1) that $H^1(K, V/\Lambda)$ is annihilated by 2 and that $2p_{ij} \in \mathbb{Z}$ for all i,j, since $\overline{\Lambda}_K \subset P(B)$. As $\alpha_i/2 \notin \Lambda$ for any i [5], (A_2) can be restated as

(A_2') if $m_{ij} = 2$, $p_{ij} = p_{ji} \mod \mathbb{Z}$ and $p_{ij} \notin \mathbb{Z}$ only if $\alpha_i \sim_\Lambda \alpha_j$.

From (A_3) follows by addition that if $\{i_1, \ldots, i_k\}$ is a circuit in Γ^0, then

$$(*) \quad (p_{i_1 i_k}+p_{i_1 i_2})\alpha_{i_1} + (p_{i_2 i_1}+p_{i_2 i_3})\alpha_{i_2} + \ldots + (p_{i_k i_{k-1}}+p_{i_k i_1})\alpha_{i_k} \in \Lambda_K.$$

Since a coboundary $K \to V_K/P(B)$ corresponding to an element $v+P(B)$ lifts to the coboundary $K \to V/\Lambda$ corresponding to $v+\Lambda$, a cohomology class $\{\overline{t}\} \in H^1(K, V_K/P(B))$ is in the image of ϕ if and only if there exists a cocycle $\overline{T}: K \to V/\Lambda$ for which

$$T(s_i) = t(s_i) \mod V^K \oplus P(B) \quad . \qquad (10)$$

Then

$$\langle T(s_i), \check{\alpha}_j\rangle = \langle t(s_i), \check{\alpha}_j\rangle \mod \mathbb{Z} \quad \text{for all } i,j. \qquad (11)$$

Theorem 1. <u>A class</u> $\{\bar{t}\} \in H^1(K, V_K/P(B))$ <u>belongs to the image of</u> ϕ <u>if and only if the following conditions are satisfied:</u>

(B_1) $2t(s_i) \in \bar{\Lambda}_K + 2P(B)$ <u>for all</u> i;

(B_2) <u>if</u> $m_{ij} = 2$, <u>then</u> $p_{ij} = p_{ji} \bmod \mathbb{Z}$ <u>and</u> $p_{ij} \notin \mathbb{Z}$ <u>only if</u> $\alpha_i \sim_\Lambda \alpha_j$;

(B_3) (*) <u>holds for every circuit</u> $\{i_1, \ldots, i_k\}$ <u>in</u> Γ^o.

<u>Proof</u>. Suppose that there exists a cocycle $\bar{T}: K \to V/\Lambda$ satisfying (10). Then $2T(s_i) = 2t(s_i) \bmod 2\Lambda^*$, so that $2t(s_i) \in \Lambda + 2\Lambda^*$ by (A_1). Since $2t(s_i) \in V_K$, we in fact have $2t(s_i) \in \bar{\Lambda}_K + 2P(B)$ by (3). Conditions (B_2) and (B_3) follow from conditions (A_2') and (A_3) for T in view of (11).

Conversely, suppose $\bar{t}$ is a cocycle $K \to V_K/P(B)$ satisfying (B_1)-(B_3). Let $a_i \in \Lambda^*$ be such that $2t(s_i) - 2a_i \in \Lambda$. When $m_{ij} = 3$, define

$$b_{ij} = (t(s_i)-a_i) + (t(s_j)-a_j) - p_{ij}\alpha_i - p_{ji}\alpha_j.$$

Then $b_{ij} \in \Lambda^*$ by (A_3), $b_{ij} = b_{ji}$ and $2b_{ij} \in \Lambda$. If $\{i_1, \ldots, i_k\}$ is a circuit in Γ^o, (*) implies that

$$b_{i_1 i_2} + \cdots + b_{i_k i_1} \in \Lambda. \tag{12}$$

It follows that there exist $c_i \in \Lambda^*$ such that $2c_i \in \Lambda$ and

$$b_{ij} + c_i + c_j \in \Lambda \quad \text{for all } i,j. \tag{13}$$

Indeed, if Σ is a spanning tree of a connected component of Γ^o and σ is a particular vertex in Σ, define $c_\sigma = 0$ and $c_i = b_{i_1 i_2} + \cdots + b_{i_{s-1} i_s}$ if $i \in \Sigma$ and $\{i_1, \ldots, i_s\}$ is the path from $i_1 = \sigma$ to $i_s = i$ in Σ. If $j \notin \Sigma$ is such that $m_{ij} = 3$ and $\{j_1, \ldots, j_t\}$ is the path from $j_1 = \sigma$ to $j_t = j$ in Σ, then $\{i_1, \ldots, i_s, j_t, \ldots, j_2\}$ is a circuit in Γ^o, so that

$$b_{i_1 i_2} + \cdots + b_{i_{s-1} i_s} + b_{ij} + b_{j_t j_{t-1}} + \cdots + b_{j_2 j_1} \in \Lambda$$

by (12), i.e. $c_i + b_{ij} + c_j \in \Lambda$, proving (13).

