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REMARKS ON METACRYSTALLOGRAPHIC GROUPS

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1. INTRODUCTION

The term metacrystallographic group which appears in the title of this paper is not a generally accepted one. I have been using it since a few years [1] for any of those groups whose definition comes logically after a definition of crystallographic groups. Several kinds of metacrystallographic groups were introduced in the literature during the last 30 years under a variety of names (a short list of synonyms can be found in [1]), and some much earlier [2].

All metacrystallographic groups considered in this paper are invariance groups of certain functions defined on crystals regarded as discrete sets of points in "ordinary space" or on finite subsets of such sets. Metacrystallographic groups can thus be used to establish a classification of such functions in a similar sense as space groups were used to establish a classification of crystals. For example, the metacrystallographic groups called magnetic space groups have extensively been used to assign classification labels to certain vector functions, called spin arrangements, which describe magnetically ordered crystals.

The only purpose of this paper is to formulate the definitions of several kinds of metacrystallographic groups using in all cases the same mathematical terminology, and to describe concisely some consequences of these definitions. The above mentioned problem of classification of functions defined on crystals will here not be discussed at all, although this problem is, from a physical point of view, one of the main reasons for being interested in metacrystallographic groups.

I may mention that this paper considerably overlaps with an earlier paper of mine [1], but the arrangement of the subject is different, and the emphasis is on different aspects of the subject. In particular, various definitions of equivalence classes of metacrystallographic groups are now explicitly formulated and more carefully compared.

2. GENERALITIES ON FUNCTIONS WHOSE INVARIANCE GROUPS ARE METACRYSTALLOGRAPHIC GROUPS

In this paper ordinary space or, for short, space means a 3-dimensional Euclidean point space in the sense of the usual (Weyl's [3]) definition. A crystallographic group is then any proper or improper subgroup of a space group, which in turn is a subgroup of the Euclidean group $E(3)$ of space. The elements of $E(3)$ are called, as usual, isometries. Most definitions and theorems of this paper can easily be rephrased for any dimension n.

Let Φ be the set of all functions $f: X \to Y$ from a set $X = \tilde{K}r_1$

into a set Y, the two sets X and Y being kept fixed. Here $\tilde{K}$ is any crystallographic group; r_1 is a point of space; $\tilde{K}r_1$ is the orbit of r_1 generated by $\tilde{K}$ or, in other words, the (discrete) point set generated by $\tilde{K}$ from r_1 (if $\tilde{K}$ is a space group, then $\tilde{K}r_1$ is a crystal). The symmetry group, Sym Kr_1, of Kr_1 consists of all symmetry elements of $\tilde{K}r_1$, that is, of all those isometries of space which map $\tilde{K}r_1$ onto itself; hence: $(\text{Sym } \tilde{K}r_1)r_1 = \tilde{K}r_1$, and $\tilde{K} \subseteq \text{Sym } Kr_1$ (each subgroup of Sym $\tilde{K}r_1$ is called an invariance group of $\tilde{K}r_1$, and each crystallographic group which generates the point set $\tilde{K}r_1$ is called a generating group of the latter). In particular, if $\tilde{K}$ is a space group, then the function space Φ consists of all functions defined on $X = \tilde{K}r_1$ and having values belonging to some specified set Y.

Remark on notation. A tilde above a letter, as in $\tilde{K}$, indicates here and everywhere in this paper that the letter denotes a group; the same letter without a tilde then denotes an element of that group. However, some groups, like $E(3)$, are denoted by capital script letters. The unit element of a group will usually be denoted by E.

By the definition of a point set $\tilde{K}r_1$ its symmetry group $\tilde{K}$ is associated with it. Also some group or groups can always be associated with the set Y. Even if Y has no algebraic structure at all, one can always associate with Y the symmetric group on Y or a subgroup of it. In particular, if Y is finite and consists of d elements, one can associate with Y a group of permutations of degree d. Let the group associated with Y be $\tilde{H}$, and let $\tilde{G}$ be some group defined in terms of $\tilde{K}$ and $\tilde{H}$. The group $\tilde{G}$ will usually, but not always, be the direct product $\tilde{K} \times \tilde{H}$. Suppose next that an action A of $\tilde{G}$ on the function space Φ is defined, that is, a mapping ψ of the Cartesian product $\tilde{G} \times \Phi$ into Φ is defined such that the set of all ordered pairs $([G]f, f)$ is a permutation of Φ; here $G \in \tilde{G}$, $f \in \Phi$, and $[G]f \in \Phi$ is the image of $(G,f) \in \tilde{G} \times \Phi$ under the mapping ψ. If $[G]f = f$, then G is called a symmetry element of the function f with respect to the action A. The group constituted by all the symmetry elements of f (that is, the stabilizer of f in $\tilde{G}$) is called the symmetry group, Sym f, of f. Any subgroup of Sym f is called an invariance group of f, and as such is a metacrystallographic group. The symmetry group, and invariance groups, of f are thus unambiguously defined only after an action A has been specified. What a metacrystallographic group actually is, depends thus on Φ, $\tilde{G}$ and A.

