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SPIN GROUPS

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Synopsis

Suggestions of Naish, Kitz, and Brinkman and Elliott to introduce groups that are more general than magnetic space groups for describing spin arrangements in magnetic crystals have not been carried out by these authors in a general and mathematically rigorous way. These deficiencies are removed in this paper by defining such more general groups, which we call spin groups (and of which magnetic groups are a special case), starting out from first principles and deducing some fundamental properties of these groups: in particular, the structure of the most general symmetry spin group of a spin arrangement is derived. The principles of constructing all spin groups and using spin groups to classify all spin arrangements are described. Also the effect of such spin-group symmetries on elastic magnetic neutron diffraction is briefly discussed.

1. *Introduction.* The term "spin" in the title and the text of this paper stands for the long descriptive phrase "magnetic moment of an atom in a magnetically ordered crystal". As is well known, spins in such a crystal are distributed and oriented according to a pattern which often shows a high degree of symmetry. To a good approximation a pattern of this kind can be described by a function $\boldsymbol{S}(\boldsymbol{r})$, defined on the set of sites $\boldsymbol{r}$ which constitute the crystal and whose values are spins $\boldsymbol{S}$. Such a function $\boldsymbol{S}(\boldsymbol{r})$ is often called a "spin arrangement"; a more precise definition $\boldsymbol{S}(\boldsymbol{r})$ is given in section 2. An often used classification of all possible spin arrangements consists in assigning to each spin arrangement a "classification label" defined in terms of "magnetic groups", and in particular "magnetic space groups" (the latter are also called "Shubnikov groups"), in ref. 1. Definitions and description of magnetic groups and a method of constructing them, the way these groups are used to classify spin arrangements, and some historical remarks on the subject can be found in a review paper by Opechowski and Guccione[2]). This classification problem has further been discussed by Opechowski and Dreyfus[1]), who have also established the equivalence of the classification of spin arrangements based on the use of magnetic groups and another classification based on the use of representations of space groups[3]).

It should be emphasized that magnetic groups are groups of space–time transformations. On the other hand, spins, that is, the values of a function $\boldsymbol{S}(\boldsymbol{r})$, are vectors of a carrier space (the "spin space") of a specific representation of the subgroup of all space–time transformations, called later in this paper the "Newton group". It follows that each element of a magnetic group induces (*via* the homomorphism which that representation constitutes) a uniquely defined transformation of the spin space onto itself. Each element of a magnetic group thus consists of two coupled transformations (one of space–time, the other of spin space). Such a pair may leave a spin arrangement invariant, or, in other words, be a "magnetic symmetry element" of the latter. All such symmetry elements of a spin arrangement constitute its "magnetic symmetry group". However for a given spin arrangement there may exist transformations of spin space alone which leave it invariant. A pair consisting of a transformation of space–time and a transformation of spin space, and which is not an element of any magnetic group, may also happen to leave that spin arrangement invariant. The purpose of this paper is to define and discuss groups which contain such "non-magnetic symmetry elements" in addition to magnetic symmetry elements. We shall call such groups "spin groups" because among them there are groups of spin-space transformations only, while no magnetic group has this property. Magnetic groups form a subclass of the class of all spin groups.

Suggestions to generalize magnetic groups in this sense, and tentative descriptions of some of the groups that we call spin groups, can be found in papers by Naish[4,5]) published in 1962 and 1963, Kitz[6]) in 1965, and by Brinkmann and Elliott[7,8]) in 1966. It is remarkable that Kitz makes no reference to Naish, and Brinkmann and Elliott make in turn no reference to either Naish or Kitz. This is however of little consequence because in none of these papers a sufficiently general, rigorous definition of spin groups is formulated which in special cases would reduce to the definition of magnetic groups. Furthermore some of the statements in Kitz's, and in Brinkmann and Elliott's papers are rather misleading. Also these authors do not make clear what spin groups are, independently of the examples used by them to illustrate their possible importance. That is why we believe that a systematic discussion of these new groups is desirable, and the purpose of this paper is to do just that. The definition of spin groups in section 2 is preceded by an explicit statement of some well-known preliminary definitions, and somewhat meticulous description of the notation used in this paper. In section 3, we discuss the structure of spin groups; in particular we define "spin-only groups" and "nontrivial spin groups", and we also discuss the relation between magnetic groups and spin groups. A gross classification of spin groups is outlined in section 4. In section 5 we give some examples of spin groups, and of the use of spin groups for defining classification labels of spin arrangements. "Spin translation groups", defined in section 4, as a subclass of the class of all spin groups, have already been applied by Litvin[9]) to the problem of interpretation of diffraction patterns resulting from magnetic scattering of neutrons by spin arrangements. "Spin-space groups", which constitute another class of spin groups (see section 4), could be used for the same purpose in a similar way; this would however require an enormous amount of preliminary work, as one can judge from the case of spin translation groups (see section 6). [A word of warning: the term "spin group" has been used by Brinkmann and Elliott (see ref. 8, page 343), in a sense which is not the same as that used in the present paper⁺.]

2. *Spin arrangements and spin symmetry groups.* First of all we introduce the following notation and terminology: $E_s(3) \times E_t(1)$ is "space–time", that is, the product space of a three-dimensional euclidean point space called the "physical space" (or simply "space") and a one-dimensional euclidean point space called "time"; $(\boldsymbol{r}, t)$ is a point of space–time in some coordinate system.

$\mathsf{E}_s(3) \times \mathsf{E}_t(1)$ is the direct product of the euclidean group consisting of all proper and improper rotations, and all translations of $E_s(3)$, and the euclidean group consisting of time inversion and all time translations of $E_t(1)$. This direct product group will be called, as has been proposed recently[10]), the "Newton group". (The Newton group is a subgroup of the Poincaré group, consisting of all those elements of the latter for which the velocity parameter is zero.)

$((R \mid \boldsymbol{v}), (A \mid \tau))$ is an element of the Newton group; here R is any 3×3 (proper or improper) rotation matrix, $\boldsymbol{v}$ is any 3×1 (column) translation matrix, A is an element of the "time-inversion group" A consisting of the unit element $E = 1$ and time inversion $E' = -1$, and τ is any real number (that specifies a time translation). An element of the Newton group maps a point $(\boldsymbol{r}, t)$ to the point $((R \mid \boldsymbol{v})\, \boldsymbol{r}, (A \mid \tau)\, t)$, where $(R \mid \boldsymbol{v})\, \boldsymbol{r} = R\boldsymbol{r} + \boldsymbol{v}$, $(A \mid \tau) = At + \tau$.