Now define $T(s_i) = t(s_i) - a_i + c_i$. Then (10) is fulfilled, $2T(s_i) \in \Lambda$, (A_2') follows from (B_2), whereas if $m_{ij} = 3$,

$$\begin{aligned} T(s_i) + T(s_j) &= (t(s_i)-a_i) + (t(s_j)-a_j) + c_i + c_j \\ &= p_{ij}\alpha_i + p_{ji}\alpha_j + b_{ij} + c_i + c_j \\ &= \langle T(s_i), \check{\alpha}_j\rangle \alpha_i + \langle T(s_j), \check{\alpha}_i\rangle \alpha_j \mod \Lambda \end{aligned}$$

by (11) and (13), proving (A_3).

It remains to calculate the group $H^1(K, V_K/P(B))$. In fact, (B_2) shows that it is sufficient to consider cocycles satisfying

$$p_{ij} = p_{ji} \bmod \mathbb{Z} \text{ if } m_{ij} = 2,$$

which we shall call <u>symmetric</u>. As all coboundaries are symmetric, the classes of such cocycles define a subgroup $H^1_{sym}(K, V_K/P(B))$, to which we shall restrict our attention. Condition (A_2) can again be replaced by (A_2') for symmetric cocycles (but not in general since $\alpha_i/2 \in P(B)$ for null α_i).

Given a symmetric cocycle $\overline{t}: K \to V_K/P(B)$, let X be the $m \times m$ matrix (x_{ij}), where x_{ij} is the class of $2p_{ij}$ in $\mathbb{Z}/2\mathbb{Z}$ (and thus equal to 0 or 1). Since an element $v \in V_K$ belongs to P(B) if and only if $\langle v, \check{\alpha}_k \rangle \in \mathbb{Z}$ for all k, condition (9) and (A_1)-(A_3) translate into the following properties of X:

(C_1) $x_{ii} = 0$ for all i;

(C_2) if $m_{ij} = 2$, $x_{ij} = x_{ji}$, with $x_{ij} \neq 0$ only if $\alpha_i \sim \alpha_j$;

(C_3) if $m_{ij} = 3$, $x_{jk} = x_{ik} + x_{ij}n_{ik} + x_{ji}n_{jk} \bmod 2\mathbb{Z}$ for all k.

The last condition can be viewed as expressing the j-th row of X in terms of the i-th row and the single unknown x_{ji}. Conversely, if X is such a matrix, the function $t_X: \{s_1, \ldots, s_m\} \to V_K$ given by

$$t_X(s_i) = (\textstyle\sum_k x_{ik}\omega_k)/2$$

defines a cocycle $\overline{t}_X: K \to V_K/P(B)$.

If $\overline{t}$ is a coboundary, $t(s_i) = c_i \alpha_i \bmod P(B)$ for some $c_i \in \mathbb{R}$, with (9) forcing $2c_i \in \mathbb{Z}$. The matrix X then equals $(2d_i n_{ij})$, taken mod $2\mathbb{Z}$; in other words, the rows of X are multiples by 0 or 1 of the rows of $\overline{N}$, the matrix N taken mod 2 .

Suppose that the general form of X contains χ unknowns. Since N has $m - \nu$ nonzero rows, one can eliminate $m - \nu$ of these unknowns to obtain a vector space (over $\mathbb{Z}/2\mathbb{Z}$) of matrices X which correspond in a 1:1 fashion to the elements of $H^1_{sym}(K, V_K/P(B))$. In particular, it follows that

$$H^1_{sym}(K, V_K/P(B)) \cong (\mathbb{Z}/2\mathbb{Z})^{\chi - m + \nu}.$$

One can then use Theorem 1 to see which of these matrices X correspond to classes $\{\overline{t}_X\}$ in the image of ϕ for a particular Λ.