Two large classes of metacrystallographic groups of the kind just described have widely been discussed in the literature: colour groups (here Y is a finite set with no algebraic structure) and spin groups or vector groups (here Y is a 3-deimensional Euchidean vector space). Other large classes of metacrystallographic groups are obtained in the case where the set $X = \tilde{K}r_1$ is embedded in some larger set X' so that Φ becomes a space of functions from X' into Y. The metacrystallographic groups called magnetic groups are obtained by embedding X in space-time

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It should be noted that in part of the literature the elements of the symmetry group are called symmetry operations while the term symmetry element is used for the axis of a rotation, the mirror plane of a reflection, etc..

while Y is the 3-dimensional carrier space of a representation of a group $\tilde{G}$ suitably defined. The metacrystallographic groups called super-space groups are obtained by taking $\tilde{K}$ to be a space group, X' to be a (3+j)- dimensional Euclidean point space ($j \geq 1$), and Y a 3-dimensional Euclidean vector space. If in the case of function spaces for which colour groups and spin groups are defined the definitions of action are modified in a way which involves the wreath product of groups, then one obtains two new classes of metacrystallographic groups, the colour W-groups and the spin W-groups. Still another large class of metacrystallographic groups is obtained by considering sets of functions defined on the same set $X=\tilde{K}r_1$ but having values in more than one set Y; such groups are sometimes called multiple symmetry groups.

Several other kinds of metacrystallographic groups have been considered in the literature, but, rightly or wrongly, they do not seem to me of actual or virtual importance in physics, and nothing will be said about them in the sequel; see [4].

In formulating the definitions of colour groups, spin groups, magnetic groups, etc., it will be convenient to make use of the term subdirect product [5], whose meaning is as follows. Let $\tilde{F} \times \tilde{L}$ be the direct product of any two groups. If an element of $\tilde{F} \times \tilde{L}$ is denoted by (F,L), where $F \in \tilde{F}$ and $L \in \tilde{L}$, then F and L called the $\tilde{F}$-part and $\tilde{L}$-part of (F,L) respectively. A subgroup $\tilde{J}$ of $\tilde{F} \times \tilde{L}$ is called a subdirect product of $\tilde{F} \times \tilde{L}$ if the distinct $\tilde{F}$-parts of the elements of $\tilde{J}$ constitute the group $\tilde{F}$, and the distinct $\tilde{L}$-parts of the elements of $\tilde{J}$ the group $\tilde{L}$.

3. COLOUR GROUPS

This is the case where

$$X = \tilde{K}r_1, \; Y = \{c_1, c_2, \ldots, c_d\}, \; d > 1.$$

The finite set Y is not assumed to have any algebraic structure, and therefore its elements, $c_1, c_2, \ldots, c_d$, may be anything, but they are usually called colours, and Y is then called a colour set. The value $c \in Y$ of a function f from $X=\tilde{K}r_1$ onto Y at the point $r \in \tilde{K}r_1$ will be denoted by c(r), and the d-colour function f itself that is, the set of the pairs (r;c(r)) by {r;c(r)}. Since to each point of $\tilde{K}r_1$ a colour is assigned in this way, the function f is also called a coloured point set or a d-colour point set.

If action of $\tilde{K}$ on the space Φ of colour functions {r;c(r)} was defined in the usual way, that is, if under action of $\tilde{K}$ on Φ, a colour function {r;c(r)} is mapped to the function

$$\text{(A1)} \qquad [K]\{r;c(r)\} = \{r;c(K^{-1}r)\} \text{ for any } K \in \tilde{K},$$

then invariance groups of these functions would simply be crystallographic groups;

no new groups would be obtained. However, by making use of a transitive group $\tilde{P}$ of permutations of the colour set Y, one can define an action of the direct product $\tilde{K} \times \tilde{P}$ on Φ. The simplest way of doing that is to require that an element (K,P) of $\tilde{K} \times \tilde{P}$ acting on $\{r;c(r)\}$ map it to

(A2) $$[K\|P]\{r;c(r)\} = \{r;\ Pc(K^{-1}r)\} \text{ for any } K \in \tilde{K} \text{ and } P \in \tilde{P}.$$

In words: a point r in the colour point set $[K\|P]\{r;c(r)\}$ has the colour Pc to which the colour c of the point $K^{-1}r$ in $\{r;c(r)\}$ is mapped by the permutation P of the set Y. The assumed transitivity of $\tilde{P}$ means that the colour of any point in a coloured point set can be mapped to any other of the d colours by some permutation belonging to $\tilde{P}$. A coloured point set that is not invariant under $K \in \tilde{K}$ in the sense of (A1) may very well be invariant under $(K,P) \in \tilde{K} \times \tilde{P}$ in the sense of (A2) for an appropriate choice of P. This observation leads to the following definition.