V_1^+ is a three-dimensional carrier space of the irreducible matrix representation $((R \mid \boldsymbol{v}), (A \mid \tau)) \to D_1^+ (R \mid \boldsymbol{v}) \times \Gamma^- (A \mid \tau)$ of the Newton group, where $D_1^+ (R \mid \boldsymbol{v}) = \delta_R R$, $\delta_R = \det R$ and $\Gamma_1^- (A \mid \tau) = \delta_A$, $\delta_A = 1$ if $A = E$; $\delta_A = -1$ if $A = E'$. Therefore, to an element $((R \mid \boldsymbol{v}), (A \mid \tau))$ of the Newton group corresponds a transformation of the vector space V_1^+ onto itself. Under such a transformation a vector $\boldsymbol{S}$ of V_1^+ is mapped to a vector denoted by $[(R \mid \boldsymbol{v}), (A \mid \tau)]\, \boldsymbol{S}$. Choosing a basis in V_1^+ we shall write

$$[(R \mid \boldsymbol{v}), (A \mid \tau)]\, S^i = \sum_{j=1}^{3} [D_1^+ (R \mid \boldsymbol{v}) \times \Gamma_1^- (A \mid \tau)]_{ij}\, S^j = \delta_A\, \delta_R \sum_{j=1}^{3} R_{ij} S^j, \quad (1)$$

where $i = 1, 2, 3$.

⁺ After this work was completed we have received from Mr. T. Dreyfus, Université de Genève, preprints of two Communications of the Joint Institute for Nuclear Research, Dubna 1973, USSR (P4-7513 and P4-7514) by V.A. Koptsik, J.N. Kotzev and Ah.-N.M. Kuzhukeev, in which, in connection with the problem of symmetry and classification of spin arrangements, the authors describe groups which are generalizations of magnetic space groups and which (with an appropriate interpretation of their terminology) seem to be identical with spin groups. However, their treatment of the problem is essentially different from ours.

We consider a subset $C_s(3) \times E_t(1)$ of space–time where $C_s(3)$ consists of those points $\boldsymbol{r}$ in $E_s(3)$ at which the atoms in a crystal are located. A "spin arrangement" is defined as a function $\boldsymbol{S}(\boldsymbol{r}, t)$ which maps points $(\boldsymbol{r}, t)$ of $C_s(3) \times E_t(1)$ to vectors $\boldsymbol{S}$ of the vector space V_1^+. The vector space V_1^+ will be called the "spin space" and the vectors $\boldsymbol{S}$ are called "spins". Because the spin space is the carrier space of a representation of the Newton group, each transformation $((R \mid \boldsymbol{v}), (A \mid \tau))$ of space–time implies the transformation given by eq. (1) of the spin space. Consequently, a spin arrangement $\boldsymbol{S}(\boldsymbol{r}, t)$ is transformed by an element of the Newton group into the spin arrangement denoted by $[(R \mid \boldsymbol{v}), (A \mid \tau)]\, \boldsymbol{S}(\boldsymbol{r}, t)$ where

$$\begin{aligned}
&[(R \mid \boldsymbol{v}), (A \mid \tau)]\, S^i(\boldsymbol{r}, t) \\
&= \sum_{j=1}^{3} [D_1^+ (R \mid \boldsymbol{v}) \times \Gamma_1^- (A \mid \tau)]_{ij}\, S^j ((R \mid \boldsymbol{v})^{-1} \boldsymbol{r}, (A \mid \tau)^{-1} t) \\
&= \delta_A\, \delta_R \sum_{j=1}^{3} R_{ij} S^j\, [(R \mid \boldsymbol{v})^{-1} \boldsymbol{r}, (A \mid \tau)^{-1} t], \qquad i = 1, 2, 3.
\end{aligned} \tag{2}$$

We will interpret the symbol $[(R \mid \boldsymbol{v}), (A \mid \tau)]$ as an operator on the space of all spin arrangements on a given crystal.

Since we are interested in spin arrangements defined on a specified crystal $C_s(3)$, we consider only the subgroup of the Newton group which transforms that crystal $C_s(3)$ onto itself. In other words, we consider the subgroup $\mathsf{F} \times \mathsf{E}_t(1)$ of the Newton group, where F consists of all elements $F = (R \mid \boldsymbol{v})$ of the space group of the crystal $C_s(3)$. We restrict ourselves to the case of static spin arrangements, that is to spin arrangements invariant under time translations $\boldsymbol{S}(\boldsymbol{r}, t + \tau) = \boldsymbol{S}(\boldsymbol{r}, t)$ and therefore replace $(A \mid \tau)^{-1} t$ by t on the right-hand side of eq. (2). We also restrict our discussion to the subgroup $\mathsf{G} = \mathsf{F} \times \mathsf{A}$ of $\mathsf{F} \times \mathsf{E}_t(1)$, the invariance of spin arrangements under time translations always being understood without being stated explicitly. Eq. (2) becomes for elements (F, A) of G:

$$[F, A]\, S^i(\boldsymbol{r}, t) = \delta_A\, \delta_R \sum_{j=1}^{3} R_{ij} S^j (F^{-1}\boldsymbol{r}, t). \tag{3}$$

We will introduce a new notation $[\delta_A \delta_R R \parallel (R \mid \boldsymbol{v}), A]$ for the operator $[F, A]$ in eq. (3), where to the right of the double vertical bar is the element (F, A) of the group G, a transformation of space–time, and to the left is the matrix which describes the corresponding transformation of spin space. In this notation eq. (3) becomes

$$[\delta_A \delta_R R \parallel F, A]\, S^i(\boldsymbol{r}, t) = \delta_A\, \delta_R \sum_{j=1}^{3} R_{ij} S^j (F^{-1}\boldsymbol{r}, t), \tag{4}$$

where $F = (R \mid \boldsymbol{v})$.

Because of the assumed invariance of spin arrangements under time translations, $\boldsymbol{S}(\boldsymbol{r}, t) = \boldsymbol{S}(\boldsymbol{r}, t')$ for any t and t', and in particular for $t' = -t$. Therefore the same value of t appears on both sides of eqs. (3) and (4). For this reason we shall write from now on $\boldsymbol{S}(\boldsymbol{r})$ instead of $\boldsymbol{S}(\boldsymbol{r}, t)$, as is customary. Eq. (3) becomes

$$[F, A]\, S^i(\boldsymbol{r}) = \delta_A\, \delta_R \sum_{j=1}^{3} R_{ij} S^j (F^{-1}\boldsymbol{r}) \tag{5}$$

and eq. (4) becomes

$$[\delta_A \delta_R R \parallel F]\, S^i(\boldsymbol{r}) = \delta_A\, \delta_R \sum_{j=1}^{3} R_{ij} S^j (F^{-1}\boldsymbol{r}), \tag{6}$$

where the symbol A appearing to the right of the double bar in eq. (4) has been omitted, corresponding to our having dropped t in $\boldsymbol{S}(\boldsymbol{r}, t)$. Eq. (5) is the definition of the spin arrangement into which $\boldsymbol{S}(\boldsymbol{r})$ is transformed by an element of G in the notation of Opechowski and Dreyfus[1]) and eq. (6) is the same definition in the new notation.