2. Some special cases.

Suppose first that K is finite; then the subsets of B corresponding to the connected components of Γ belong to the well-known 'types' A-G [1]. It is convenient to consider types A_1 and B_2 to be C_1 and C_2 in this context. Null elements α_i of B are then precisely the last elements in components of type C_n for some $n \geq 1$. We call such an α_i <u>odd</u> or <u>even</u> according to whether n is odd or even. If $n \geq 2$, we denote by α_{i-1} the unique element in B joined to α_i (in Γ). One can see from the tables in [1] that in a component of type C_n, the weights ω_n and ω_{n-1} are equal, mod 2P(B), to $\alpha_n/2$ and 0 if n is odd, and to 0 and $\alpha_n/2$ if n is even.

Solving equations (C_1)-(C_3), one sees [2] that elements of $H^1_{sym}(K,V_K/P(B))$ correspond in a 1:1 fashion to matrices X whose nonzero entries x_{ij} occur only when

(a) α_i, α_j are distinct and null, when $x_{ij} = x_{ji}$;

(b) α_i, α_j belong to a component B' of type A_3, B_3, B_4 or D_4, when the only exceptions are $x_{13} = x_{31} = x_{23}$ and also, in the case of D_4, $x_{14}=x_{41}=x_{24}$ and $x_{34}=x_{43}=x_{23}+x_{24} \bmod 2\mathbb{Z}$.

(c) α_i is the last element of a component of type C_n ($n \geqslant 2$) and $\alpha_j = \alpha_{i-1}$.

By Theorem 1, the class $\{\bar{t}_X\}$ belongs to the image of ϕ for a particular Λ if and only if the following conditions hold:

(D_1) if α_i, α_j are distinct and null, then $x_{ij} = 0$ unless $\alpha_i \sim_\Lambda \alpha_j$;

(D_2) if α_i is null and $\alpha_i/2 \notin \bar{\Lambda}_K$, then

$$\sum_{\alpha_k \text{ odd}} x_{ik} + x_{i,i-1}e = 0 \bmod 2\mathbb{Z},$$

where $e = 1$ if α_i is even and $e = 0$ if α_i is odd;

(D_3) if α_i, α_j belong to a component B' of type A_3, then $x_{ij} = 0$ unless $(\alpha_1 - \alpha_3)/2 \in \Lambda_K$ and $P(B') \subset \bar{\Lambda}_K$.

(D_4) if α_i, α_j belong to a component B' of type B_3, B_4 or D_4, then $x_{ij} = 0$ unless $P(B') \subset \Lambda_K$.

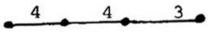
Suppose $T_1,\dots,T_h$ are the equivalence classes mod Λ of null elements in B. Let τ_r be the cardinality of T_r and call T_r <u>even</u> if <u>every</u> element in T_r is even. Also say that T_r is of Type I if $\alpha_i/2 \notin \bar{\Lambda}_K$ for some (and hence all) $\alpha_i \in T_r$ and of Type I' otherwise. Let ζ be the number of even T_r of Type I, ν_1 the number of components in B of type C_1 and ξ the number of components in B of type A_3, B_3 and B_4 which satisfy the restrictions in (D_3) and (D_4), <u>plus</u> twice the number of components of type D_4 that do so. A counting argument then shows that

$$\dim_{\mathbb{Z}/2\mathbb{Z}} \mathrm{Im}(\phi) = \sum_{\text{type I}} (\tau_r-1)(\tau_r-2)/2 + \sum_{\text{type I'}} \tau_r(\tau_r-1)/2 + \nu - \nu_1 - \zeta + \xi .$$

Together with (6), this provides a general formula for $\dim_{\mathbb{Z}/2\mathbb{Z}} H^1(K,V/\Lambda)$. Note also that a map of the form (2) can belong to the normaliser $N(K,\Lambda)$ only if all $d_i = 1$, and thus ${}^{\pi}N = N$; therefore the group $N(K,\Lambda)/K$ is isomorphic to a subgroup of such graph automorphisms π of Γ .

Secondly, instead of assuming K to be finite, suppose merely that $m_{ij} \leqslant 3$ for all i,j, so that Γ is an ordinary graph. Null elements of B then correspond to isolated vertices in Γ. A connected component of Γ is called <u>special</u> if it is a complete s-partite graph for $s = 2$ or 3. Solution of equations (C_1)-(C_3) then leads [5] to the conclusion that elements of $H^1_{sym}(K,V_K/P(B))$ are in 1:1 correspondence with matrices X whose nonzero entries x_{ij} occur only if α_i and α_j are both null or belong to the same special component. Since the only special components which correspond to finite groups are of type A_2, A_3 or D_4, perhaps this helps to explain the exceptional role played by these types (A_2 is too small) in the finite case.