(D1) A group $\tilde{B}$ is called a <u>d-colour group</u> if it satisfied the following conditions:

(C1): $\tilde{B}$ is a subdirect product $\tilde{B}(\tilde{K};\tilde{P})$ of $\tilde{K} \times \tilde{P}$, where $\tilde{K}$ is a crystallographic group and $\tilde{P}$ is a transitive group of permutations of a finite set consisting of $d \geq 2$ elements;

(C2): $\tilde{B}$ is an invariance group of some d-colour function in the sense of (A2).

A colour group $\tilde{B}(\tilde{K};\tilde{P})$ is called a <u>colour space group</u>, a <u>colour lattice group</u>, etc., according as $\tilde{K}$ is a space group, a lattice group, a point group, etc. 2-colour groups are often called <u>black-and-white groups</u>, or <u>Shubnikov groups</u>.

Colour groups have also been defined in a slightly different ways by modifying (C1): by replacing in (C1) the words "crystallographic groups" by the words "discrete group of isometries" (then $\tilde{K}$ could be, for example, the icosahedral group); or the words "subdirect product" by the word "subgroup" (this would mean regarding crystallographic groups as colour groups, the one-colour groups).

Colour groups for d>2 were first introduced by Belov and Tarkova [6]; a definition involving permutations of a colour set was proposed by Van der Waerden and Burckhardt [7]. Groups here called 2-colour groups were first considered by Heesch [2].

Since for any colour function $\{r;c(r)\}$

$$[E\|P]\{r;c(r)\} = \{r;Pc(r)\} \neq \{r;c(r)\} \text{ if } P \neq E,$$

it follows from (C2) that no colour groups contains any of the elements (E,P) of $\tilde{K} \times \tilde{P}$, except if P=E. (In fact, a definition of colour groups in which this property of subdirect products of $\tilde{K} \times \tilde{P}$ is postulated instead of (C2) is equivalent to (D1)). Using this property of colour groups one can show that a subdirect product $\tilde{B}(\tilde{K};\tilde{P})$ is a colour group only if there exists a homomorphism ρ of $\tilde{K}$ onto $\tilde{P}$; in

other words, if ρ is a representation of $\tilde{K}$ by the transitive group $\tilde{P}$ of permutations (a colour group $\tilde{B}(\tilde{K};\tilde{P})$ is thus isomorphic onto $\tilde{K}$). From the theory of permutation representations it follows then that each representation of $\tilde{K}$ by a transitive group of permutations of degree d can be identified with a homomorphism ρ of $\tilde{K}$ onto a transitive group of permutations of the set $\tilde{K} : \tilde{L}$ of the left cosets of some subgroup $\tilde{L}$ of index d in $\tilde{K}$. Conversely, one can show that if $\tilde{K}$ is homomorphic onto $\tilde{P}$, then each subdirect product $\tilde{B}(\tilde{K};\tilde{P})$ is an invariance group of suitably defined coloured point set, that is, by (C2), $\tilde{B}(\tilde{K};\tilde{P})$ is indeed a colour group. In other words, a subdirect product $\tilde{B}(\tilde{K};\tilde{P})$ is a colour group if and only if there exists a permutation representation ρ: $\tilde{K} \to \tilde{P}$. Since each non-trivial permutation representation of $\tilde{K}$ by $\tilde{P}$ is determined by exactly one subgroup ${}^{d}\tilde{L}$ of index $d \geq 2$ in $\tilde{K}$, each such permutation representation ρ can be specified by a symbol $\tilde{B}[\tilde{K}({}^{d}\tilde{L})]$ or, for short, $\tilde{K}({}^{d}\tilde{L})$, and the same symbol can and will be used to specify a d-colour group. The colour groups $\tilde{K}({}^{d}\tilde{L})$ with a fixed group $\tilde{K}$ are said to constitute <u>the family of $\tilde{K}$</u>.

The problem of finding all colour groups is thus reduced to the problem of finding all proper subgroups of finite index in each crystallographic group. However, one is really not interested in finding all colour groups, but only one colour group from each equivalence class of colour groups after such equivalence classes have been defined conveniently. What is convenient depends of course on what one wants to do with colour groups. In particular, it may be convenient not to regard any d-colour groups belonging to the same family as equivalent [8]. If one disregards this extreme point of view, then, as far as I know, four different kinds of equivalence classes of colour groups constituting a family of $\tilde{K}$ have been considered in the literature:

(D2.1) Two colour groups $\tilde{K}(\tilde{L}^{(1)})$ and $\tilde{K}(\tilde{L}^{(2)})$ are called <u>equivalent</u> if $\tilde{L}^{(1)}$ and $\tilde{L}^{(2)}$ are conjugate subgroups of $\tilde{K}$ [7].