The operators $[\delta_A\, \delta_R R \parallel R \mid \boldsymbol{v}]$ are operators on the space of all spin arrangements on a given crystal and consist of pairs of transformations, a transformation of space–time and a transformation of spin space. A characteristic of the operators $[\delta_A\, \delta_R R \parallel R \mid \boldsymbol{v}]$ which correspond to elements of G is that the same proper or improper rotation matrix R appears both to the right and to the left of the double bar. We now introduce additional operators on the space of all spin arrangements on a given crystal which are transformations of spin space only, and are identity transformations of space–time. These operators will be denoted by $[B \parallel E \mid 0]$ where B is a 3×3 matrix describing any proper or improper rotation of the spin space. Consequently a spin arrangement $\boldsymbol{S}(\boldsymbol{r})$ is transformed by an operator $[B \parallel E \mid 0]$ into the spin arrangement

$$[B \parallel E \mid 0]\, S^{(i)}(\boldsymbol{r}) = \sum_{j=1}^{3} B_{ij} S^{(j)} (\boldsymbol{r}). \tag{7}$$

Since both the operators $[B \parallel E \mid 0]$ and the operators $[\delta_A\, \delta_R R \parallel R \mid \boldsymbol{v}]$ are defined on the same space (the space of all spin arrangements on a given crystal), we can define their products $[B \parallel E \mid 0]\, [\delta_A\, \delta_R R \parallel R \mid \boldsymbol{v}] = [\delta_A\, \delta_R BR \parallel R \mid \boldsymbol{v}]$. All such products will generate a group which is the direct product $\boldsymbol{\Omega}_B \times \boldsymbol{\Omega}_F$ of the group $\boldsymbol{\Omega}_B$ consisting of all operators of the form $[B \parallel E \mid 0]$, and the group $\boldsymbol{\Omega}_F$ consisting of all operators of the form $[E \parallel R \mid \boldsymbol{v}]$, where $(R \mid \boldsymbol{v})$ is an element of the space group F of the crystal. (While B is thus an arbitrary proper or improper rotation of the spin space, R is subject to the usual crystallographic restrictions.)

From eqs. (4) and (7) we conclude that an element of $\boldsymbol{\Omega}_B \times \boldsymbol{\Omega}_F$ acts on a spin arrangement as follows:

$$[B \parallel R \mid \boldsymbol{v}]\, S^{(i)}(\boldsymbol{r}) = \sum_{j=1}^{3} B_{ij} S^{(j)} [(R \mid \boldsymbol{v})^{-1}\, \boldsymbol{r}]. \tag{8}$$

A spin arrangement is said to be "invariant" under $[B \| R \mid \boldsymbol{v}]$ if $[B \| R \mid \boldsymbol{v}]\, \boldsymbol{S}(\boldsymbol{r}) = \boldsymbol{S}(\boldsymbol{r})$. We shall also say in such a case that $[B \| R \mid \boldsymbol{v}]$ is a "symmetry element" of $\boldsymbol{S}(\boldsymbol{r})$. The set of all symmetry elements of $\boldsymbol{S}(\boldsymbol{r})$ is called the "symmetry group" of $\boldsymbol{S}(\boldsymbol{r})$. We now define a spin group: a subgroup of $\boldsymbol{\Omega}_B \times \boldsymbol{\Omega}_F$ will be called a "spin group" if it is the symmetry group of some spin arrangement.

It should be pointed out that the definitions (4), (6), (7) and (8) of operators are somewhat different from those introduced in ref. 9 on spin translation groups. This modification of definitions does not require any changes in tables 1 and 2 of ref. 9, except replacing primes by horizontal bars (which corresponds to replacing E' by $\bar{E}$, as defined here in section 3).

3. *Structure of spin groups.* In this section we first consider the structure and a method of deriving subgroups of the direct product of two arbitrary groups. We then determine the structure of spin groups.

Let $\mathscr{B}$ and $\mathscr{F}$ be two arbitrary groups. $\mathscr{B} \times \mathscr{F}$ is the direct product of the groups $\mathscr{B}$ and $\mathscr{F}$ whose elements are denoted by $(B \| F)$. The identity, product, and inverse of elements of $\mathscr{B} \times \mathscr{F}$ are respectively, $(E \| E)$, $(B_1 \| F_1)(B_2 \| F_2) = (B_1 B_2 \| F_1 F_2)$ and $(B \| F)^{-1} = (B^{-1} \| F^{-1})$. Although we shall be interested only in the cases where $\mathscr{F}$ is the euclidean group of the "physical space" and $\mathscr{B}$ is the group of the 3×3 matrices which represent all proper and improper rotations of the "spin space", the following argument is quite general.

Let X denote an arbitrary subgroup of $\mathscr{B} \times \mathscr{F}$. Then the left-hand side members of the elements $(B \| F)$ of X form a subgroup B of $\mathscr{B}$, the right-hand side elements form a subgroup F of $\mathscr{F}$. We will say that X belongs to the "family of B and F" if the left-hand side and right-hand side members constitute, respectively, the groups B and F.

A method of deriving all subgroups X of $\mathscr{B} \times \mathscr{F}$ belonging to the family of B and F is based on an "isomorphism theorem" which Zamorzaev[11]) used recently in connection with a study of groups which are related to spin symmetry groups (a proof of this theorem is given in the appendix): let X be a group belonging to the family of B and F, and let $\mathsf{b} = \mathsf{B} \cap \mathsf{X}$ and $\mathsf{f} = \mathsf{X} \cap \mathsf{F}$; then the quotient groups B/b and F/f are isomorphic.

Using this isomorphism theorem one constructs all groups belonging to the family of B and F as follows. First one finds all normal subgroups f of F and b of B such that F/f is isomorphic to B/b. For each pair of subgroups f and b and each isomorphism between F/f and B/b, both F and B are written as coset decompositions

$$\mathsf{F} = \mathsf{f} + F_2\mathsf{f} + \cdots + F_n\mathsf{f},$$

$$\mathsf{B} = \mathsf{b} + B_2\mathsf{b} + \cdots + B_n\mathsf{b},$$

where $F_i\mathsf{f}$ and $B_i\mathsf{b}$, for every i, are cosets which are mapped on each other by the isomorphism of F/f and B/b. Next one pairs every element of the ith coset of B with every element of the ith coset of F; the symbol $(B_i\mathsf{b} \parallel F_i\mathsf{f})$ will denote this set of pairs. The set consisting of the elements of all the sets $(B_i\mathsf{b} \parallel F_i\mathsf{f})$, $i = 1,2,\ldots,n$, will then constitute a group X belonging to the family of B and F. We shall write:

$$\mathsf{X} = (\mathsf{b} \parallel \mathsf{f}) + (B_2 \parallel F_2)(\mathsf{b} \parallel \mathsf{f}) + \cdots + (B_n \parallel F_n)(\mathsf{b} \parallel \mathsf{f}). \tag{9}$$