Another example of some interest is the case when Γ is the graph



(14)

There are four equivalence classes of basic systems, corresponding to the following choices of values of elements $(n_{12},n_{21},n_{23},n_{32})$ in N: $(-2,-1,-1,-2)$; $(-1,-2,-1,-2)$; $(-2,-1,-2,-1)$; $(-1,-2,-2,-1)$. Since $\det N = -2$, the only choices for Λ in each case are Q(B) and P(B); however, the latter choice is disqualified in all but the second case because of the presence of null elements. Thus there are five lattices to consider.

For example, in the first case α_1 is null, but distinct α_i are not equivalent. We have $\rho = 3$, $\nu = 1$ and $\mu = 1$, so that $\mathrm{Im}(\gamma)$ is isomorphic to $(\mathbb{Z}/2\mathbb{Z})^2$. The elements of $H^1_{sym}(K,V_K/P(B))$ correspond to matrices X **whose only** nonzero entries are x_{12} and x_{23}. The **class** $\{\bar{t}_X\}$ belongs to the image of ϕ if and only if $x_{12}\,\omega_2$ and $x_{23}\,\omega_3$ belong to Q(B). However, $\omega_2 = -(3/2\,\alpha_1 + 3\,\alpha_2 + 2\,\alpha_3 + \alpha_4) \notin Q(B)$, while $\omega_3 = -(2\,\alpha_1 + 4\,\alpha_2 + 2\,\alpha_3 + \alpha_4) \in Q(B)$. Therefore $x_{12} = 0$, but x_{23} may equal 0 or 1. Therefore $H^1(K,V/\Lambda) \cong (\mathbb{Z}/2\mathbb{Z})^3$.

The elements $v_1 = -(\alpha_1 + 3\,\alpha_2 + 2\,\alpha_3 + \alpha_4)$, $v_2 = \alpha_2$, $v_3 = \alpha_2 + \alpha_3$ and $v_4 = \alpha_2 + \alpha_3 + \alpha_4$ form another basis of Q(B). However, if $(\cdot,\cdot)$ is the unique **symmetric** bilinear form on V left invariant by K, and normalised by $(\alpha_1,\alpha_1) = 2$, one sees that the v_i are mutually orthogonal, while $(v_1,v_1) = -1$ and $(v_i,v_i) = 1$ for $i = 2,3,4$. Thus Q(B) is the "cubic lattice" in space-time considered by Schild [9], Coxeter and Whitrow [3] and Zassenhaus and Plesken [10]. The group K is shown there to consist of <u>all</u> integral Lorentz transformations. (The calculation of $H^1(K,V/\Lambda)$ in [10] is, however, erroneous.)

3. The group $H^1(K^+,V/\Lambda)$.

The rotation subgroup K^+ of K consists of those elements of K which can be written as a product of an even number of the s_i's. Choose an element $\alpha_0 \in B$ and let $g_i = s_i s_0$ for $i \neq 0$; then $g_i \in K^+$.

Since $g_i g_j^{-1} = s_i s_j$, the g_i's generate K^+ and the obvious relations

$$g_i^{m_{i0}} = 1, \quad (g_i g_j^{-1})^{m_{ij}} = 1 \tag{15}$$

form a presentation of K^+ [1,p.38]. We exclude the trivial case of $\dim V_K = 1$; it is then clear from (7) that $V^{K^+} = V^K$.

In general, if G is a group, H a normal subgroup of G and A a G-module, we have the exact sequence

$$0 \to H^1(G/H,A^H) \xrightarrow{\text{inf}} H^1(G,A) \xrightarrow{\text{res}} H^1(H,A)^G \xrightarrow{\varepsilon} H^2(G/H,A^H) \quad . \tag{16}$$

Suppose furthermore that G is the semidirect product of H and a cyclic subgroup $\{1,s\}$ of order 2. Then $H^2(G/H,A^H)$ is isomorphic to $A^G/(1+s)A^H$ and the homomorphism ε can be described as follows. If $\{t\} \in H^1(H,A)^G$, we have ${}^st - t = \delta_a$, the coboundary corresponding to some $a \in A$, unique up to elements of A^H. Then $(1+s)a \in A^G$ and ε associates the class of $(1+s)a$ to $\{t\}$. If this class is zero, i.e. if $(1+s)a = (1+s)b$ for some $b \in A^H$, the cocycle t extends to a cocycle $G \to A$ by defining $t(s)$ to be $b-a$.

