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On Bravais Classes of Magnetic Lattices

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Summary. The concept of Bravais classes is examined by looking at the extensions from which n-dimensional space groups are obtained. It is shown how n-dimensional magnetic space groups, too can be derived from extensions of abelian groups. This leads to a natural classification, which interprets in terms of extensions that given by OPECHOWSKI and GUCCIONE. Bravais classes of magnetic lattices are defined by generalization of the concept of arithmetically equivalent holohedries. A new group is introduced: the magnetic linear group $ML(n, Z)$, i.e. the group of linear basis transformations leaving invariant the magnetic lattice structure. This group is isomorphic to subgroups $ML_\nu(n, Z)$ of index $2^n - 1$ in $GL(n, Z)$, which subgroups replace $GL(n, Z)$ in the magnetic case. Some basic properties of these new groups are discussed. As illustration, the two-dimensional Bravais classes of magnetic lattices are derived.

1. Introduction

The Bravais classes of two- and three-dimensional magnetic lattices are well known [1][1]). But only recently has a mathematical definition for these equivalence classes been given, by W. OPECHOWSKI and R. GUCCIONE [2]. In their paper (here quoted as OG) one also finds an explicit definition of the Bravais classes of the usual translational lattices. In the non-magnetic case, the Bravais classes are given by the arithmetic classes of lattice holohedries and correspond, therefore, to the classes of conjugate finite subgroups of $GL(n, Z)$. In the magnetic case, however, OG use the concept of 'semidirect product' in order to have a simple definition.

In the present paper we show how this concept can be avoided. The result represents a natural generalization of the arithmetic case, as it involves, for the equivalence defining magnetic Bravais classes, conjugation with respect to a subgroup of $GL(n, Z)$. At the same time one learns how Bravais classes can be defined for more general crystallographic symmetry groups (for example, in the relativistic case, as will be discussed in a subsequent paper). For definitions and properties of magnetic symmetry groups, we refer to OG.

2. Bravais Classes of Euclidean Lattices

Let us briefly examine the euclidean case, because it forms a natural basis for our subsequent treatment. The approach indicated below is discussed in detail in a paper of E. ASCHER and A. JANNER [3] (here quoted as AJ).

We consider a n-dimensional lattice Λ in a euclidean space V of same dimension. The most general (invertible) isometries of V which leave Λ invariant are elements of space groups G obtained from extensions of a n-dimensional translation group T by an abstract crystallographic point group R with $\varphi_0: R \to \mathrm{Aut}(T)$ a monomorphism. Actually $\varphi_0(R)$ is the (no more abstract) crystallographic point group belonging to G.

[1]) Numbers in brackets refer to References, p. 682.

One has the following exact sequence:

$$0 \to T \overset{\varkappa}{\to} G \overset{\sigma}{\to} R \to 1 \quad (\varphi_0) . \tag{2.1}$$

That is:

$$T \lhd G \quad \text{and} \quad G/T \cong R . \tag{2.2}$$

Throughout this paper $\varkappa$ is the natural injection of the subgroup T and σ the canonical epimorphism (i. e. the homomorphic projection onto R considered as factor group of G). In what follows we therefore omit their indication.

Between isomorphic space groups $G \cong \overline{G}$, it is possible to construct a morphism of group extensions by:

$$\begin{tikzcd} 0 \arrow[r] & T \arrow[r] \arrow[d, "\chi_0"'] & G \arrow[r] \arrow[d, "\psi"] & R \arrow[r] \arrow[d, equal] & 1 & (\varphi_0) \\ 0 \arrow[r] & \overline{T} \arrow[r] & \overline{G} \arrow[r] & R \arrow[r] & 1 & (\overline{\varphi}_0) \end{tikzcd} \tag{2.3}$$

with χ_0 and ψ isomorphisms such that:

$$\forall\ a \in T,\ \forall\ \alpha \in R,\ \overline{\varphi}_0\, \alpha\, o\, a = \chi_0(\varphi_0\, \alpha\, o\, a)\, \chi_0^{-1} . \tag{2.4}$$

The isomorphism between G and $\overline{G}$ is then explicitly given by:

$$\psi(a, \alpha) = (\chi_0\, a, \alpha) \ \text{ for } (a, \alpha) \in G,\ \forall\ a \in T \text{ and } \forall\ \alpha \in R . \tag{2.5}$$

If one gives the one-to-one correspondence between the generators of T and those of $\overline{T}$, then χ_0 is completely defined for all $a \in T$ and $\overline{a} \in \overline{T}$. The free abelian group T is generated by a basis of the lattice Λ, therefore $T \overset{\lambda}{\cong} Z^n$, and analogously: $\overline{T} \overset{\overline{\lambda}}{\cong} Z^n$. Let us consider the following commutative diagram of group-isomorphisms:

$$\begin{tikzcd} T \arrow[r, tail, two heads, "\chi_0"] \arrow[d, "\lambda"'] & \overline{T} \arrow[d, "\overline{\lambda}"] \\ Z^n \arrow[r, tail, two heads, "\chi"] & Z^n \end{tikzcd} \tag{2.6}$$

with χ_0 as in (2.3). One has from construction: $\chi = \overline{\lambda}\, \chi_0\, \lambda^{-1}$. Through the isomorphism λ, the monomorphism φ_0 of (2.3) induces a monomorphism φ: $R \to GL(n, Z)$ given by:

$$\varphi\, \alpha = \lambda(\varphi_0\, \alpha)\, \lambda^{-1} , \qquad \forall\ \alpha \in R , \tag{2.7}$$

where $GL(n, Z)$ is the group of the n-dimensional integral matrices with determinant ± 1. In the same way one obtains another monomorphism $\overline{\varphi}$: $R \to GL(n, Z)$ by:

$$\overline{\varphi}\, \alpha = \overline{\lambda}\, (\overline{\varphi}_0\, \alpha)\, \overline{\lambda}^{-1} , \qquad \forall\ \alpha \in R . \tag{2.8}$$

Relation (2.4) becomes (for any $\alpha \in R$):

$$\overline{\varphi}\, \alpha = \chi\, (\varphi\, \alpha)\, \chi^{-1} , \text{ with } \chi \in GL(n, Z) . \tag{2.9}$$

From this last formula, there follows that $\varphi(R)$ and $\overline{\varphi}(R)$ are related through an inner automorphism of $GL(n, Z)$ and belong to the same class of conjugate finite subgroups of $GL(n, Z)$ isomorphic to R. Such class is called an arithmetic crystal class. One says that $\varphi(R)$ and $\overline{\varphi}(R)$ are arithmetically equivalent.