As an example of constructing such groups, we consider a group belonging to the family of B and F where, using the "international notation", $\mathsf{B} = \mathsf{mm2}$ and $\mathsf{F} = 4/\mathsf{m}$. We construct a group by taking $\mathsf{b} = 2$ and $\mathsf{f} = \bar{4}$. The coset decompositions are:

$$\mathsf{mm2} = 2 + m_x 2,$$

$$\bar{4}/\mathsf{m} = \bar{4} + \bar{1}\,\bar{4}.$$

The pairing of elements of corresponding cosets means that each of the four elements of $\bar{4}$ (the first coset of $4/\mathsf{m}$) are paired with each of the two elements of 2 (the first coset of mm2). This gives the eight elements:

$$(1 \parallel 1), (1 \parallel \bar{4}_z), (1 \parallel 2_z), (1 \parallel \bar{4}_z^{-1}),$$

$$(2_z \parallel 1), (2_z \parallel \bar{4}_z), (2_z \parallel 2_z), (2_z \parallel \bar{4}_z^{-1}),$$

which are denoted by $(2 \parallel \bar{4})$ in the notation $(\mathsf{b} \parallel \mathsf{f})$ used in eq. (9). The pairing of elements of the coset of $\bar{4}$ with those of the coset of 2 gives the eight elements:

$$(m_x \parallel \bar{1}), (m_x \parallel 4_z), (m_x \parallel m_z), (m_x \parallel 4_z^{-1}),$$

$$(m_y \parallel \bar{1}), (m_y \parallel 4_z), (m_y \parallel m_z), (m_y \parallel 4_z^{-1}),$$

which are the eight elements given above multiplied by $(m_x \parallel \bar{1})$. These are denoted by $(m_x \parallel \bar{1})(2 \parallel \bar{4})$ in the notation $(B_2 \parallel F_2)(\mathsf{b} \parallel \mathsf{f})$ used in eq. (9). The group obtained in this way is then:

$$\mathsf{X} = (2 \parallel \bar{4}) + (m_x \parallel \bar{1})(2 \parallel \bar{4}).$$

We now consider the case where $\mathscr{B}$ is the group of 3×3 orthogonal matrices in the spin space, and $\mathscr{F}$ is the euclidean group in the physical space. Elements $(B \parallel F)$ of the direct product $\mathscr{B} \times \mathscr{F}$ are now identified with operators $[B \parallel F]$, see eq. (8), on the set of all spin arrangements defined on a given crystal.

We now derive conditions which a subgroup of $\mathscr{B} \times \mathscr{F}$ must satisfy if it is to be a spin group as defined in section 2. Since spin arrangements are defined on crystals, every spin group belongs to a family of B and F, where F is a crystallographic group. Spin arrangements may be classified into three kinds, linear arrangements, where all spins are collinear, planar arrangements, where all spins are coplanar, and spatial arrangements which include all remaining possibilities. Every spin group contains as a subgroup a group $[\mathsf{b} \parallel E]$, denoted for simplicity by b, which consists of those elements $[B \parallel E]$ which are transformations of the spin space only, and leave a spin arrangement invariant. The group b depends only on the kind of spin arrangement, and will be called a "spin-only group". The spin-only groups for the three kinds of spin arrangements are (see Kitz[6]):

$$\mathsf{b}_l = \mathsf{C}_\infty + \bar{C}_2\mathsf{C}_\infty, \qquad \mathsf{b}_p = \{E, \bar{C}_2\}, \qquad \mathsf{b}_s = E. \tag{10}$$

Here the indices l, p, s denote linear, planar and spatial spin arrangements respectively; C_∞ is the group of matrices representing all proper rotations of the spin space about the common direction of spins; C_2 is the matrix representing a rotation through angle π, which is about an axis perpendicular to that direction in the case of b_l, and to the plane of spins in the case of b_p. Matrix C_2 multiplied by -1 is denoted by $\bar{C}_2$.

In the coset decomposition of B into cosets of a spin-only group b the coset representatives can always be chosen such that they constitute a group B^*, and such that $\mathsf{B} = \mathsf{b} \times \mathsf{B}^*$. The group B^* is not uniquely determined by the groups B and b, except in the case of spatial spin arrangement, where b is the identity group E and therefore $\mathsf{B}^* = \mathsf{B}$. However, for linear spin arrangements the group B^* can (and always will) be taken to be the identity group E or the group $\{E, \bar{E}\}$; and for planar spin arrangements the group B^* can (and always will) be taken to be a rotation group of a two-dimensional subspace of the spin space.

Spin groups are then subgroups of $\mathscr{B} \times \mathscr{F}$ belonging to a family of $\mathsf{b} \times \mathsf{B}^*$ and F, where b is a spin-only group as defined by eq. (10), B^* is a subgroup of $\mathscr{B}$, and F is a crystallographic group. Let us denote by $E, B_2^*, B_3^*, \ldots, B_n^*$, the elements of B^*. In view of eq. (9), these properties of spin groups imply that each spin group Z_b is the direct product of a spin-only group b and another group which we call a "nontrivial spin group" Z,

$$\mathsf{Z}_\mathsf{b} = \mathsf{b} \times \mathsf{Z}, \tag{11a}$$

where

$$\mathsf{Z} = [E \parallel \mathsf{f}] + [B_2^* \parallel F_2]\,[E \parallel \mathsf{f}] + \cdots + [B_m^* \parallel F_m]\,[E \parallel \mathsf{f}]. \tag{11b}$$

A nontrivial spin group Z thus belongs to the family of B^* and F, and contains a subgroup f such that F/f is isomorphic to B^*. From the isomorphism theorem formulated earlier in this section, it follows then that Z is isomorphic to F. In other words Z is an extension of f by B^*. Therefore an element of a nontrivial spin group Z is always of the form $[B(F)^* \parallel F]$, that is, each element of F is paired in Z with one and only one element of B^*. Since the spin-only groups are known [see eq. (10)], to derive all spin groups one needs only to derive all non-trivial spin groups.

We have thus shown that each spin group Z_b has a structure described by eqs. (11a) and (11b). We will now show that, conversely, each group X_b whose structure is described by these equations is the symmetry group of a spin arrangement, and therefore is a spin group.

A crystal invariant under a space group F can be partitioned into "simple crystals" each of which consists of atoms whose positions can be obtained by applying all elements of the space group F to any atom position $\boldsymbol{r}$, and is said to be generated by F from $\boldsymbol{r}$. If an atom position $\boldsymbol{r}$ in a simple crystal is such that the equation $F_l\boldsymbol{r} = F_k\boldsymbol{r}$ implies $F_l = F_k$ then the position is called a "general position"; otherwise one speaks of a "special position". A crystal consisting of n simple crystals generated by F from positions $\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_n$ will be denoted by $[\mathsf{F}; \boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_n]$.

