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WREATH GROUPS

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A new class of groups is defined for describing the symmetry of spin arrangements in magnetic crystals. The general structure of these new groups, which we name wreath groups, is determined in a mathematically rigorous manner. Wreath groups are particularly suitable for describing incommensurate spin arrangements with varying magnitudes of spins. The use of wreath groups to classify all spin arrangements and the effect of such wreath group symmetries on elastic magnetic neutron diffraction are briefly discussed.

1. Introduction

In a method based on magnetic groups, three-dimensional spin arrangements $S(r)$ are characterized by a label which in the simplest case contains a three-dimensional magnetic space group, the magnetic symmetry group of the spin arrangement, and the orientation and magnitude of a single spin[1]). For three-dimensional spin arrangements, as the incommensurate helical spin arrangement in $MnAu_2$ [2]), one needs to specify in such a label an infinity of spins since the magnetic symmetry group of such a spin arrangement is a two-dimensional magnetic space group. Using spin groups[3,4]) instead of magnetic groups, such a spin arrangement can be characterized by a label containing a single spin because the spin symmetry group of the helical spin arrangement in $MnAu_2$ is a three-dimensional spin space group. However, when using either magnetic groups or spin groups, other three-dimensional spin arrangements, as the incommensurate linear transverse-wave spin arrangement in $TbAu_2$[5]), can not be characterized by a label containing a single spin. This is because such a spin arrangement is not invariant under any three-dimensional magnetic space group or spin space group. The reason such three-dimensional spin arrangements have magnetic and spin symmetry groups of lower dimensionality has to do with the varying magnitude of the spins of such spin arrangements and the definition of magnetic and spin group elements.

Magnetic groups and spin groups are groups of pairs of coupled transformations, one of space-time and the second of spin space, the vector space of spins, i.e. the values of the function $\boldsymbol{S}(\boldsymbol{r})$. Characteristic of all magnetic and spin group elements is that the corresponding spin space transformation can be represented by a three by three proper or improper rotation matrix. Since a spin and its rotated image are of the same magnitude, the invariance of a spin arrangement under a magnetic or spin group element implies relationships, relative orientation and position, only among spins of the same magnitude. Magnetic and spin group elements can not provide relationships among spins of different magnitudes. Consequently, for three-dimensional spin arrangements, as the incommensurate linear transverse-wave spin arrangement in $TbAu_2$ with its spins of varying magnitude, the magnetic and spin symmetry groups are not three-dimensional, but of lower dimensionality.

In section 2, after a brief review of terminology and definitions of magnetic and spin groups, we introduce new transformations of spin space. These new transformations of spin space coupled with the usual transformations of space-time determine a new type of pair of coupled transformations. Characteristic of this new type of coupled transformations is that the invariance of a spin arrangement under such a coupled transformation can imply relationships among spins of different magnitudes. Groups of such coupled transformations which are symmetry groups of some spin arrangement are named "wreath groups". The structure of wreath groups are determined in section 3. In sections 4 and 5, the use of wreath groups in classifying all spin arrangements and the effect of wreath group symmetries on elastic magnetic neutron diffraction are briefly discussed.

2. Spin arrangements and wreath groups

We use the following notation and terminology[4]): $E_s(3)\times E_t(1)$ is "space-time" the product space of a three-dimensional euclidean point space called "space" and a one-dimensional euclidean point space called "time". $(\boldsymbol{r}, t)$ is a point in space-time in some coordinate system. $\mathscr{E}_s(3)\times\mathscr{E}_t(1)$ is the Newton group, the direct product of the euclidean group $\mathscr{E}_s(3)$ consisting of all proper and improper rotations and all translations of $E_s(3)$, and the euclidean group $\mathscr{E}_t(1)$ consisting of time inversion and all time translations of $E_t(1)$. An element of $\mathscr{E}_s(3)$ will be denoted by $F=(R\,|\,\boldsymbol{v})$ where R is a three by three proper or improper rotation matrix and $\boldsymbol{v}$ is a three by one column translation matrix. An element of $\mathscr{E}_t(1)$ is denoted by $(A\,|\,\tau)$ where A is an element of the time inversion group $\mathbf{A}$ consisting of the unit element $E=1$ and time inversion $E'=-1$, and τ is any real number representing a time translation.