It follows from (15) that, if Λ is a K^+-invariant lattice, a function $t: \{g_i\} \to V$ induces a cocycle $\bar{t}:K^+ \to V/\Lambda$ if and only if

$$N(s_i s_0)t(g_i) \in \Lambda \ ; \ N(s_i s_j)t(g_i) = N(s_j s_i)t(g_j) \bmod \Lambda \tag{17}$$

whenever $m_{i0} < \infty$ and $i \neq j$, $m_{ij} < \infty$ respectively. Let $u_{ij} = \langle t(g_i), \check{\alpha}_j \rangle$.

Suppose that Λ is, in fact, invariant under K (this need not always be true [2,6]) and apply (16) with $G = K$, $H = K^+$, $s = s_0$ and $A = V/\Lambda$. Then $A^G = \Lambda^*/\Lambda$, $A^H = \Lambda^\#/\Lambda$, where

$$\Lambda^\# = \{v \in V \mid v - g_i v \in \Lambda \ \text{ for all } i \neq 0\} = V^K \oplus \Lambda^\#_K ,$$

and $A^G/(1+s)A^H$ is isomorphic to

$$E(\Lambda) = P(B)/(\bar{\Lambda}_K + (1+s_0)\Lambda^\#_K). \tag{18}$$

Note that since $P(B) \subset \Lambda^\#_K$, we have $2P(B) \subset (1+s_0)\Lambda^\#_K$, which shows that $E(\Lambda)$ is annihilated by 2.

If $\{\bar{t}\} \in H^1(K^+,V/\Lambda)^K$, we have

$$({}^{s_0}\bar{t} - \bar{t})(g_i) = -2\bar{t}(g_i) + \delta_a(g_i),$$

where $a = \sum_{i\neq 0} u_{ii}\omega_i$. It follows first of all that $H^1(K^+,V/\Lambda)^K$ is equal to the subgroup $H^1(K^+,V/\Lambda)_2$ of all elements in $H^1(K^+,V/\Lambda)$ annihilated by 2. Every class in $H^1(K^+,V/\Lambda)_2$ contains a cocycle $\bar{t}$ with the property $2\bar{t} = 0$ since if, in general, $2\bar{t}$ equals a coboundary δ_v, we can replace $\bar{t}$ by $\bar{t} - \delta_{v/2}$. Confining our attention to such cocycles, for which $2u_{ij} \in \mathbb{Z}$ (we depart here from the conventions of [2]) it follows from the above discussion that the homomorphism ε associates to $\{\bar{t}\}$ the class of the element $(1+s_0)a = \sum_{i\neq 0} 2u_{ii}\omega_i \in P(B)$

in $E(\Lambda)$. We thus obtain the exact sequence

$$0 \to H^1(K/K^+, \Lambda^{\#}/\Lambda) \xrightarrow{\inf} H^1(K, V/\Lambda) \xrightarrow{\mathrm{res}} H^1(K^+, V/\Lambda)_2 \xrightarrow{\varepsilon} E(\Lambda). \quad (19)$$

To obtain further information about ε , one can work out eqns.(17) explicitly, using Lemma 1, for a cocycle $\bar{t}$ satisfying $2\bar{t} = 0$. This results in the following conditions on t (where $i,j \neq 0$):

(E_1) if $m_{i0} = 2$, $u_{ii}\alpha_i + u_{i0}\alpha_0 \in \Lambda$;

(E_2) if $m_{i0} = 3$, $t(g_i) = u_{ii}\alpha_0 + u_{i0}\alpha_i \bmod \Lambda$;

(E_3) if $m_{ij} = 2$, $(u_{ii}+u_{ji})\alpha_i = (u_{jj}+u_{ij})\alpha_j \bmod \Lambda$;

(E_4) if $m_{ij} = 3$, $t(g_i)+t(g_j) = (u_{jj}+u_{ij})\alpha_i + (u_{ii}+u_{ji})\alpha_j \bmod \Lambda$.

From (E_1) it follows immediately that $u_{ii} \in \mathbb{Z}$ unless $\alpha_i \sim_\Lambda \alpha_0$ or $m_{i0} > 2$. In calculating $\varepsilon(\{\bar{t}\})$, it therefore suffices to consider only such values of i.