If $\varphi_0(R_0)$ is the largest point group leaving Λ invariant with φ_0 a monomorphism as above, then going over to $\varphi(R_0)$ by means of (2.6) and (2.7) one defines a holohedry of the lattice Λ by:

$$H \overset{\text{Def}}{=} \varphi(R_0) \subset GL(n, Z) . \tag{2.10}$$

For a given Λ one has an infinite number of possible holohedries (corresponding to different choices of basis), all belonging to the same arithmetic crystal class. Λ determines this arithmetic class but not vice versa. What such an arithmetic class determines is a whole Bravais class of lattices. Two lattices Λ and $\overline{\Lambda}$ are said to belong to the same Bravais class if and only if they have arithmetically equivalent holohedries:

$$\Lambda \sim \overline{\Lambda} \Longleftrightarrow \overline{H} = \chi\, H\, \chi^{-1} \text{ for } \chi \in GL(n, Z) , \tag{2.11}$$

where H and $\overline{H}$ are holohedries of Λ and $\overline{\Lambda}$, respectively. Looking now at (2.3), (2.6), and (2.9) one realises that in order to obtain all non- isomorphic space groups, it is sufficient to consider one representative of each Bravais class. This representative is also called Bravais lattice. The result is independent of special choices in (2.6) precisely because it depends only on the arithmetic crystal class and not on the representative point group considered.

In crystallography it is customary to identify not all isomorphic space groups, but only those having the same orientation. To obtain all differently oriented space groups, one has to consider oriented Bravais classes. These are defined by the equivalence arising from holohedries belonging to the same proper arithmetic crystal class, i.e.:

$$\Lambda \overset{+}{\sim} \overline{\Lambda} \Longleftrightarrow \overline{H} = \chi_+\, H\, \chi_+^{-1} \text{ for } \chi_+ \in SL(n, Z) , \tag{2.12}$$

where $SL(n, Z)$ is the subgroup of $GL(n, Z)$ consisting of the automorphisms of Z^n with determinant $+1$. Only in spaces of even dimensions may one expect differences between Bravais classes with and without orientation (because a lattice always permits inversion). Actually in the two-dimensional euclidean case, there is no such difference, but this is a consequence of the particular simple case.

3. Magnetic Space Groups as Extensions

We consider n-dimensional non-trivial magnetic space groups M. According to the general theory [2] the elements of M can be classified in primed and in unprimed according to whether they are associated or not with the time inversion operation $(t \to -t)$.

The unprimed elements form a subgroup $D \subset M$ of index 2. Therefore one obtains all the magnetic space groups M of given dimension (the trivial case of 'grey' space groups included) by considering extensions:

$$1 \to D \to M \to A \to 0 \tag{3.1}$$

where D is a space group of same dimension and $A = (E, E') \simeq C_2$ is the group consisting of the identity E and the time inversion E'. The difficulties lying in this approach are due to the fact that in (3.1) the group D is in general non-abelian.

Non-trivial magnetic space groups, however, considered as abstract groups, are isomorphic to space groups, so that, from this point of view, they can equally well be obtained from extensions of abelian groups, along the lines discussed in AJ. In addition, one needs a careful discussion relative to the distribution of the primes among the elements of the group M. In other words, a magnetic space group is a group M together with a subgroup D of index two (D being a space group). We are now back again to (3.1). Nevertheless, it is very instructive to discuss magnetic space groups in the frame of the theory developed in AJ.

One then finds, for example, that the three cases M_T, M_{R0}, and $M_{R\alpha}$ considered in the systematic presentation given by OPECHOWSKI and GUCCIONE (compare with Table II of OG) have a simple interpretation in terms of commutative diagrams with exact sequences. Actually it turns out that it is convenient to split the case $M_{R\alpha}$ into a case $M_{R\alpha'}$ and into a case $M_{R\alpha''}$. OPECHOWSKI and GUCCIONE, too, consider in their book over magnetic groups [4] a somewhat equivalent separation of $M_{R\alpha}$ in $M_{R\alpha 1}$ and $M_{R\alpha 2}$. We discuss below the mutual relations of these various cases.

In the first case ($M = M_T$), all primitive translations are unprimed, and $D = D_T$, the subgroup of index two of (3.1), has the same lattice as M_T. The other cases are characterized by the presence of a magnetic lattice Λ_M left invariant by the point group $\varphi_0(R)$. In other words, $M = M_R$ has the same point group as $D = D_R$, and primed, as well as unprimed, primitive translations occur. In the second case ($M_R = M_{R0}$), all non-primitive translations are unprimed, whereas in the cases denoted by $M_{R\alpha}$ primes are distributed also among non-primitive translations. The subdivision of $M_{R\alpha}$ into two other classes cannot be explained here in a few words.

a) *The first case:* $M = M_T$

All magnetic space groups M_T belonging to the first case are obtained from extensions of the following type:

$$0 \rightarrow T \rightarrow M_T \rightarrow R_M \rightarrow 1 \quad (\varphi_0) \tag{3.2}$$

where T is a discrete translation group generating a euclidean n-dimensional lattice, R_M a corresponding crystallographic magnetic point group and φ_0 is a monomorphism as considered in Section 2.

In fact, (3.2) is part of a more complete commutative diagram with exact rows and columns:

$$\begin{array}{ccccccccc}
 & & & & 1 & & 1 & & \\
 & & & & \downarrow & & \downarrow & & \\
0 & \rightarrow & T & \rightarrow & D_T & \rightarrow & K & \rightarrow & 1 \quad (\varphi_0) \\
 & & \| & & \downarrow & & \downarrow & & \\
0 & \rightarrow & T & \rightarrow & M_T & \rightarrow & R_M & \rightarrow & 1 \quad (\varphi_0) \\
 & & & & \downarrow & & \downarrow & & \\
 & & & & A & = & A & & \\
 & & & & \downarrow & & \downarrow & & \\
 & & & & 0 & & 0 & &
\end{array} \tag{3.3}$$

where $A = (E, E') \cong C_2$.

The monomorphism φ_0 indicated in the upper extension is actually the restriction of that appearing in the lower one, to the elements of the subgroup K of R_M.

Let r stand for a set of representatives for the cosets of M_T by T in M_T. As T consists only of unprimed elements, for any unprimed element $\alpha \in R_M$, the representative $r(\alpha)$ is an unprimed element of M_T. For any primed element $\beta' \in R_M$, $r(\beta')$ is a primed element of M_T, which can be noted as:

$$r(\beta') \overset{\text{Def}}{=} r(\beta)' . \tag{3.4}$$

In this last notation, R_M appears as an abstract group, the magnetic structure of the crystallographic point group being taken over by primed and unprimed representatives $r(R_M)$.

There follows that all unprimed elements of M_T are of the form:

$$(a, \alpha) \overset{\text{Def}}{=} a\, r(\alpha) \in D_T\,, \quad \forall\, a \in T\,, \quad \forall\, \alpha \text{ (unprimed)} \in R_M\,, \quad \text{(i.e. } \forall\, \alpha \in K)\,, \tag{3.5}$$

whereas the primed ones are given by:

$$(a, \beta') \overset{\text{Def}}{=} a\, r(\beta') = a\, r(\beta)' \in M_T - D_T\,, \quad \forall\, a \in T\,, \quad \forall\, \beta' \text{ (primed)} \in R_M \quad \text{(i.e. } \forall\, \beta' \in R_M - K)\,. \tag{3.6}$$

We observe that using (3.4) and according to (1.1) of AJ:

$$\varphi_0\, \beta' \circ a \overset{\text{Def}}{=} r(\beta')\, a\, r(\beta')^{-1} = r(\beta)\, a\, r(\beta)^{-1} \overset{\text{Def}}{=} \varphi_0\, \beta \circ a\,, \tag{3.7}$$

so that R_M operates (through φ_0) as an abstract group on T (and not as a magnetic group). One easily verifies that the elements of the factor set m: $R_M \times R_M \to T$ are, as they have to be, always unprimed elements.