(D2.2) Two colour groups $\tilde{K}(\tilde{L}^{(1)})$ and $\tilde{K}(\tilde{L}^{(2)})$ are called <u>equivalent</u> if $\tilde{L}^{(1)}$ and $\tilde{L}^{(2)}$ are conjugate subgroups of the normalizer of $\tilde{K}$ in the proper affine group (that is, in the orientation preserving subgroup of the affine group); in other words, if there exists an orientation preserving affine transformation N such that

$$N \tilde{K} N^{-1} = \tilde{K} \quad \text{and} \quad N \tilde{L}^{(1)} N^{-1} = \tilde{L}^{(2)}.$$

(D2.3) This is a variant of (D2.2) which is obtained by omitting in (D2.2) the words "proper" and "orientation preserving".

(D2.4) Two colour groups $\tilde{L}^{(1)}$ and $\tilde{L}^{(2)}$ are called <u>equivalent</u> if there exists an automorphism of $\tilde{K}$ which maps $\tilde{L}^{(1)}$ onto $\tilde{L}^{(2)}$ [9].

In general, these four definitions of equivalence of colour groups give rise to four distinct partitions of a family of colour groups into equivalence classes: the greater the integer m in (D2.m), the coarser the partition. However, in many

special cases two or more such partitions are identical. For example, if $\tilde{K}, \tilde{L}^{(1)}$, and $\tilde{L}^{(2)}$, are space groups, then the partition of the family of $\tilde{K}$ in the sense of (D2.4) will always be identical, by Bieberbach's Theorem, with its partition in the sense of (D2.3), and even in the sense of (D2.2) provided $\tilde{L}^{(1)}$ and $\tilde{L}^{(2)}$ do not form an enantiomorphic pair. On the other hand, the partition of the family of the point group D_{2h} in the sense of (D2.4) and the partition in the sense of (D2.3) are different. The difference between the equivalence in the sense of (D2.1) and in the sense of (D2.2) may be illustrated by considering, for example, the family of a point group D_4.

If one adopts the usual definition of equivalence classes of crystallographic groups, according to which two crystallographic groups are called <u>equivalent</u> if they are conjugate subgroups of the proper affine group (and there are good reasons in physical crystallography to adopt this definition!), then it is most natural to give preference to (D2.2) as the definition of equivalence of colour groups. In fact, the published lists [12,4] of colour point groups give one representative of each equivalence class in the sense of (D2.2).

Equivalence of colour lattice groups has of course to be defined separately in the spirit of the Bravais definition of equivalence classes of lattice groups (not much is known about colour lattice groups [10]).

A straightforward generalization of (D2.2) to the case where two groups do not belong to the same family is as follows:

(D3) Two colour groups $\tilde{K}^{(1)}(\tilde{L}^{(11)})$ and $\tilde{K}^{(2)}(\tilde{L}^{(22)})$ are called <u>equivalent</u> if there exists an orientation preserving affine transformation S such that

$$S\,\tilde{K}^{(1)}S^{-1} = \tilde{K}^{(2)} \text{ and } S\,\tilde{L}^{(11)}\,S^{-1} = \tilde{L}^{(22)}$$

Only in the case of 2-colour groups have all equivalence classes in the sense of (D2.2) of colour point groups and colour space groups been determined: there are 58 of the former, and 1191 of the latter [11,4]. All equivalence classes of d-colour point groups, $d \geq 2$, are also known [4,12]: there are 212 of them. Some general theorems concerning the numbers of various equivalence classes of d-colour 2-dimensional space groups in the sense of (D2.4) are also available [9].

4. <u>SPIN GROUPS</u>

This is the case where $X = \tilde{K}r_1$ and Y is a 3-dimensional Euclidean vector space. In connection with applications of spin groups (to be defined presently) in the theory of magnetically ordered crystals, the vector space Y has been called the <u>spin space</u>, the term <u>spin</u> being used for a magnetic moment vector of an atom (not to be confused with the electron spin!). Spins are thus vectors which constitute the spin space Y. A function $\sigma=\{r;v(r)\}$ from $X = \tilde{K}r_1$ into Y, where v(r) is the spin v at the point $r \in \tilde{K}r_1$, is then called a <u>spin arrangement</u> (it will be here

always assumed that not all values of σ are $v = 0$). If $\tilde{K}$ is a space group, then a spin arrangement becomes a simple model for a magnetically ordered crystal. However, no physical interpretation of functions $\{r;v(r)\}$ is used in defining spin groups; the latter could just as well be called vector groups.