Suppose now that K is finite. If B contains a component B' of type other than C_1, we can choose $\alpha_0 \in B'$ in such a way that it is joined to precisely one element $\alpha_1 \in B'$, with $n_{01} = -1$. Then $\alpha_0 = 2\omega_0 - \omega_1$, so that the class of ω_1 is zero in $E(\Lambda)$. Therefore, by Lemma 7.1 in [2] (with α_0 chosen as the first root in case B' is of type D_n, $n \geqslant 5$), we have $\varepsilon(\{\bar{t}\}) = 2u_{11}\omega_1 = 0$, unless B' is of type A_3, B_3, B_4 or D_4, when $\varepsilon(\{\bar{t}\}) = 2u_{22}\omega_2$ in the first three cases and $\varepsilon(\{\bar{t}\}) = 2u_{22}\omega_2 + 2u_{33}\omega_3$ in the fourth. In the case of B_3 or B_4, $u_{22} \notin \mathbb{Z}$ only if $\alpha_0 \sim \alpha_2$, which implies that $\omega_2 \in \Lambda_K$ and hence $\varepsilon(\{\bar{t}\}) = 0$. In the case of D_4, if not all of $\alpha_0, \alpha_2, \alpha_3$ are equivalent mod Λ, we can assume that α_0 is not equivalent to the other two, which forces u_{22} and u_{33} to be in $\mathbb{Z}$; otherwise, ω_2 and ω_3 are in Λ_K, so that again $\varepsilon(\{\bar{t}\}) = 0$.

We are thus left with the case when all components of B are of type C_1 or A_3. If π is such a component, let ω_π be the weight corresponding to the last element in π, and let Λ_e be the sublattice of index 2 in P(B) spanned by Q(B) and all elements of the form $2\omega_\pi$ and $\omega_\pi + \omega_{\pi'}$ $(\pi \neq \pi')$. Also let $T_1, \dots, T_h$ be the equivalence classes mod Λ of null elements in B. Call Λ a <u>special</u> lattice if it satisfies

(i) $\bar{\Lambda}_K = \Lambda_e$;

(ii) $2\omega_\pi \in \Lambda_K$ for all π ;

(iii) T_i has an even number of elements for $i = 1, \dots, h$;

(iv) if B is of type $C_1 \times \dots \times C_1$, $\Lambda_K \neq \Lambda_e$.

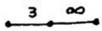
It is demonstrated in [2] that ε assumes a nonzero value precisely when Λ is a special lattice. Furthermore, apart from the case when B is of type $C_1 \times \dots \times C_1$ and $\Lambda_K = \Lambda_e$, $\Lambda_K^{\#} = P(B)$ if K is finite.

Therefore $E(\Lambda)$ is cyclic of order **2** for special Λ, which shows that the image of res is then of index 2. It also follows that the first group in (19) is isomorphic to $(\mathbb{Z}/2\mathbb{Z})^{\mu}$, with μ as defined earlier; in the exceptional case, it is isomorphic to $(\mathbb{Z}/2\mathbb{Z})^{\lambda}$, where $\lambda = \dim V^K$, unless $\dim V^K$ is odd and $\overline{\Lambda}_K = \Lambda_K$, when $\lambda = \dim V^K + 1$.

Once $H^1(K^+, V/\Lambda)_2$ has been determined from (19), the calculation of $H^1(K^+, V/\Lambda)$ reduces to that of the subgroup $2H^1(K^+, V/\Lambda)$, in view of the exact sequence

$$0 \longrightarrow H^1(K^+, V/\Lambda)_2 \longrightarrow H^1(K^+, V/\Lambda) \longrightarrow 2H^1(K^+, V/\Lambda) \longrightarrow 0.$$

When K is finite, the latter is usually zero or quite small [2]. However, in general it may happen, as in the case of



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(when K^+ is isomorphic to the modular group) that $H^1(K^+, V) \neq 0$ and $2H^1(K^+, V/\Lambda)$ contains factors isomorphic to $\mathbb{R}/\mathbb{Z}$. One also has to consider separately lattices Λ which are only invariant under K^+. It is shown in [2] that if K is finite and $\dim V_K \geqslant 3$, the normaliser of K^+ equals the normaliser of K.

A translation between our notation and that of classical crystallography for $\dim V \leqslant 3$ can be found in [2] and [4]. For further relevant results, see [7] and [8].

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