The Bravais classes of these non-magnetic lattices are precisely the non-magnetic ones. The first case is also the simplest one.

b) *The cases* $M = M_R$

These cases need a preliminary discussion in common. Magnetic space groups M_R are obtained from extensions of the following type:

$$0 \to T_M \to M_R \to R \to 1 \quad (\varphi_0)\,, \tag{3.8}$$

with T_M a magnetic translation group generating a n-dimensional magnetic lattice Λ_M and R a non-magnetic crystallographic point group. φ_0 is a monomorphism: $R \to \mathrm{Aut}(T_M)$. By $\mathrm{Aut}(T_M)$ we mean the group of automorphisms of the magnetic lattice Λ_M into itself, so that $\varphi_0(R)$ maps unprimed elements on unprimed ones, and primed on primed i.e.:

$$\forall\, \alpha \in R\,, \quad \varphi_0\, \alpha \in \mathrm{Aut}\,(T_M) \text{ implies:}$$

$$\varphi_0\, \alpha \circ a \in T^D \quad \text{for} \quad \forall\, a \in T^D \tag{3.9}$$

$$\varphi_0\, \alpha \circ b' \in T - T^D \quad \text{for} \quad \forall\, b' \in T - T^D\,. \tag{3.10}$$

T^D is the subgroup of index two of T_M consisting of the unprimed elements of T_M.

The choice of a basis in Λ_M, which corresponds to choosing the generators of T_M, and the isomorphic mapping of these on the generators of Z^n, leads to a n-dimensional faithful integral representation $ML(n, Z)$ of $\mathrm{Aut}(T_M)$ with $ML(n, Z) \subset GL(n, Z)$. The magnetic linear group $ML(n, Z)$ can be interpreted as the group of linear transformations which transform a basis of Λ_M into all the other ones of the same magnetic type (see Section 5). This justifies the notation. Some basic properties of $ML(n, Z)$ are discussed in Section 5. We consider the isomorphism λ:

$$T_M \overset{\lambda}{\rightarrowtail\!\!\twoheadrightarrow} Z^n . \tag{3.11a}$$

According to (2.7), there follows from (3.8):

$$\varphi\,\alpha = \lambda\,(\varphi_0\,\alpha)\,\lambda^{-1}\,, \quad \forall\,\alpha \in R\,, \tag{3.11b}$$

but now φ is a monomorphism: $R \to ML(n, Z) \subset GL(n, Z)$.

Choosing different representatives for the cosets of T_M in M_R, one obtains equivalent extensions (i.e. extensions having systems (φ_0, m) and $(\overline{\varphi}_0, \overline{m})$, respectively, which are equivalent). Equivalent extensions define isomorphic groups [3].

The point is that, in the case of magnetic space groups, we cannot simply identify isomorphic groups. We can do so only if we can find an isomorphism which maps primed elements into primed ones (and therefore unprimed into unprimed). In the case of such an isomorphism we may speak of a magnetic-group-isomorphism. Henceforth, by isomorphic magnetic groups, we mean groups related by this special type of isomorphism (preserving the magnetic structure), for which we adopt the notation:

$$M \approxeq \overline{M}\,. \tag{3.12}$$

Let us now consider the diagram representing two equivalent extensions (3.8):

$$\begin{array}{ccccccccc} 0 \to & T_M & \to & M_R & \to & R & \to 1 & (\varphi_0) \\ & \| & & \downarrow{\scriptstyle\mu} & & \| & & \\ 0 \to & T_M & \to & \overline{M}_R & \to & R & \to 1 & (\overline{\varphi}_0)\,. \end{array} \tag{3.13}$$

According to A(52)/A(56) in AJ, M_R and $\overline{M}_R$ are related by the isomorphism μ induced by a different choice of the representatives of the cosets by T_M, namely:

$$\mu\,r(\alpha) = u(\alpha)\,\overline{r}(\alpha)\,, \quad \forall\,\alpha \in R\,. \tag{3.14}$$

The mapping u: $R \to T_M$ satisfies the conditions implying that (φ_0, m) and $(\overline{\varphi}_0, \overline{m})$ are two equivalent systems from R to T_M, related by ($\forall\,\alpha, \beta \in R$):

$$\varphi_0\,\alpha\circ a = u(\alpha)\,(\overline{\varphi}_0\,\alpha\circ a)\,u(\alpha)^{-1}\,, \tag{3.15}$$

$$m(\alpha, \beta) = u(\alpha)\,[\overline{\varphi}_0\,\alpha\circ u(\beta)]\,\overline{m}(\alpha, \beta)\,u(\alpha\,\beta)\,, \tag{3.16}$$

with of course $u(\varepsilon) = 1$. The isomorphism μ is then given by:

$$\mu[a\,r(\alpha)] = a\,u(\alpha)\,\overline{r}(\alpha)\,, \quad \forall\,a \in T_M\,, \quad \forall\,\alpha \in R\,. \tag{3.17}$$

From the above relations one can see that μ is a magnetic-group-isomorphism if and only if all $u(R)$ are unprimed (i.e. $u\colon R \to T^D$). Primed u's change the distribution of primes among the r's (possibly among the m's, too) and may therefore lead (but not necessarily) to different magnetic space groups.

For this reason, we cannot restrict ourselves to inequivalent extensions. Note that this difficulty does not arise in (3.2). All this is a consequence of the fact that a magnetic group is a group together with a given subgroup of index two.

Actually, the diagram (3.8) has to be seen as part of a more complete commutative diagram with exact rows and columns, given by:

$$\begin{tikzcd} & 0 \arrow[d] & 1 \arrow[d] & & \\ 0 \arrow[r] & T^D \arrow[r] \arrow[d] & D_R \arrow[r] \arrow[d, "\varrho"'] & R_M \arrow[r] \arrow[d, equal] & 1 \quad (\tilde{\varphi}_0) \\ 0 \arrow[r] & T_M \arrow[r] \arrow[d] & M_R \arrow[r] \arrow[d] & R_M \arrow[r] & 1 \quad (\varphi_0) \\ & A \arrow[r, equal] \arrow[d] & A \arrow[d] & & \\ & 0 & 0 & & \end{tikzcd} \tag{3.18}$$

with A as in (3.1). The injection ϱ, which determines the relation between $\tilde{\varphi}_0$ and φ_0, depends on the case considered (M_{R0}, $M_{R\alpha'}$ or $M_{R\alpha''}$).