Next the action of a group $\tilde{K} \times \tilde{\Omega}$ on the space Φ of spin arrangements is defined, where $\tilde{\Omega}$ is any subgroup of the group $O(3)$ of all orthogonal transformations of the spin space Y: an element (K,Ω) of $\tilde{K} \times \tilde{\Omega}$, acting on a spin arrangement $\{r;v(r)\}$, maps the latter to the spin arrangement

$$\text{(A3)} \qquad [K\|\Omega]\{r;v(r)\} = \{r;\Omega v(K^{-1}r)\}$$

In words: at a point r in the spin arrangement $[K\|\Omega]\{r;v(r)\}$ there is the spin Ωv to which the spin v at the point K^{-1} r in the spin arrangement $\{r;v(r)\}$ is mapped by the orthogonal transformation Ω. It should perhaps be emphasized that, according to (A3), the orthogonal part R of an isometry $K = (R|\ell)$ has no effect on the spins of a spin arrangement. Using (A3) one is led to the following definition [13,1]:

(D4) A group $\tilde{s}$ is called a spin group (or a vector group) if it satisfies the following conditions:

(S1): $\tilde{s}$ is a subdirect product $\tilde{s}(\tilde{K};\tilde{\Omega})$ of $\tilde{K} \times \tilde{\Omega}$, where $\tilde{K}$ is a crystallographic group, and $\tilde{\Omega}$ is a non-trivial group of orthogonal transformations of the spin space;

(S2): $\tilde{s}$ is an invariance group of some spin arrangement in the sense of (A3).

Unlike colour groups, which cannot contain any elements of the form (E,P) with $P \neq E$, a spin group $\tilde{s}$ may very well contain elements of the form (E,Ω) with $\Omega \neq E$. All such elements of $\tilde{s}$ form a normal subgroup $\tilde{s}_0$, which is called a spin-only group because it acts non-trivially only in the spin space. Spin-only groups satisfy (S1) with $\tilde{K} = \tilde{E}$ (trivial group). A spin-only group can thus be identified with a group of orthogonal transformations of the spin space.

One can show that each spin group $\tilde{s}(\tilde{K};\tilde{\Omega})$ is a direct product of a spin only group $\tilde{s}_0$ and a spin group $\tilde{z}(\tilde{K};\tilde{Q})$ which is a subdirect product of $\tilde{K} \times \tilde{Q}$, where $\tilde{Q} \subseteq \tilde{\Omega}$, and which does not contain any elements of the form (E,Q) with $Q \neq E$. Any spin group which has no such elements is called a non-trivial spin group. Furthermore it turns out that $\tilde{z}(\tilde{K},\tilde{Q})$ is a spin group if and only if $\tilde{z}$ is homomorphic onto $\tilde{Q}$. This implies that if ρ is such a homomorphism, and $\tilde{z}_K$ is a (normal) subgroup of z which consists of all the elements of the form (K,E), where $K \in \ker \rho$, then $\tilde{z}(\tilde{K},\tilde{Q})$ can be decomposed into cosets of $\tilde{z}_K$ as follows:

$$\tilde{z}(\tilde{K},\tilde{Q}) = \tilde{z}_K + (K_2,Q_2)\,\tilde{z}_K + \ldots + (K_q,Q_q)\,\tilde{z}_K;$$

here q is the order of $\tilde{Q}$, and $Q_i = Q(K_i)$ is the image of K_i under ρ; $K_1 = E$, $K_2, \ldots, K_q$, are the coset representatives of $\ker \rho$ in $\tilde{K}$. A symbol $\tilde{z}(\rho:\tilde{K} \to \tilde{Q})$ thus completely specifies a non-trivial spin group. If $\tilde{K}$ is a space group, or a

point group, etc., then the spin group $z(\rho:\tilde{K} \to \tilde{Q})$ is called a spin space group, or a spin lattice group, or a spin point group, etc.

The spin groups $z(\rho:\tilde{K} \to \tilde{Q})$ with a fixed $\tilde{K}$ are said to constitute the family of $\tilde{K}$, those with fixed $\tilde{K}$ and $\tilde{Q}$ the family of $\tilde{K}$ and $\tilde{Q}$, and those with fixed $\tilde{K}$, $\tilde{Q}$, and ker ρ , the family of $\tilde{K}$, $\tilde{Q}$ and ker ρ. It follows that the number of spin groups in the latter family is equal to the number of isomorphisms of $\tilde{K}/\ker \rho$ onto $\tilde{Q}$, that is, to the number of automorphisms of $\tilde{Q}$.