Consider a crystal $[\mathsf{F}; \boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_n]$, that is, an atom arrangement for which F is its space group. Suppose that $\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_n$ are general positions with $n \geqq 3$, and F is the symmetry group of the crystal. On this crystal we will now construct a spin arrangement whose symmetry group is a given group $\mathsf{X}_\mathsf{b} = \mathsf{b} \times \mathsf{X}$, where X is defined by the right-hand side of eq. (11b) in which F has been replaced by some proper or improper subgroup L of F. It is well known[1,2]) that the coset decomposition of F is

$$\mathsf{F} = \mathsf{L} + \mathsf{L}F_2 + \mathsf{L}F_3 + \cdots;$$

then a simple crystal $\mathsf{F}\boldsymbol{r}_j$ can be regarded as composed of a certain number of interlocking simple atom arrangements generated by L from the atoms located at $\boldsymbol{r}_j$, $F_2\boldsymbol{r}_j$, $F_3\boldsymbol{r}_j, \ldots$ Therefore we can replace the symbol $[\mathsf{F}; \boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_n]$ by the symbol $[\mathsf{L}; \boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3, \ldots]$.

To each atom position $\boldsymbol{r}_j$ appearing in $[\mathsf{L}; \boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3, \ldots]$ we assign a spin $\boldsymbol{\sigma}_j$ such that: 1) each $\boldsymbol{\sigma}_j$ is invariant under the spin-only group b, but are not all collinear in the case of $\mathsf{b} = \mathsf{b}_\mathrm{p}$, not all coplanar in the case of $\mathsf{b} = \mathsf{b}_\mathrm{s}$; 2) no two spins $\boldsymbol{\sigma}_j$ and $\boldsymbol{\sigma}_k$, $j \neq k$, have the same magnitude. A spin arrangement on $[\mathsf{L}; \boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3, \ldots]$ is now constructed by assigning to the atom located at $L\boldsymbol{r}_j$ the spin $B^*(L)\,\boldsymbol{\sigma}_j$:

$$S(L\boldsymbol{r}_j) = B^*(L)\,\boldsymbol{\sigma}_j.$$

It is not difficult to verify that the symmetry group of the spin arrangement obtained in this way is in fact the group X_b. We shall say that this spin arrangement is "generated" by X from the spins $\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \boldsymbol{\sigma}_3, \ldots$

We would like to mention that even if the spins of a spin arrangement all have the same magnitude, it may not be possible to generate it by a spin group from a single spin [see example 2, case (b), and example 3, in section 5 below].

In the case of a spin arrangement generated by a group defined by eq. (11) from a single spin $\boldsymbol{\sigma}$, the number of distinct spin orientations in such a spin arrangement does not exceed the order m of the group B^*. For example, in the case of a ferromagnetic spin arrangement (that is, one spin orientation) B^* is the identity group; and in the case of a linear antiferromagnetic spin arrangement (that is, two distinct spin orientations) B^* is the group of order 2 consisting of E and $\bar{E}$.

We are now in a position to describe the relations between magnetic groups (as defined in ref. 2), spin groups, and nontrivial spin groups. First of all we observe that, since $\mathsf{b}_s = \mathsf{E}$, a spin group of a spatial spin arrangement is always a nontrivial spin group. Next we show that it is possible to make correspond to each magnetic group m a group $[\mathsf{m}]$ of operators $[B^*(F) \parallel F]$ such that m and $[\mathsf{m}]$ are isomorphic. To see that, it is sufficient to recall that an element of m has the form $(F, A(F))$, where $A(F)$ is an element of time-inversion group. Therefore acting with $(F, A(F))$ on a spin arrangement $S(\boldsymbol{r})$ gives rise to another spin arrangement, which in the notation of eq. (5) is denoted by $[F, A(F)]\, S(\boldsymbol{r})$, and in the operator notation of eq. (6) becomes $[\delta_{A(F)}\delta_R R \parallel F]\, S(\boldsymbol{r})$, where $F = (R \mid \boldsymbol{v})$. Hence to each element $(F, A(F))$ of m we can make correspond the operator $[\delta_{A(F)}\delta_R R \parallel F]$, and the group m is isomorphic to the spin group $[\mathsf{m}]$ constituted by these operators. This means that the group $[\mathsf{m}]$ is a spin group because using $[\mathsf{m}]$ one can generate a spatial spin arrangement whose symmetry group is $[\mathsf{m}]$ itself.

4. *Principles of the derivation and classification of nontrivial spin groups.* We have already indicated in section 3 the general principle of a derivation of spin groups based on the isomorphism theorem. We will now apply that general principle to specific classes of nontrivial spin groups.

Since only nontrivial spin groups will be considered in this section we will drop the adjective "nontrivial", thus in this section "spin group" will mean "nontrivial spin group". Correspondingly we will write B for the group previously denoted by B^*. A spin group belonging to a family of B and F will be called a spin space group, a spin translation group, or a spin point group, according as F is, respectively, a space group, translation group, or point group. We will divide these three kinds of spin groups into classes in a way analogous to the well-known classification of space groups, translation groups, and point groups into, respectively, 230, 14 and 32 classes.

4.1. Spin point groups. Spin point groups, denoted by R_s, belong to a family of B and R, where B is a subgroup of $\mathscr{B}$ and R is a point group belonging to one of the 32 classes of point groups. To derive all spin point groups one proceeds as follows. For a specific group R one first finds all normal subgroups r of R and then those groups B which are isomorphic to R/r. Each pair of groups B and r, and each isomorphism between B and R/r determines, because of the isomorphism theorem of section 3 in the case where **b** = E, one spin point group belonging to the family of B and R. By taking each group R in turn, one finds in this way all spin point groups.

For the purpose of classifying spin point groups we denote by $\mathscr{K}$ the linear group GL (3) in spin space, and by $\mathscr{A}$ the affine group GIL (3) in physical space. Spin groups, which are subgroups of $\mathscr{B} \times \mathscr{F}$, are also subgroups of $\mathscr{K} \times \mathscr{A}$. Spin point groups are classified into classes of conjugate subgroups of $\mathscr{K} \times \mathscr{A}$, that is two spin point groups are said to belong to the same "class of spin point "groups" if they are conjugate subgroups of $\mathscr{K} \times \mathscr{A}$. (This is analogous to the classification of point groups R into 32 classes of conjugate subgroups of $\mathscr{A}$.) One finds that there are 655 classes of spin point groups[12]).

For example, taking a specific point group R belonging to the class **mm2** one finds in this way 28 spin point groups. However, the number of classes of spin point groups turns out to be in this case only 13.

4.2. Spin translation groups. Spin translation groups, denoted by T_s, belong to a family of B and T, where B is a subgroup of $\mathscr{B}$, and T is a translation group belonging to one of the 14 Bravais classes of translation groups. A method of deriving all spin translation groups is described in detail in ref. 9.