After these general remarks, we may treat these three remaining cases separately.

c) *The second case:* $M = M_{R0}$

One obtains all magnetic space groups of the type M_{R0} by choosing unprimed representatives $r(\alpha)$ for any $\alpha \in R$. There follows that the factor set $m(R, R)$ involves only unprimed elements because of the relation:

$$r(\alpha)\, r(\beta) = m(\alpha, \beta)\, r(\alpha\, \beta)\,, \qquad \forall\; \alpha, \beta \in R\,. \tag{3.19}$$

Therefore the unprimed elements of M_{R0} are:

$$(a, \alpha) \overset{\text{Def}}{=} a\, r(\alpha) \in D_{R0}\,, \qquad \forall\; a \in T^D, \qquad \forall\; \alpha \in R\,, \tag{3.20}$$

and the primed ones appear as:

$$(b', \alpha) \overset{\text{Def}}{=} b'\, r(\alpha) \in M_{R0} - D_{R0}\,, \qquad \forall\; b' \in T - T^D\,, \quad \forall\; \alpha \in R\,. \tag{3.21}$$

The relations (3.20) and (3.21) correspond precisely to the characterization given by OG for the second case.

In the case $M_R = M_{R0}$ the injection ϱ of diagram (3.18) is the natural one, and the monomorphism $\tilde{\varphi}_0$ is simply the restriction of φ_0 to the elements of the subgroup $\mathrm{Aut}(T^D)$ of $\mathrm{Aut}(T_M)$.

d) *The third and the fourth case:* $M = M_{R\alpha}$

Magnetic space groups of this type are those which cannot be obtained by choosing unprimed representatives $r(\alpha)$ only; primed ones must also be chosen. This is a common property of the third and fourth case. Distinction between primed and unprimed representatives give a partition into J and I, respectively, of the set of indices numbering the elements of R. For clarity, we denote by:

α_i: any element of R with $r(\alpha_i)$ an unprimed representative ($i \in I$)
β_j: any element of R with $r(\beta_j)'$ a primed representative ($j \in J$)

$$\left.\begin{array}{l} a_\nu\text{: any element of } T_D \\ b'_\nu\text{: any element of } T_M - T^D \end{array}\right\} \nu \text{ is a numbering index.} \tag{3.22}$$

According to (3.22) the elements of $M_{R\alpha}$ can be divided into one of the following four sets:

$$\begin{array}{ll} \text{1st set:} & (a_\nu, \alpha_i) \overset{\text{Def}}{=} a_\nu\, r(\alpha_i) \\ \text{2nd set:} & (b'_\nu, \alpha_i) \overset{\text{Def}}{=} b'_\nu\, r(\alpha_i) \\ \text{3rd set:} & (a_\nu, \beta_j) \overset{\text{Def}}{=} a_\nu\, r(\beta_j)' \\ \text{4th set:} & (b'_\nu, \beta_j) \overset{\text{Def}}{=} b'_\nu\, r(\beta_j)' , \end{array} \tag{3.23}$$

for any element of (3.22).

The first and the fourth set of (3.23) constitute together the group $D_{R\alpha}$. The first set alone in general does not form group, because for example in:

$$r(\alpha_i)\, r(\alpha_k) = m(\alpha_i, \alpha_k)\, r(\alpha_i\, \alpha_k) , \quad \forall\, i, k \in I , \tag{3.24}$$

one does not know a priori if $m(\alpha_i, \alpha_k)$ and $r(\alpha_i\, \alpha_k)$ are primed elements or not of $M_{R\alpha}$.

The partition of Opechowski and Guccione [4] of $D_{R\alpha}$ into $D_{R\alpha 1}$ and $D_{R\alpha 2}$ is based on the distinction between the case in which the first set of (3.23) forms a group (denoted by Q or $Q_{\tau 0}$), and the case in which it does not.

Our partition of $D_{R\alpha}$ into $D_{R\alpha'}$ and $D_{R\alpha''}$ distinguishes between factor sets involving only unprimed elements and those involving primed elements as well.

Looking at (3.24) one sees that the two classifications are more or less equivalent. We have not succeeded, however, in proving whether or not they always are equivalent, or if in some cases they are not. We keep, therefore, the two different notations mentioned above. They are:

(i) According to Opechowski and Guccione.

Case $M_{R\alpha 1}$: if the first set (3.23):

$$\{a_\nu\, r(\alpha_i) \mid \forall\, a_\nu \in T^D , \quad \forall\, \alpha_i \in R , \quad i \in I\} \overset{\text{Def}}{=} Q \tag{3.25}$$

forms a subgroup of $D_{R\alpha 1}$.

Case $M_{R\alpha 2}$: if the first set (3.23) does not form a subgroup of $D_{R\alpha 2}$. (3.26)

(ii) According to our subdivision.

Case $M_{R\alpha'}$: if the factor set involves only unprimed elements, i.e.:

$$m\colon\ R \times R \to T^D \tag{3.27}$$

Case $M_{R\alpha''}$: if for given $\gamma, \delta \in R$,

$$m(\gamma, \delta)' \in T - T^D . \tag{3.28}$$

The following propositions indicate the mutual relations between (i) and (ii) (insofar as investigated).

Proposition 1.

A magnetic space group of the type $M_{R\alpha'}$ is also of the type $M_{R\alpha 1}$.

Proof: The product of any two elements of the first set (3.23) is given by:

$$[a_\nu\, r(\alpha_i)]\,[a_\mu\, r(\alpha_k)] = a_\nu\,(\varphi_0\,\alpha_i\; o\; a_\mu)\; m(\alpha_i, \alpha_k)\; r(\alpha_i\,\alpha_k) . \tag{3.29}$$

Per hypothesis $m(\alpha_i, \alpha_k) \in T^D$, therefore $r(\alpha_i\,\alpha_k)$ is unprimed and (3.29) is an element of the same first set. The inverse of any element of the first set belongs to the set: $[a_\nu\, r\,(\alpha_i)]^{-1} = [\varphi_0\,\alpha_i^{-1}\; o\; a_\nu^{-1}]\; m(\alpha_i^{-1}, \alpha_i)^{-1}\, r(\alpha_i^{-1})$. There follows that this set is a subgroup Q of $D_{R\alpha'}$.

Corollary 1.

The group Q of proposition 1 is a subgroup of index two of $D_{R\alpha'}$ (and therefore of index four of $M_{R\alpha'}$).

Proof: The product of any two elements of $D_{R\alpha'}$ not in Q is an element of Q:

$$[b'_\nu\, r(\beta_j)']\,[b'_\mu\, r(\beta_k)'] = b'_\nu\,(\varphi_0\,\beta_j\; o\; b'_\mu)\; m(\beta_j, \beta_k)\; r(\beta_j\,\beta_k) . \tag{3.30}$$

Proposition 2.

A magnetic space group of the type $M_{R\alpha 2}$ is also of the type $M_{R\alpha''}$.