How to define equivalence classes of non-trivial spin groups? As in the case of colour groups, there is a choice of answers to this question. However, there is one answer which seems to be more convenient than others from the point of view of physical crystallography. From that point of view two spin groups, $\tilde{z}(\rho_1:\tilde{K}^{(1)} \to \tilde{Q}^{(1)})$ and $\tilde{z}(\rho_2:\tilde{K}^{(2)} \to \tilde{Q}^{(2)})$, will certainly not be regarded as equivalent if the crystallographic groups $\tilde{K}^{(1)}$ and $\tilde{K}^{(2)}$ are not equivalent in the usual sense (already defined here), or $\tilde{Q}^{(1)}$ and $\tilde{Q}^{(2)}$ are not conjugate subgroups of the linear group GL(3). It thus remains to define the equivalence of non-trivial spin groups which constitute the family of $\tilde{K}$ and $\tilde{Q}$.

(D5) Let

$$\tilde{z}^{(1)}(\rho_1: \tilde{K} \to \tilde{Q}) \quad \text{and} \quad \tilde{z}^{(2)}(\rho_2: \tilde{K} \to \tilde{Q})$$

be any two spin groups belonging to the family of $\tilde{K}$ and $\tilde{Q}$. Furthermore let N be an element of the normalizer of $\tilde{K}$ in the proper affine group, and M be an element of the normalizer of $\tilde{Q}$ in GL(3). Finally let ρ_3 be the homomorphism of $\tilde{K}$ onto $\tilde{Q}$ under which NKN^{-1} is mapped to MQM^{-1} if K is mapped to Q under the homomorphism ρ_1. The spin groups $\tilde{z}^{(1)}$ and $\tilde{z}^{(2)}$ are called equivalent if $\rho_3 = \rho_2$ for some N and some M.

(As in the case of colour lattice groups, the definition of equivalence classes of spin lattice groups has to be adapted to the usual definition of Bravais classes of lattice groups; see [14], where also a list of the Bravais classes of spin lattice groups is given).

It turns out that there are 566 equivalence classes of spin point groups in the sense of (D5); here it may be mentioned that in the case of spin point groups, the groups $\tilde{Q}$ are necessarily crystallographic. A list of the representatives of all these equivalence classes (one point spin group for each class) can be found in [15,16] . This list provides striking illustrations of the implications of the definition (D5). Little is known about spin space groups.

5. MAGNETIC GROUPS

This is the case where $X = \tilde{K}r_1$ is regarded as embedded in a larger set X', the Cartesian product of $\tilde{K}r_1$ and the one-dimensional Euclidean point space $E_t(1)$($E_t(1)$ is one of the many meanings of the term time in physics): $X' = \tilde{K}r_1 \times E_t(1)$. Elements of X' are thus points $x = (r,t)$ of space-time, where $r \in \tilde{K}r_1$ and $t \in E_t(1)$.

The Euclidean group $E_t(1)$ of $E_t(1)$ consists of all time isometries, $(A|\tau)$, where $(E|\tau)$ is a time translation and A is one of the two elements, E (unit element) and E' (time inversion), of the time-inversion group $\tilde{A}$ (that is, of $O(1)$). The set Y is a 3-dimensional Euclidean vector space which is assumed to be the carrier space of a matrix representation of the groups $\tilde{K} \times E_t(1)$. This group is a subgroup of the direct product $N = E(3) \times E(1)$ of the Euclidean group of space $E(3)$ and the Euclidean group $E_t(1)$ of time, just defined. It is important to realize for what follows that the structure of the group N (sometimes called the Newton group [17]) can also be regarded as a semidirect product group:

$$N = (\mathcal{U} \times R_+) \circledS T;$$

here T is the group of all space-time translations, R_+ is the group $SO(3)$ of all proper rotations of space, and $\mathcal{U}$ is the discrete space-time group, which consists, of the unit element, space inversion I, time inversion E', and space-time inversion $I' = E'I$ ($\mathcal{U}$ has the structure of the "vierergruppe": $\mathcal{U} = \tilde{A} \times \tilde{I}$, where $\tilde{I}$ is the space-inversion group).

The fact that the vector space Y is the carrier space of a matrix representation of $\tilde{K} \times E_t(1)$ uniquely determines an action of this group on a space of functions from X' into Y, once such a representation is specified: if, relative to some basis of Y, the matrix $\Gamma(K,\chi)$ represents an element (K,χ) of $\tilde{K} \times E_t(1)$, then a function $f = \{(r,t);\ v(r,t)\}$ from X' into Y will be mapped under action of (K,χ) to the function

$$\text{(A4)} \qquad [K,\chi]\{(r,t);\ v(r,t)\} = \{(r,t);\ \Gamma(K,\chi)v(K^{-1}r,\chi^{-1}t)\}$$