Classifying the translation groups T into classes of conjugate subgroups of $\mathscr{A}$ results, as is well known, in no classification at all, all groups T belonging to the same unique class. It follows that if we were to classify the spin translation groups into classes of conjugate subgroups of $\mathscr{K} \times \mathscr{A}$ we would find a classification independent of T; in fact, we would find a classification of the subgroups of the orthogonal group in physical space which as a classification of spin translation groups is too "coarse" for our purposes. To obtain a more satisfactory classification we therefore define, again in analogy with what one does to classify the translation groups, the "holohedry" H_s of a spin translation group T_s. The holohedry H_s of T_s is the group of all elements $[B \parallel R \mid 0]$ of $\mathscr{B} \times \mathscr{F}$ such that

$$[B^{-1} \parallel R^{-1} \mid 0]\, \mathsf{T}_s\, [B \parallel R \mid 0] = \mathsf{T}_s .$$

Let us consider now the subgroup of $\mathscr{B} \times \mathscr{F}$ generated by T_s and the holohedry H_s of T_s. One can show that the subgroup so defined is the semidirect product $\mathsf{H}_s \wedge \mathsf{T}_s$ of its subgroups H_s and T_s. Two spin translation groups will be said to belong to the same "Bravais class of spin translation groups" if the semidirect products $\mathsf{H}_s \wedge \mathsf{T}_s$ for the two spin translation groups are conjugate subgroups of $\mathscr{K} \times \mathscr{A}$. A list of all Bravais classes of three-dimensional spin translation groups has been given by Litvin[9]).

4.3. Spin space groups. A spin space group denoted by F_s belongs to a family of B and F, where B is a subgroup of $\mathscr{B}$ and F is a space group. A spin space group F_s will be called "symmorphic" or "nonsymmorphic" according as F is a symmorphic or a nonsymmorphic space group.

We have seen in section 3 that every element of a spin group, hence in particular of a spin space group, F_s, is of the form $[B(F) \parallel F]$ where $B(F)$ denotes that element of B which is associated with the element F of F. The elements of the form $[B(t) \parallel E \mid t]$ constitute a normal subgroup T_s of F_s, the spin translation subgroup T_s belonging to the family of $B(T)$ and T. We shall denote the coset representatives of T_s in F_s by $[B(R) \parallel R \mid \tau(R)]$.

From the definition of the holohedry H_s of a spin translation group T_s, and the fact that T_s is a normal subgroup of F_s, it follows that the elements $[B(R) \parallel R \mid 0]$ {for nonsymmorphic spin space groups, these are $[B(R) \parallel R \mid \tau(R)]$ on setting $\tau(R) = 0$}, are contained in the holohedry H_s of T_s. In symmorphic spin space groups, the set of elements $\{[B(R) \parallel R \mid 0]\}$ constitute a group, a spin point group R_s contained in the holohedry H_s of T_s. In nonsymmorphic spin space groups the set of elements $\{[B(R) \parallel R \mid \tau(R)]\}$ do not in general constitute a group, but the $B(R)$, for all R, satisfy the relations

$$B(R_i)\, B(R_j) = B(t_{ij})\, B(R_i R_j), \tag{12}$$

where $t_{ij} = \tau(R_i) + R_i \tau(R_j) - \tau(R_i R_j)$ belongs to T.

Consequently, a method of deriving all spin space groups is as follows. We first consider the case of symmorphic spin space groups. Let F be a symmorphic space group, the semidirect product of its translation group T and its point group R, and let T_s be a spin translation group belonging to a family of $B(T)$ and T, and R_s a spin point group belonging to a family of $B(R)$ and R, and contained in the holohedry H_s of T_s. One constructs all symmorphic spin space groups F_s belonging to a family of B and F by taking the semidirect product of each spin translation group T_s with each of the spin point groups R_s contained in the holohedry H_s of T_s. By taking, in turn, all symmorphic space groups F one obtains all symmorphic spin space groups.

Let F be a nonsymmorphic space group containing the translation group T and the rotations of the point group R, and let T_s be a spin translation group belonging to a family of $B(T)$ and T. One constructs all nonsymmorphic spin space groups F_s belonging to a family of B and F by taking the semidirect product of each proper spin translation group T_s with each set of elements $\{[B(R) \parallel R \mid \tau(R)]\}$ where $\{[B(R) \parallel R \mid 0]\}$, the corresponding set where $\tau(R) = 0$, is a set of elements contained in the holohedry H_s of T_s and such that the $B(R)$, for all R of R, satisfy relations (12). By taking in turn all nonsymmorphic space groups F one obtains all nonsymmorphic spin space groups.

We classify spin space groups as follows. Two spin space groups are said to belong to the same "class of spin space groups" if they are conjugate subgroups of $\mathscr{K} \times \mathscr{A}$ and if the element $[K \parallel L \mid v]$ of $\mathscr{K} \times \mathscr{A}$, which transforms one subgroup into the other is such that $\det K > 0$ and $\det L > 0$. The latter condition is imposed to obtain a classification analogous to the usual classification of crystallographic space groups, where two space groups are defined to belong to the same class of space groups if they are conjugate subgroups of $\mathscr{A}$ and if the element $(L \mid \boldsymbol{v})$ of $\mathscr{A}$ which transforms one subgroup into the other is such that $\det L > 0$.

5. *Classification labels of spin arrangements by means of spin groups.* In this section we discuss three examples of assigning a spin group to a given spin arrangement.

5.1. Example 1. This is the case of a simple spiral spin arrangement considered in ref. 2, p. 160. The simple crystal on which this spin arrangement is defined is generated by the group $P422$ from a point $\boldsymbol{r}_0 = (\frac{1}{2}, \frac{7}{8}, 0)$ using the edge lengths of a tetragonal unit cell as units. In terms of magnetic groups this spin arrangement is uniquely specified by a "Cl′ label" in the sense of Opechowski and Dreyfus[1]) as follows:

$$[P4_z2_x2_{xy}; p4_z; S(\boldsymbol{r}_0) = (S_x, S_y, 0); S((1 \mid 00n)\, \boldsymbol{r}_0) = R^n_\psi S(\boldsymbol{r}_0)].$$

This label indicates that the spin arrangement is specified by two groups: the trivial two-dimensional magnetic space group $p4$, and an infinite rotation group $\langle R_\psi \rangle$ generated by a rotation R_ψ through angle ψ about the z axis. Using spin groups these two groups can be replaced for the purpose of specifying the spin arrangement by a single spin group. The corresponding label is as follows:

$$[P4_z2_x2_{xy};\ \mathrm{b}_{p_z} \times P_{11R_\psi}(4_z \parallel 4_z)(\bar{2}_a \parallel 2_x)(\bar{2}_{ab} \parallel 2_{xy});\ S(\boldsymbol{r}_0) = S\boldsymbol{a}].$$