Proof: Consider two elements of the first set (3.23) with product not lying in the same set. This product then lies in the fourth set (3.23):

$$[a_\nu\, r(\alpha_i)]\,[a_\mu\, r(\alpha_k)] = a_\nu(\varphi_0\,\alpha_i\; o\; \alpha_\mu)\; m(\alpha_i, \alpha_k)'\; r(\beta_j)' , \tag{3.31}$$

with $\beta_j = \alpha_i\,\alpha_k$. Therefore $m(\alpha_i, \alpha_k)'$ is necessarily primed.

From the above propositions one sees that a necessary and sufficient condition for having the case $M_{R\alpha 1}$ is:

$$m(\alpha_i, \alpha_k) \in T^D , \qquad \forall\; \alpha_i, \alpha_k \in R \quad \text{with} \quad i, k \in I . \tag{3.25a}$$

(3.25a) is a weaker condition than (3.27). However, it ensures already that the following other factors are also unprimed:

$$m(\alpha_i, \beta_j) \text{ and } m(\beta_j, \alpha_i) \in T^D, \;\; \forall\; \alpha_i, \beta_j \in R \text{ with } i \in I, j \in J . \tag{3.32}$$

In fact: $[b'_\nu\, r(\beta_j)']\, r(\alpha_i)$ is not an element of the group Q, because $r(\alpha_i) \in Q$ but $b'_\nu\, r(\beta_j)' \notin Q$, it is therefore an element of the fourth set (3.23):

$$[b'_\nu\, r(\beta_j)']\; r(\alpha_i) = b'_\nu\; m(\beta_j, \alpha_i)\; r(\beta_j\,\alpha_i)' , \tag{3.33}$$

implying $m(\beta_j, \alpha_i) \in T^D$. In the same way and by considering $r(\alpha_i)\;[b'_\nu\; r(\beta_j)']$ one gets: $m(\alpha_i, \beta_j) \in T^D$.

What (3.25a) not necessarily ensures (at least at the present stage of investigation) is that $m(\beta_j, \beta_k)$ also is unprimed. The requirement of this last property for all $j, k \in J$ is equivalent to that of Q being a subgroup of index two of $D_{R\alpha 1}$. With one of these conditions, $M_{R\alpha 1}$ becomes equivalent to $M_{R\alpha'}$ and we arrive at the following proposition:

Proposition 3.

If the group Q of (3.25) is a subgroup of index two of $D_{R\alpha 1}$ (and therefore of index four of $M_{R\alpha 1}$), then the magnetic space group $M_{R\alpha 1}$ is of type $M_{R\alpha'}$.

Proof: Q being a subgroup of index two of $D_{R\alpha 1}$, the product of any two elements of the fourth set (3.23) is an element of Q:

$$[b'_\nu\, r(\beta_j)'] \, [b'_\mu\, r(\beta_k)'] = b'_\nu (\varphi_0\, \beta_j \circ b'_\mu)\, m(\beta_j, \beta_k)\, r(\beta_j\, \beta_k) \,, \tag{3.34}$$

thus $m(\beta_j, \beta_k) \in T^D$. (3.34), (3.25a), and (3.32) give (3.27).

According to the detailed investigation of OPECHOWSKI and GUCCIONE [4], all three-dimensional magnetic space groups of the type $M_{R\alpha 1}$ satisfy the condition of proposition 3.

Let us remark that in the case $M_{R\alpha'}$, the four sets (3.23) are cosets of $M_{R\alpha'}$ relative to Q. Take for example the following four elements of $M_{R\alpha'}$:

$$(e, \varepsilon), \quad (b'_0, \varepsilon), \quad (e, \beta_0) \quad \text{and} \quad (b'_0, \beta_0) \,,$$

with $r(\beta_0)'$ and b'_0 primed. Then (3.23) becomes:

$$\begin{aligned} &\text{1st coset:} && (a_\nu, \alpha_i) \in (e, \varepsilon)\, Q \\ &\text{2nd coset:} && (b'_\nu, \alpha_i) \in (b'_0, \varepsilon)\, Q \\ &\text{3rd coset:} && (a_\nu, \beta_j) \in (e, \beta_0)\, Q \\ &\text{4th coset:} && (b'_\nu, \beta_j) \in (b'_0, \beta_0)\, Q \,. \end{aligned} \tag{3.23a}$$

The following corollary shows how $M_{R\alpha'}$ can also be obtained from extensions of T_M by R_M exactly in the way explained by OG.

Corollary 3.

In all magnetic space groups of the type $M_{R\alpha'}$ the point group R has a subgroup

$$K \overset{\text{Def}}{=} \{\forall\ \alpha_i \in R \mid i \in I\} \quad \text{of index two.}$$

Proof:

$$r(\alpha_i)\, r(\alpha_k) = m(\alpha_i, \alpha_k)\, r(\alpha_i\, \alpha_k) \,, \tag{3.35}$$

$r(\alpha_i\, \alpha_k)$ being unprimed, $\alpha_i\, \alpha_k = \alpha_l$ with $l \in I$. Therefore $\{\alpha_i \mid i \in I\}$ forms a subgroup K of R. The product of any two elements β_j, β_k not belonging to K lies in K:

$$r(\beta_j)'\, r(\beta_k)' = m(\beta_j, \beta_k)\, r(\beta_j\, \beta_k) \,, \tag{3.36}$$

giving $\beta_j\, \beta_k = \alpha_h \in K$.

In other words, we can equally well have the primes on the elements β_j of R according to:

$$r(\beta_j)' \overset{\text{Def}}{=} r(\beta'_j) \,, \qquad \forall\ j \in J \,. \tag{3.37}$$

In the case of space groups of type $M_{R\alpha'}$ the injection ϱ of diagram (3.18) is explicitly given by:

$$\varrho[a_\nu\, \tilde{r}(\alpha_i)] = a_\nu\, r(\alpha_i) \,, \quad \forall\ a_\nu \in T^D \,, \quad \forall\ \alpha_i \in K$$

$$\varrho[a_\nu\, \tilde{r}(\beta_j)] = a_\nu\, b'_0\, r(\beta_j)' \overset{\text{Def}}{=} b'_\nu\, r(\beta_j)' \,, \tag{3.38}$$

for $\forall\ a_\nu \in T^D$ and uniquely given $b_0' \in T_M - T^D$ (i.e. $\forall\ b_\nu' \overset{\text{Def}}{=} a_\nu\, b_0' \in T_M - T^D$), and $\forall\ \beta_j \in R_M - K$.