In what follows it will always be assumed that such a function f is time-independent, that is, $[E,(E|\tau)]f = f$ for all time-translations $(E|\tau)$. This makes it possible to simplify notations: $\{r;v(r)\}$ will stand for f, and χ can be replaced by $A \in \tilde{A}$, so that (A4) becomes

$$\text{(A5)} \qquad [K||A]\{r;v(r)\} = \{r;\ \Gamma(K,A)\ v(K^{-1}r)\} \text{ where } (K,A) \in \tilde{K} \times \tilde{A}.$$

What the matrix representation Γ is, depends on the role played in physical theory by the vectors which constitute the vector space Y. According to the standard assumptions of the theory of electromagnetism, the field vectors, such as electric field E, magnetic induction B, polarization D, magnetization M, all generate the same representations of the R_+ by the matrices of $SO(3)$, but two different representations of the discrete space-time group $\mathcal{U}$: vectors E and P (and therefore also an electric dipole p) are multiplied by -1, +1, -1, under I, E', I', (representation Γ_+), while vectors B and M (and therefore also a magnetic

dipole, that is, a spin S) are multiplied by +1, -1, -1 (representation Γ_-). This means that in the case of electric dipole arrangements $\{r;p(r)\}$ the definition (A5) of action becomes:

$$\text{(A6)} \qquad [K\|A]\{r;p(r)\} = \{r;\ Rp(K^{-1}r)\},\quad K = (R|\ell) \in \tilde{K},$$

where $(R|\ell)$ denotes an isometry whose orthogonal part is R , and the same letter R is used for the matrix which represents that orthogonal part in the representation Γ_+. On the other hand, in the case of spin arrangements $\{r;S(r)\}$ the definition (A5) becomes:

$$\text{(A7)} \qquad [K\|A]\{r;S(r)\} = \{r;\ \eta_A\delta_R RS(K^{-1}r)\},\ K = (R|\ell) \in \tilde{K},$$

where δ_R = Det R, and η_A = +1 or -1 according as A=E or E'. Using (A6) and (A7), one is in a position to define <u>electric groups</u> and <u>magnetic groups</u>.

(D6) A group $\tilde{m}$ is called a <u>magnetic group</u> if it satisfies the following conditions:

(M1): $\tilde{m}$ is a subdirect product $\tilde{m}(\tilde{K})$ of $\tilde{K} \times \tilde{A}$, where $\tilde{K}$ is a crystallographic group, and $\tilde{A}$ is the time-inversion group;

(M2): $\tilde{m}$ is an invariance group of some spin arrangement in the sense of (A7).

A magnetic group $\tilde{m}(\tilde{K})$ is called a <u>magnetic space group</u>, or <u>magnetic point group</u>, or etc., according as $\tilde{K}$ is a space group, or a point group, or etc.

Remarks similar to those which immediately follow Definition (D2) can be repeated in this case. In particular, replacing the words "subdirect product" by the word "subgroup" would result in a definition of magnetic groups according to which each crystallographic group is a magnetic group. If such a modified definition is adopted, the crystallographic groups are called <u>trivial magnetic groups</u>, while all other magnetic groups are called <u>non-trivial magnetic groups</u> [18].

In the case of electric dipole arrangements, and the action (A6), a definition <u>mutatis mutandis</u>, identical with (D6) easily leads to the conclusion that the direct product $\tilde{K} \times \tilde{A}$ itself is, for any crystallographic group $\tilde{K}$, which does not contain space inversion I, an electric group. That is why this term is very rarely used.

Coming back to magnetic groups, it immediately follows from (M2) that no magnetic group contains the element (E,E') of $\tilde{K} \times \tilde{A}$. In fact, a definition of magnetic groups in which this property of subdirect products of $\tilde{K} \times \tilde{A}$ is postulated instead of (M2) is equivalent to (D6). Starting out from this property, one can easily show that a subdirect product $\tilde{m}(\tilde{K})$ of $\tilde{K} \times \tilde{A}$ is a magnetic group if and only if there exists a homomorphism ρ of $\tilde{K}$ onto $\tilde{A}$. The argument is the same as in the case of colour groups, and since the order of $\tilde{A}$ is 2, there are, for a fixed $\tilde{K}$, as many magnetic groups as there are subgroups ${}^2\tilde{L}$ of index 2 in $\tilde{K}$. Each (if there are any!) of these magnetic groups can thus be specified by the symbol $\tilde{m}[\tilde{K}({}^2\tilde{L})]$