A crystal is a subset $C_s(3)$ of points in $E_s(3)$, the points being the positions at which atoms are located. A crystal $C_s(3)$ is "invariant" under an element F

of $\mathscr{C}_s(3)$, and F is said to be a "symmetry element" of the crystal, if for each point r of $C_s(3)$, $Fr = (R \mid v)r = Rr + v$ is also a point of $C_s(3)$. The set of all such symmetry elements constitutes a group $\mathbf{F}$ called the "symmetry group" of the crystal.

Consider a subset $C_s(3) \times E_t(1)$ of space-time. A "spin arrangement" is defined as a function $S(r, t)$ which maps points (r, t) of $C_s(3) \times E_t(1)$ to vectors S of a vector space V^+. V^+ is a three-dimensional carrier space of the irreducible representation $((R \mid v), (A \mid \tau)) \rightarrow D_1^+(R \mid v) \times \Gamma_1^-(A \mid \tau)$ of the Newton group, where $D_1^+(R \mid v) = \delta_R R$, $\delta_R = \det R$, and $\Gamma_1^-(A \mid \tau) = \delta_A$, $\delta_A = +1$ if $A = E$, $\delta_A = -1$ if $A = E'$. The vector space V^+ is called "spin space" and vectors S "spins".

We are interested in spin arrangements defined on a crystal $C_s(3)$ and restrict ourselves to the case of static spin arrangements, the invariance of spin arrangements under time translation always being understood without being explicitly stated. Consequently, we shall write $S(r)$ instead of $S(r, t)$ and consider the subgroup $\mathbf{G} = \mathbf{F} \times \mathbf{A}$ of the Newton group, where $\mathbf{F}$ is the symmetry group of the crystal $C_s(3)$ and $\mathbf{A}$ is the time inversion group.

Because spin space is a carrier space of an irreducible representation of the Newton group, each transformation $G = (F, A)$ of $\mathbf{G} = \mathbf{F} \times \mathbf{A}$ implies a transformation $\delta_A \delta_R R$ of spin space. Consequently, a spin arrangement $S(r)$ is transformed by an element $G = (F, A)$ of $\mathbf{G}$ into the spin arrangement denoted by $[\delta_A \delta_R R \| F] S(r)$, where

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

We interpret the symbol $[\delta_A \delta_R R \| F]$ as an operator on the space of all spin arrangements on a given crystal. A spin arrangement $S(r)$ is invariant under an element $G = (F, A)$ of $\mathbf{G} = \mathbf{F} \times \mathbf{A}$ if

$$[\delta_A \delta_R R \| F] S(r) = S(r), \tag{2}$$

and G is said to be a a "magnetic symmetry element" of the spin arrangement. The set of all such magnetic symmetry elements constitutes a group $\mathbf{M}$ called the "magnetic symmetry group"[1]) of the spin arrangement.

Additional operators on the space of all spin arrangements on a given crystal have been introduced in defining the concept of the "spin symmetry group" of a spin arrangement[3,4]). These additional operators are denoted by $[B \| E]$ where B is a three by three rotation matrix representing any proper or improper rotation of spin space. A spin arrangement $S(r)$ is transformed by an operator $[B \| E]$ into the spin arrangement denoted by $[B \| E] S(r)$, where

$$[B \| E] s^i(r) = \sum_{j=1}^{3} B_{ij} S^j(r).$$

All products of operators $[\delta_A\delta_R R\|F]$ and $[B\|E]$ 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 $[B\|E]$, and the group $\boldsymbol{\Omega}_F$ consisting of all operators of the form $[E\|F]$ where F is an element of the symmetry group F of the crystal $C_s(3)$. An element $[B\|F]$ of $\boldsymbol{\Omega}_B \times \boldsymbol{\Omega}_F$ transforms a spin arrangement $\boldsymbol{S}(\boldsymbol{r})$ into a spin arrangement denoted by $[B\|F]\boldsymbol{S}(\boldsymbol{r})$, where

$$[B\|F]S^i(\boldsymbol{r}) = \sum_{j=1}^{3} B_{ij} S^j(F^{-1}\boldsymbol{r}). \tag{3}$$

A spin arrangement $\boldsymbol{S}(\boldsymbol{r})$ is invariant under an element $[B\|F]$ of $\boldsymbol{\Omega}_B \times \boldsymbol{\Omega}_F$ if

$$[B\|F]\boldsymbol{S}(\boldsymbol{r}) = \boldsymbol{S}(\boldsymbol{r}) \tag{4}$$

and $[B\|F]$ is said to be a "symmetry element" of the spin arrangement. The set of all such symmetry elements of $\boldsymbol{S}(\boldsymbol{r})$ constitutes a group called the "spin symmetry group" of the spin arrangement[3,4]).