Here b_{p_z} is the spin-only group of any planar spin arrangement in the xy plane. The nontrivial group is given in a modified international notation consisting of symbols which denote the generators of the group; P_{11R_ψ} is the nontrivial spin translation group generated by $(1 \parallel 1 \mid 100)$, $(1 \parallel 1 \mid 010)$, $(R_\psi \parallel 1 \mid 001)$, and is a subgroup of a nontrivial spin group generated by these translations and the elements $(4_z \parallel 4_z)$, $(\bar{2}_a \parallel 2_x)$, $(\bar{2}_{ab} \parallel 2_{xy})$; $\boldsymbol{b}$ is a unit vector perpendicular to $\boldsymbol{a}$ in the xy plane. This nontrivial spin group is then used to generate the spin arrangement from $S(\frac{1}{2}, \frac{7}{8}, 0)$ which will then clearly be identical with the spin arrangement generated from the same spin by the two groups appearing in the Cl′ label.

5.2. Example 2. This is the case of the spin arrangement defined on a crystal generated by the space group $Pbnm$ from an atom located at $\boldsymbol{r}_1 = (x, y, \frac{1}{4})$; the spin arrangement is specified by the following Cl′ label:

(a) $[Pbnm; P_{2a}2_1/m'; S(\boldsymbol{r}_1) = (S_x, S_y, 0), S(\boldsymbol{r}_3) = (S_y, -S_x, 0)]$

here $r_3 = (\frac{1}{2} + x, \frac{1}{2} - y, \frac{3}{4})$. For details, see ref. 1, p. 482, where this spin arrangement was (incorrectly) assumed to be that of the Dy spins in $DyCrO_3$. The actual spin arrangement (see Van Laar[13]) in this case is

(b) $[Pbnm; P_{2a}2_1/m'; \boldsymbol{S}(\boldsymbol{r}_1) = (S_x, S_y, 0), \boldsymbol{S}(\boldsymbol{r}_3) = (S_x, -S_y, 0)]$.

The difference between the spin arrangements (a) and (b) is that in case (a) $\boldsymbol{S}(\boldsymbol{r}_1) \cdot \boldsymbol{S}(\boldsymbol{r}_3) = 0$ while this is not so in case (b).

Using spin groups the corresponding labels are:

(a) $[Pbnm; \mathrm{b}_{p_z} \times P_{2_z2_z1}\,(4_z \parallel b)\,(4_z^{-1} \parallel n)\,(1 \parallel m); \boldsymbol{S}(\boldsymbol{r}_1) = (S_x, S_y, 0)]$,

(b) $[Pbnm; \mathrm{b}_{p_z} \times P_{2_z2_z1}\,(2_z \parallel 2_1)/(1 \parallel m);$

$\boldsymbol{S}(\boldsymbol{r}_1) = (S_x, S_y, 0), \boldsymbol{S}(\boldsymbol{r}_3) = (S_x, -S_y, 0)]$.

We see that in case (a) using a spin group makes it possible to generate the spin arrangement from a single spin while this was not possible using the Cl′ label. However it is in general not true that replacing the Cl′ classification (based on magnetic groups) by the classification based on spin groups will lead to a reduction in the minimum number of spins from which a spin arrangement can be generated; this is clearly illustrated with case (b).

5.3. Example 3. This is the case of the spin arrangement of the Tb spins in $TbCrO_3$ whose Cl′ label is (see ref. 1, p. 481):

$$[Pbnm; P_{2b}2_1'nm'; \boldsymbol{S}(\boldsymbol{r}_1) = \boldsymbol{S}(\boldsymbol{r}_2) = (S_x, S_y, 0)],$$

where $\boldsymbol{r}_1 = (x, y, \frac{1}{4})$ and $\boldsymbol{r}_2 = (1 - x, 1 - y, \frac{3}{4})$. The corresponding label based on the use of spin groups is:

$$[Pbnm; \mathrm{b}_{p_z} \times P_{12_z1}\,(2_y \parallel 2_1)\,(2_y \parallel n)\,(1 \parallel m), \boldsymbol{S}(\boldsymbol{r}_1) = \boldsymbol{S}(\boldsymbol{r}_2) = (S_x, S_y, 0)].$$

Just as in case (b) in example 2, it is not possible to generate this spin arrangement from a single spin.

6. *Spin groups and magnetic scattering of neutrons.* In this section we briefly indicate how the symmetry spin groups of a spin arrangement $\boldsymbol{S}(\boldsymbol{r})$ manifests itself in elastic magnetic scattering of unpolarized neutrons by a single magnetic crystal represented in our theory by $\boldsymbol{S}(\boldsymbol{r})$. For simplicity we consider the case of a spin arrangement in which all spins have the same magnitude and the same magnetic structure factor f. The generalization to the case of an arbitrary spin arrangement is straightforward. As is well known, the cross section for such a scattering process is usually taken to be

$$\sigma(\boldsymbol{k}) = |\boldsymbol{P}(\boldsymbol{k})|^2 - |\boldsymbol{k} \cdot \boldsymbol{P}(\boldsymbol{k})/k|^2, \tag{13}$$

where $\boldsymbol{k}$ is the scattering vector, k is its magnitude, and $\boldsymbol{P}(\boldsymbol{k})$ is the scattering amplitude. To indicate that the latter is a functional of $\boldsymbol{S}(\boldsymbol{r})$ we introduce for a moment a more explicit notation, $\boldsymbol{P}(\boldsymbol{k}; \boldsymbol{S}(\boldsymbol{r}))$, and denote by $\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_a, \ldots$, the atom sites constituting the crystal on which $\boldsymbol{S}(\boldsymbol{r})$ is defined. Then

$$\boldsymbol{P}(\boldsymbol{k}; \boldsymbol{S}(\boldsymbol{r})) = f \sum_a \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_a} \boldsymbol{S}(\boldsymbol{r}_a). \tag{14}$$

If the spin arrangement $\boldsymbol{S}(\boldsymbol{r})$ is replaced by the spin arrangement $[B \| R | \boldsymbol{v}]\, \boldsymbol{S}(\boldsymbol{r})$ then the scattering amplitude becomes

$$\boldsymbol{P}(\boldsymbol{k}; [B \| R | \boldsymbol{v}]\, \boldsymbol{S}(\boldsymbol{r})) = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{v}} B\boldsymbol{P}(R^{\mathrm{T}}\boldsymbol{k}, \boldsymbol{S}(\boldsymbol{r})), \tag{15}$$

where R^{T} is the transpose of R. Therefore the invariance of $\boldsymbol{S}(\boldsymbol{r})$ under $[B \| R | \boldsymbol{v}]$ implies:

$$\boldsymbol{P}(\boldsymbol{k}; \boldsymbol{S}(\boldsymbol{r})) = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{v}} B\boldsymbol{P}(R^{\mathrm{T}}\boldsymbol{k}, \boldsymbol{S}(\boldsymbol{r})). \tag{16}$$