In addition to (3.18), the following two other diagrams with exact rows and columns can be constructed:

$$\begin{tikzcd}
 & 0 \arrow[d] & 1 \arrow[d] & 1 \arrow[d] & \\
0 \arrow[r] & T^D \arrow[r] \arrow[d] & Q \arrow[r] \arrow[d, "\pi"'] & K \arrow[r] \arrow[d] & 1 \ (\varphi_0') \\
0 \arrow[r] & T_M \arrow[r] \arrow[d] & M_{R\alpha'} \arrow[r] \arrow[d] & R_M \arrow[r] \arrow[d] & 1 \ (\varphi_0) \\
0 \arrow[r] & A \arrow[r] \arrow[d] & A \times A \arrow[r] \arrow[d] & A \arrow[r] \arrow[d] & 0 \\
 & 0 & 0 & 0 &
\end{tikzcd} \tag{3.39}$$

with $A \simeq C_2$ as in (3.1). The monomorphism π is the natural injection and, therefore, φ_0' is the restriction of φ_0 (this latter being the same as in (3.18)) to the elements of T^D and of K.

$$\begin{tikzcd}
 & & 1 \arrow[d] & 1 \arrow[d] & \\
0 \arrow[r] & T^D \arrow[r] \arrow[d, equal] & Q \arrow[r] \arrow[d, "\sigma"'] & K \arrow[r] \arrow[d] & 1 \ (\varphi_0') \\
0 \arrow[r] & T^D \arrow[r] & D_{R\alpha'} \arrow[r] \arrow[d] & R_M \arrow[r] \arrow[d] & 1 \ (\tilde{\varphi}_0) \\
 & & A \arrow[r, equal] \arrow[d] & A \arrow[d] & \\
 & & 0 & 0 &
\end{tikzcd} \tag{3.40}$$

with $\tilde{\varphi}_0$ as in (3.18) and φ_0' as in (3.39). The injection σ is defined by:

$$\sigma[a_\nu\, r(\alpha_i)] = a_\nu\, \tilde{r}(\alpha_i)\,, \quad \forall\ a_\nu \in T^D\,, \quad \forall\ \alpha_i \in K\,, \tag{3.41}$$

so that φ_0' is the restriction of $\tilde{\varphi}_0$ to the elements of K.

From (3.38) and (3.41) there follows:

$$\varrho\, \sigma = \pi\,, \tag{3.42}$$

with π as in (3.39).

Proposition 4.

Symmorphic magnetic space groups $M_{R\alpha}$ are of the type $M_{R\alpha'}$.

Proof: In this case the extension (3.8) is a split-extension, the factor set may be chosen to be the trivial one, thus unprimed, and (3.27) is verified.

What we indicate here is only a first step towards a theory of extensions for magnetic space groups. In particular the case $\mathrm{M}_{R\alpha''}$ needs further investigation. However, our reformulation of the results already obtained by OG (and summarized in Table I) is sufficient in order to arrive at a simple definition of the Bravais classes of magnetic lattices.

Table I. *Classification of magnetic space groups*

Type	Magnetic space group M	Point group R	Translation group T	Representatives of the cosets of M by T in M: $r(R)$	$\varphi(R)$ finite subgroup of	Factor set $m(R, R)$
I	M_T	R_M with a subgroup K of index 2	T unprimed elements only	primed and unprimed representatives	$GL(n, Z)$	unprimed
II	$M_{R\,0}$	R	T_M primed and unprimed elements	unprimed representatives only	$ML(n, Z)$	elements
III	$M_{R\,\alpha'}$	R_M with a subgroup K of index 2		primed and unprimed representatives		only
IV	$M_{R\,\alpha''}$	R				primed and unprimed elements

4. Bravais Classes of Magnetic Lattices

Magnetic lattices occur only with magnetic space groups of the type M_R; from now on we restrict ourselves to these groups (simply noted M).

Given two isomorphic magnetic space groups ($M \cong \overline{M}$) we are able to construct a morphism of group extensions in the same way as in (2.3):

$$\begin{tikzcd} 0 \arrow[r] & T_M \arrow[r, "\varkappa_0"] \arrow[d, "\chi_0"'] & M \arrow[r] \arrow[d, "\psi"'] & R \arrow[r] \arrow[d, equal] & 1 \quad (\varphi_0) \\ 0 \arrow[r] & \overline{T}_M \arrow[r, "\overline{\varkappa}_0"'] & \overline{M} \arrow[r] & R \arrow[r] & 1 \quad (\overline{\varphi}_0) \end{tikzcd} \tag{4.1}$$

with monomorphisms φ_0: $R \to \mathrm{Aut}(T_M)$ and $\overline{\varphi}_0$: $R \to \mathrm{Aut}(\overline{T}_M)$ and ψ a magnetic-group-isomorphism.

According to AJ (A34), χ_0 is an isomorphism; it even preserves the magnetic structure, because in our case (with $\varkappa_0$ and $\overline{\varkappa}_0$ natural injections) χ_0 is the restriction to T_M of ψ. But of course T_M and $\overline{T}_M$ generate in general two different magnetic lattices Λ_M and $\overline{\Lambda}_M$. For this reason it is convenient to go over to Z^n by means of the diagram (2.6) so that according to (3.11a, b), $\mathrm{Aut}(T_M)$ is replaced by $ML(n, Z)$. This subgroup is determined only after specification of how the elements of $\mathrm{Aut}(T_M)$ act on basis vectors of Λ_M and for a given type of lattice basis (see Section 5).

It is convenient to choose a covariant transformation (compare with (5.2)) of a so-called magnetic basis (i.e. a basis consisting of primed elements only). Doing so, and supposing that these primed elements (generators) are mapped by λ on the generators of Z^n, one gets a uniquely defined subgroup $ML_0(n, Z)$ of $GL(n, Z)$. The integral matrices elements of $ML_0(n, Z)$ are in one-to-one correspondence with the transformations of a magnetic basis into an arbitrary other magnetic basis of the same lattice Λ_M. The same can be done for the lower extension of (4.1), and we can now replace that diagram by:

$$\begin{tikzcd} 0 \arrow[r] & Z^n \arrow[r, "\varkappa"] \arrow[d, "\chi"'] & M \arrow[r] \arrow[d, "\psi"'] & R \arrow[r] \arrow[d, equal] & 1 \; (\varphi) \\ 0 \arrow[r] & Z^n \arrow[r, "\bar{\varkappa}"'] & \bar{M} \arrow[r] & R \arrow[r] & 1 \; (\bar{\varphi}) \end{tikzcd} \tag{4.2}$$

with $\varkappa = \varkappa_0\, \lambda^{-1}$, $\bar{\varkappa} = \varkappa_0\, \bar{\lambda}^{-1}$, $\chi = \bar{\lambda}\, \chi_0\, \lambda^{-1}$ and monomorphisms φ and $\bar{\varphi}$: $R \to ML_0(n, Z)$ related to φ_0 and to $\bar{\varphi}_0$ by (2.7) and (2.8), respectively. As χ_0 is a magnetic-group-isomorphism and after the special choices discussed above, we have:

$$\chi \in ML_0(n, Z)\ . \tag{4.3}$$

There follows from AJ(A62):

$$\bar{\varphi}(R) = \chi\, \varphi(R)\, \chi^{-1}\ , \tag{4.4}$$

so that $\bar{\varphi}(R)$ and $\varphi(R)$ belong to the same class of conjugate finite subgroups of $ML_0(n, Z)$.

The results obtained do not depend on the particular choice: the only important point is to fix once for all the subgroup $ML_\nu(n, Z)$ considered.