or, for short, $\tilde{K}(^{2}\tilde{L})$; they are said to constitute the family of $\tilde{K}$ ($\tilde{K}$ has no family at all if it does not have sub-groups of index 2). Since the group $\tilde{A}$ and the symmetric group $^{2}\tilde{P}$ are isomorphic, one can establish a one-to-one correspondence between the magnetic groups which constitute the family of $\tilde{K}$ and the 2-colour groups (black-and-white groups) belonging to the family of $\tilde{K}$, by pairing a netic group $\tilde{m}[\tilde{K}(^{2}\tilde{L}^{(1)})]$ with a colour group $\tilde{B}[\tilde{K}(^{2}\tilde{L}^{(2)})]$ if and only if $^{2}\tilde{L}^{(1)} = {}^{2}\tilde{L}^{(2)}$. A magnetic group and a black-and-white group which are the two members of such a pair are often identified. More generally the terms "magnetic groups" and "black-and-white groups" are often regarded as synonyms. Such an identification is often useful, especially as the generally accepted definition of equivalence of magnetic groups is, mutatis mutandis, identical with the definition (D2.2) of equivalence of black-and-white groups. It then follows, for example, that the number of equivalence classes of magnetic space groups is 1191 (they are arranged into families in [18 1]). However, when considering physical consequences of a magnetic space group $\tilde{M}$ being the symmetry group of a magnetically ordered crystal it is essential to take into account the fact time inversion E' appears in some elements (K,E') of $\tilde{M}$. And this not only in quantum mechanical theories, where time inversion becomes an antiunitary operator while isometries become unitary operators, but also in classical theories; for example, in the case of magneto-electric effects [17]. It is in connection with the theory of magnetic order in crystals, where time inversion plays an important rôle, that the term "magnetic space group" was introduced by Landau and Lifshitz [19].

Each magnetic group can also be identified with an appropriate non-trivial spin group (but the converse is of course not true!); what the "appropriate" spin-group is, can be easily shown [13, 1]. However, here again one may miss some physical consequences of magnetic symmetry by considering spin groups and disregarding the role of time inversion. On the other hand, it has been shown [14] that the knowledge of spin lattice groups may make the interpretation of incomplete data concerning magnetic neutron diffraction less ambiguous.

An extensive catalogue of experimentally determined magnetically ordered crystals with classification labels [20] assigned to them using magnetic space groups is available [21]. A similar catalogue, although less complete, where the classification labels make use of spin space groups, is also available [22]. A comparison of these two kinds of classification labels can be found in [13]. The idea of using groups later called spin space groups for specifying the symmetry of magnetically ordered crystals is due to Naish [23].

6. COLOUR W-GROUPS AND SPIN W-GROUPS

An element of a colour group acting on a coloured point set $\{r;c(r)\}$ has the same effect on a colour c_i at all the points r which have the colour c_i. This is so because the action (A2) is defined in a way such that a permutation P of the

colour set does not depend on what r is. It has been pointed out by Koptsik and Kotzev [24,4] that by using the wreath product $\tilde{P} \circledW \tilde{K}$ of $\tilde{P}$ by $\tilde{K}$, instead of the direct product $\tilde{K} \times \tilde{P}$, one can define an action in such a way that a permutation of a colour set does depend on r. This can also be done, using the wreath product $\tilde{\Omega} \circledW \tilde{K}$ instead of the direct product $\tilde{K} \times \tilde{\Omega}$, in the case of spin arrangements $\{r;v(r)\}$. Having defined the action of such a wreath products on colour point sets (that is, colour functions) and on spin arrangements (that is, vector functions) respectively, one next defines colour W-groups and spin W-groups as invariance groups of such colour functions and vector function in the sense of this action. The definitions of colour W-groups and spin W-groups can be formulated in exactly the same "mathematical style" as the definitions of colour groups and spin groups formulated in Sections 3 and 4 of this paper. Such a definition of colour W-groups is formulated explicitly, and its immediate consequences discussed in [1]. A formulation of a similar definition of spin W-groups does not present any difficulty. For further development of this subject the reader may be referred to the publications of Koptsik and Kotzev [25,26].

7. CONCLUDING REMARKS

Only some of the several kinds of metacrystallographic groups mentioned in Section 2 were explicitly defined and further discussed in this paper. I wanted only to present, and to illustrate with a few examples, a fairly general uniform mathematical way of introducing such groups. Because this mathematical way is often different from that followed by other authors, and as a result the mathemathical style, terminology and notation are also quite different, it is not always a simple matter to compare these various treatments of the subject; and, in any case, it would take very many pages to do so. For example, even the term "colour group" is sometimes used in the literature for a much wider class of metacrystallographic groups than in this paper. In fact, the term "colour groups" or sometimes "generalized colour groups" seems occasionally to mean what I call here "metacrystallographic groups", and the term "colour symmetry" seems to refer to any symmetry which cannot be described by means of crystallographic groups [4,24].

The limited length of this paper has prevented me from properly defining and further discussing the super space groups, which I could only very briefly characterize in Section 2. The idea to introduce such groups for a mathematical description of the so-called modulated crystal structures is due to De Wolff [27]. It has been further developed into a formal mathematical theory by Janner and Janssen [28,29]. Super space groups may well become as important in describing the various modulated crystal structures as space groups are in the case of "ordinary" crystals.

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