In particular if $\boldsymbol{S}(\boldsymbol{r})$ is generated by a nontrivial spin translation group T_s from a spin $\boldsymbol{S}(\boldsymbol{r}_1)$, and therefore is invariant under T_s, then, denoting the elements of T_s by $[B(\boldsymbol{t}) \| E | \boldsymbol{t}]$, we may rewrite eqs. (14) and (16) as follows [we now omit $\boldsymbol{S}(\boldsymbol{r})$ in the argument of $\boldsymbol{P}$]:

$$\boldsymbol{P}(\boldsymbol{k}) = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_1} \sum_{\boldsymbol{t}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{t}} B(\boldsymbol{t})\, \boldsymbol{S}(\boldsymbol{r}_1), \tag{17}$$

$$\boldsymbol{P}(\boldsymbol{k}) = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{t}} B(\boldsymbol{t})\, \boldsymbol{P}(\boldsymbol{k}). \tag{18}$$

To avoid infinities when summing over $\boldsymbol{t}$ we introduce the usual cyclic boundary conditions. The group T_s becomes then a finite group of order N. If we furthermore write

$$C(\boldsymbol{k}) = \sum_{\boldsymbol{t}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{t}} B(\boldsymbol{t}), \tag{19}$$

eq. (17) can be rewritten as

$$\boldsymbol{P}(\boldsymbol{k}) = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_1} C(\boldsymbol{k})\, \boldsymbol{S}(\boldsymbol{r}_1) \tag{20}$$

and eq. (18), summed over $\boldsymbol{t}$, becomes

$$[C(\boldsymbol{k}) - NE]\, \boldsymbol{P}(\boldsymbol{k}) = 0, \tag{21}$$

where E is a unit 3×3 matrix as before. From eq. (21) it follows that either

$$\boldsymbol{P}(\boldsymbol{k}) = 0, \tag{22}$$

or

$$\det\,[C(\boldsymbol{k}) - NE] = 0. \tag{23}$$

The fact that the homomorphism $\boldsymbol{t} \to e^{i\boldsymbol{k}\cdot\boldsymbol{t}}\, B(\boldsymbol{t})$ is a representation $\Gamma(\boldsymbol{k})$ of T_s implies that the matrix $C(\boldsymbol{k})$, being the sum of all matrices belonging to $\Gamma(\boldsymbol{k})$, satisfies the following relations:

$$\begin{aligned} &C(\boldsymbol{k}) \neq 0 && \text{if } \Gamma(\boldsymbol{k}) \text{ contains the identity representation of } \mathsf{T}_s;\\ &C(\boldsymbol{k}) = 0 && \text{otherwise;}\\ &C(\boldsymbol{k})^2 = C(\boldsymbol{k}). \end{aligned} \tag{24}$$

Eqs. (20), (21) and (24) imply:

$$P(\boldsymbol{k}) = (1/N)\, e^{i\boldsymbol{k}\cdot\boldsymbol{r}_1}\, C(\boldsymbol{k})\, S(\boldsymbol{r}_1). \tag{25}$$

The vectors $C(\boldsymbol{k})\, S(\boldsymbol{r}_1)$ have been tabulated by Litvin[9]) for all nontrivial spin translation groups and all vectors $\boldsymbol{k}$ for which $C(\boldsymbol{k}) \neq 0^{+}$.

In the case of an arbitrary spin group one can use eq. (16) in a way similar to that described in the above example, although the computations would in general be much more complicated.

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APPENDIX

We prove here the isomorphism theorem of section 3, according to which if X is a subgroup of $\mathscr{B} \times \mathscr{F}$ belonging to a family of B and F then B/b is isomorphic to F/f where $\mathsf{b} = \mathsf{B} \cap \mathsf{X}$ and $\mathsf{f} = \mathsf{X} \cap \mathsf{F}$. We will use the symbol $\simeq$ for the expression "is isomorphic to", and the notation $\mathsf{H} < \mathsf{G}$ to indicate that H is a normal subgroup of G.

Since X is a subgroup of $\mathsf{B} \times \mathsf{F}$ and $\mathsf{F} < \mathsf{B} \times \mathsf{F}$ it follows from the second isomorphism theorem (we here use Rotman's terminology; see ref. 14), that $\mathsf{f} < \mathsf{X}$

$^{+}$ Corrections to the caption of fig. 2 of Litvin[9]) are noted here: F and G, which represent possible values of $C(\boldsymbol{k})\, \boldsymbol{S}$, should read

$$F = \frac{1}{2}\begin{pmatrix} S_{\bar{x}} - iS_{\bar{y}} \\ iS_{\bar{x}} + S_{\bar{y}} \\ 0 \end{pmatrix}, \qquad G = \frac{1}{2}\begin{pmatrix} S_{\bar{x}} + iS_{\bar{y}} \\ -iS_{\bar{x}} + S_{\bar{y}} \\ 0 \end{pmatrix}$$

and all indices x, y and z should be replaced by $\bar{x}$, $\bar{y}$ and $\bar{z}$.

and $\mathsf{X}/\mathsf{f} \simeq \mathsf{XF}/\mathsf{F}$, where XF denotes the set of products XF. Since X belongs to a family of B and F this latter result becomes $\mathsf{X}/\mathsf{f} \simeq \mathsf{B}$. In a similar manner one can show that $\mathsf{b} < \mathsf{X}$ and $\mathsf{X}/\mathsf{b} \simeq \mathsf{F}$. Because $\mathsf{b} < \mathsf{X}$ and $\mathsf{f} < \mathsf{X}$, and b and f have only the identity element in common, we have $\mathsf{b} \times \mathsf{f} < \mathsf{X}$. From $\mathsf{f} < \mathsf{b} \times \mathsf{f} < \mathsf{X}$ and $\mathsf{b} < \mathsf{b} \times \mathsf{f} < \mathsf{X}$, using the third isomorphism theorem[14]) and the isomorphisms $\mathsf{X}/\mathsf{f} \simeq \mathsf{B}$ and $\mathsf{X}/\mathsf{b} \simeq \mathsf{F}$ derived above, we find

$$\mathsf{X}/(\mathsf{b} \times \mathsf{f}) \simeq \mathsf{X}/\mathsf{b}/(\mathsf{b} \times \mathsf{f})/\mathsf{b} \simeq \mathsf{F}/\mathsf{f}$$

and

$$\mathsf{X}/(\mathsf{b} \times \mathsf{f}) \simeq \mathsf{X}/\mathsf{f}/(\mathsf{b} \times \mathsf{f})/\mathsf{f} \simeq \mathsf{B}/\mathsf{b}.$$

Hence B/b is isomorphic to F/b.

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