We may now define a *magnetic holohedry* H of a given magnetic lattice Λ_M by:

$$H \overset{\text{Def}}{=} \varphi(R_0) \subset ML_0(n, Z) \tag{4.5}$$

where $\varphi(R_0)$ is the largest point group leaving Λ_M invariant and φ is a monomorphism referred, as above, to a magnetic basis of Λ_M.

Definition of magnetic Bravais classes

Two magnetic lattices Λ_M and $\bar{\Lambda}_M$ are said to belong to the same Bravais class if and only if their magnetic holohedries H and $\bar{H}$ respectively, are conjugate subgroups of $ML_0(n, Z)$:

$$\Lambda_M \approx \bar{\Lambda}_M \Longleftrightarrow \bar{H} = \chi\, H\, \chi^{-1} \text{ for } \chi \in ML_0(n, Z)\ . \tag{4.6}$$

Looking at (4.2) one sees that in order to obtain all isomorphic magnetic space groups, it is sufficient to consider one representative of each magnetic Bravais class. In particular as extensions of a given type (φ fixed) always admit the trivial (or split) extension which yields symmorphic magnetic space groups, our definition is equivalent to that indicated by OG in terms of semi-direct products (consider in (4.2) the split-extensions for $R = R_0$ as above, together with (4.4), (4.5), and (4.6)).

5. Basic Properties of the Magnetic Linear Group $ML(n, Z)$

We consider an arbitrary basis of a given n-dimensional magnetic lattice Λ_M and the corresponding translation group T_M:

$$T_M = \{e_1, e_2 \ldots e_j \ldots e_n\}\ , \tag{5.1}$$

and we fix the correspondence between the elements A of $GL(n, Z)$ and the basis transformations of the basis in Λ_M by:

$$\bar{e}_j(A) = \sum_{k=1}^{n} A_{jk}\, e_k\,, \quad \forall\, A \in GL(n, Z)\,, \quad j = 1, 2, \dots n\,. \tag{5.2}$$

In (5.1) at least one of the basis vectors is primed. In general we may distinguish between primed indices (if the corresponding basis vectors are primed) and unprimed indices (if not). We define as *basis of the same type,* those bases which have the same sequence of primed and unprimed indices. In particular, denoting by p the number of primed indices we have: $1 \leqslant p \leqslant n$. For a magnetic basis (as defined in Section 4): $p = n$.

Proposition 5.

For n-dimensional magnetic lattices the total number of different types of basis is $N = 2^n - 1$.

Proof: For $p = k$ there are $\binom{n}{k}$ different types of basis. Altogether, therefore:

$$N = \sum_{k=1}^{n} \binom{n}{k} = 2^n - 1\,.$$

Proposition 6.

There is alway an element $T_{\nu\mu} \in GL(n, Z)$ which transforms a basis of type μ into one of type ν ($\nu, \mu = 0, 1, \dots, N-1$).

Proof: To every permutation of the order of the elements of the basis there corresponds an element of $GL(n, Z)$. If $p < n$ one can always increase p by one in the following manner. Suppose e'_k primed and e_j unprimed elements of the basis. Define:

$$\bar{e}'_j = e_j + e'_k \quad \text{and} \quad \bar{e}_h = e_h \quad \text{for} \quad h \neq j\,. \tag{5.3}$$

By (5.2) there corresponds to the transformation (5.3) an element of $GL(n, Z)$. One gets $T_{\nu\mu}$ by suitable combination of these transformations.

Corollary 6.

The element $T_{\nu\mu}$ of proposition 6 transforms every basis of type μ into one of type ν.

Proof: This follows directly from the construction of $T_{\nu\mu}$ indicated above.

Proposition 7.

The elements of $GL(n, Z)$ which transform (according to (5.2)) a basis of a given type ν into another of the same type form a subgroup $ML_\nu(n, Z)$ of index $2^n - 1$, isomorphic to $ML(n, Z)$, and to $\mathrm{Aut}(T_M)$.

Proof: From the definition there follows directly that $ML_\nu(n, Z) \subset GL(n, Z)$. That $ML_\nu(n, Z) \simeq ML(n, Z) \simeq \mathrm{Aut}(T_M)$ is a consequence of the fact that the elements of $\mathrm{Aut}(T_M)$ and of $ML(n, Z)$ are uniquely given once one knows how they transform the generators of T_M, i.e. the corresponding basis of Λ_M. To demonstrate that the index is $2^n - 1$, we show that there is a set of $2^n - 1$ elements $S_\mu \in GL(n, Z)$, $\mu = 0, 1, \dots, N-1$, such that for any $A \in GL(n, Z)$:

$$A = S_\mu\, B, \text{ with a uniquely determined } B \in ML_\nu(n, Z)\,. \tag{5.4}$$

Consider a basis of type ν. Every element $A \in GL(n, Z)$ can be classified according to the type of basis (say μ) into which it transforms the basis ν. Take $T_{\nu\mu}$ as in proposition 6. Then:

$$T_{\nu\mu} A \stackrel{\text{Def}}{=} B \in ML_\nu(n, Z) . \tag{5.5}$$

For a fixed ν, choose $2^n - 1$ such transformations $T_{\nu\mu}$. By:

$$S_\mu \stackrel{\text{Def}}{=} T_{\nu\mu}^{-1} \tag{5.6}$$

these form the desired set. The unicity of the decomposition (5.4) follows from the group properties of $GL(n, Z)$ and from the fact that A as above transforms every basis of type ν into one of type μ.

We now consider the homomorphism: $Z \to Z_2$, i.e.:

$$A \rightsquigarrow A \ (\text{mod } 2) , \qquad \forall\ A \in GL(n, Z) \tag{5.7}$$

obtained by using the elements of the Galois field $GF(2)$ instead of integers. The homomorphic image of $GL(n, Z)$ is then $GL(n, 2)$, which is a finite group of order [5]:

$$| \, GL(n, 2) \, | = (2^n - 1)\,(2^n - 2) \ldots (2^n - 2^{n-1}) . \tag{5.8}$$

Denote by $ML_\nu(n, 2)$ the image of the subgroups $ML_\nu(n, Z)$ under the homomorphism (5.7). There follows corollary 7.

Corollary 7.

The order of $ML_\nu(n, 2)$ is:

$$| \, ML_\nu(n, 2) \, | = (2^n - 2)\,(2^n - 2^2) \ldots (2^n - 2^{n-1}) .$$

Proof: Propositions 6 and 7 remain true under the homomorphism (5.7). This because the transformation by (5.2) of a primed basis vector into a primed, or into a unprimed one, depends only on A (mod 2). Therefore the $ML_\nu(n, 2)$ are subgroups of index $2^n - 1$ in $GL(n, 2)$.

Remark.

In Section 4 we have denoted by $\nu = 0$ the magnetic-basis-type ($p = n$). In this case, and using (5.2), one sees that those elements of $GL(n, Z)$ which also belong to $ML_0(n, Z)$ have in each row an odd number of odd rational integers.

First example: $n = 2$

$$GL(2, 2) \cong D_3 = \{s, t\} , \quad \text{with} \quad s^3 = t^2 = (s\,t)^2 = e .$$

The order is:

$$| \, GL(2, 2) \, | = (2^2 - 1)\,(2^2 - 2) = 6 .$$

The six elements are:

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}.$$

For $ML_\nu(2, 2)$ we have:

$$| \, ML_\nu\,(2, 2) \, | = (2^2 - 2) , \ \text{therefore} \ ML_\nu(= 2, 2) \cong C_2$$

and the index is $2^2 - 1 = 3$.

In particular for the types of basis:

$$\nu = 0 \quad T_{M0} = \{e_1', e_2'\} \quad \text{(magnetic basis)}, \quad ML_0\,(2,2) = \left\{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\right\}$$

$$\nu = 1 \quad T_{M1} = \{e_1', e_2\} \quad ML_1(2, 2) = \left\{\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}\right\}$$

$$\nu = 2 \quad T_{M2} = \{e_1, e_2'\} \quad ML_2(2, 2) = \left\{\begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}\right\}.$$

Second example: $n = 3$

$GL(3, 2) \cong LF(2, 7)$, linear fractional group of order 168 and abstract definition [6]:

$$r^3 = s^3 = (r\,s)^4 = (r^{-1}\,s)^4 = e\,.$$

In our case for example:

$$r = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \text{ and } s = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix}.$$

$ML_\nu(3, 2) \cong 0$, octahedral group of order 24, index 7 and abstract definition:

$$u^4 = v^2 = (u\,v)^3\,.$$

For $ML_0(3, 2)$ take e.g.:

$$u = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \text{ and } v = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

6. The Two-Dimensional Magnetic Bravais Classes

To illustrate how our considerations apply in practical cases, we derive here the magnetic Bravais classes for the two-dimensional case. Two magnetic lattices having the same magnetic Bravais class have arithmetically equivalent holohedries, which are in one-to-one relation with the non-magnetic Bravais classes. One therefore starts from these (supposed known) and discusses the equivalence of the corresponding magnetic lattices.

a) *Oblique lattices*

$$R_0 = C_2 = \{\alpha\} \quad \text{with} \quad \alpha^2 = \varepsilon\,.$$

The non-magnetic Bravais class is: $P = \{a, b\}$ with $\varphi\,a\,o\,a = -\,a$, $\varphi\,\alpha\,o\,b = -\,b$ i.e. holohedry

$$H = \left\{\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}\right\}.$$

The corresponding magnetic lattices are: $P_1 = \{a, b'\}$, $P_2 = \{a', b\}$, $P_3 = \{a', b'\}$ or expressed in magnetic bases: $P_1 = \{a + b', b'\}$, $P_2 = \{a', a' + b\}$, $P_3 = \{a', b'\}$.

All these lattices have the same holohedry H and belong therefore to the single magnetic Bravais class P'.

b) *Rectangular lattices*

$$R_0 = C_{2v} = \{\alpha, \beta\} \quad \text{with} \quad \alpha^2 = \beta^2 = (\alpha\,\beta)^2 = \varepsilon\,.$$

The non-magnetic Bravais class is: $R = \{a, b\}$ with:

$$\varphi\,\alpha\,o\,a = -a\,; \qquad \varphi\,\alpha\,o\,b = -b\,; \qquad \varphi\,\beta\,o\,a = a\,; \qquad \varphi\,\beta\,o\,b = -b$$

i.e. holohedry

$$H = \left\{\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right\}.$$

The corresponding magnetic lattices expressed in magnetic bases are:

$$R_1 = \{a - b', b'\}\,, \quad R_2 = \{a', a' + b\}\,, \quad R_3 = \{a', b'\}$$

with magnetic holohedries given respectively by:

$$H_1 = \left\{\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 1 & 2 \\ 0 & -1 \end{pmatrix}\right\}, \quad H_2 = \left\{\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 2 & -1 \end{pmatrix}\right\},$$

$$H_3 = \left\{\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right\}.$$

Now $H_1 \approx H_2$ because:

$$\lambda\,H_1\,\lambda^{-1} = H_2 \quad \text{for} \quad \lambda = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \in ML_0(2, Z)$$

but H_3 belongs to another magnetic Bravais class. To establish this, it is sufficient for this to consider the second generator of H_1 and H_3, respectively:

$$\lambda\,H_1\,\lambda^{-1} = H_2 \quad \text{implies}$$

$$\lambda \begin{pmatrix} 1 & 0 \\ 2 & -1 \end{pmatrix} = \begin{pmatrix} \pm 1 & 0 \\ 0 & \mp 1 \end{pmatrix} \lambda\,,$$

and one finds that the possible values for $\lambda \in GL(2, Z)$ are:

$$\lambda = \pm \begin{pmatrix} 1 & 0 \\ \mp 1 & \pm 1 \end{pmatrix} \notin ML_0(2, Z)\,, \text{ or } \lambda = \pm \begin{pmatrix} \pm 1 & \mp 1 \\ 1 & 0 \end{pmatrix} \notin ML_0(2, Z).$$

There are two rectangular magnetic Bravais classes and R_1, $R_2 \in R'_{a,b}$, $R_3 \in R'_c$.

c) *Diamond lattices*

$$R_0 = C_{2v} = \{\alpha, \beta\}$$

as above.

The non-magnetic Bravais class is: $D = \{a, b\}$ with:

$$\varphi\,\alpha\,o\,a = -a\,; \qquad \varphi\,\alpha\,o\,b = -b\,; \qquad \varphi\,\beta\,o\,a = b\,; \qquad \varphi\,\beta\,o\,b = a\,.$$

The corresponding holohedry is:

$$H = \left\{ \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right\}.$$

For primed a, this holohedry implies also primed b. The only compatible magnetic lattice is therefore $D' = \{a', b'\}$ with holohedry H. By every other choice of the magnetic bases, one obtains magnetically equivalent holohedries so that there is only one magnetic Bravais class of this type.

d) *Square lattices*

This case can be discussed exactly as under c). There is only one magnetic Bravais class $Q' = \{a', b'\}$ corresponding to a non-magnetic square lattice $Q = \{a, b\}$.

e) *Hexagonal lattices*

$$R_0 = C_{6v} = \{\alpha, \beta\} \quad \text{with} \quad \alpha^6 = \beta^2 = (\alpha\,\beta)^2 = \varepsilon\,.$$

The non-magnetic Bravais class is: $E = \{a, b\}$ with:

$$\varphi\,\alpha\,o\,a = a - b\,; \qquad \varphi\,\alpha\,o\,b = a\,; \qquad \varphi\,\beta\,o\,a = a\,; \qquad \varphi\,\beta\,o\,b = a - b\,.$$

The corresponding holohedry is:

$$H = \left\{ \begin{pmatrix} 1 & -1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 1 & -1 \end{pmatrix} \right\}.$$

One sees from $\varphi(\alpha)$ that this holohedry is not compatible with a magnetic lattice.

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