Two characteristics of the operators on the space of all spin arrangements on a given crystal defined above in eqs. (1) and (3) are :

1) The action of the left-hand-side component of the operators $[\delta_A\delta_R R\|F]$ and $[B\|F]$ is independent of the position $\boldsymbol{r}$. That is, the three by three matrices $\delta_A\delta_R R$ and B acting in spin space on the components S^j of the spins $\boldsymbol{S}(F^{-1}\boldsymbol{r})$, on the right-hand-side of eqs. (1) and (3), are not dependent on the position $\boldsymbol{r}$.

2) A necessary condition for operators $[\delta_A\delta_R R\|F]$ and $[B\|F]$ to be symmetry elements of a spin arrangement $\boldsymbol{S}(\boldsymbol{r})$ is that, for all $\boldsymbol{r}$, the magnitude of the spins $\boldsymbol{S}(\boldsymbol{r})$ and $\boldsymbol{S}(F^{-1}\boldsymbol{r})$ must be the same. This follows from the action of operators on a spin arrangement defined in eqs. (1) and (3), and the definition of a symmetry element in eqs. (2) and (4).

We shall now introduce new operators on the space of all spin arrangements on a given crystal, new operators which do not necessarily possess the two above characteristics of operators previously defined in eqs. (1) and (3). These new operators will be denoted by $[\boldsymbol{V}(\boldsymbol{r})\|E]$ where $\boldsymbol{V}(\boldsymbol{r})$ is a function which maps points $\boldsymbol{r}$ of the crystal $C_s(3)$ to spins $\boldsymbol{V}$ of the vector space V^+. The action of an operator $[\boldsymbol{V}(\boldsymbol{r})\|E]$ on a spin arrangement $\boldsymbol{S}(\boldsymbol{r})$ is defined as follows: A spin arrangement $\boldsymbol{S}(\boldsymbol{r})$ is transformed by an operator $[\boldsymbol{V}(\boldsymbol{r})\|E]$ into a spin arrangement denoted by $[\boldsymbol{V}(\boldsymbol{r}')\|E]\boldsymbol{S}(\boldsymbol{r})$ (the argument $\boldsymbol{r}$ of the function $\boldsymbol{V}(\boldsymbol{r})$ has been replaced by $\boldsymbol{r}'$ to distinguish it from the argument of the spin arrangement $\boldsymbol{S}(\boldsymbol{r})$) and defined by

$$[\boldsymbol{V}(\boldsymbol{r}')\|E]\boldsymbol{S}(\boldsymbol{r}) = \boldsymbol{S}(\boldsymbol{r}) + \boldsymbol{V}(\boldsymbol{r}). \tag{5}$$

Since both $\boldsymbol{S}(\boldsymbol{r})$ and $\boldsymbol{V}(\boldsymbol{r})$ are spins, vectors in the vector space V^+, the vector sum on the right-hand side of eq. (5) is well defined. The action of an operator $[V(r')\|E]$ on a spin arrangement $S(r)$ is position dependent. That is, the value of the function $V(r')$ added to the right-hand side of eq. (5) is dependent on the value of the spin arrangement's argument r, its position, of the spin arrangement $S(r)$ on the left-hand side of eq. (5).

The set of all operators $[V(r)\|E]$ where $V(r)$ is a function which maps points r of the crystal to vectors V of spin space, can be promoted to a group Ω_V by defining the product of two operators $[V_1(r)\|E]$ and $[V_2(r)\|E]$ as:

$$[V_1(r)\|E][V_2(r)\|E] = [V_1(r) + V_2(r)\|E].$$

We consider the set of all pairs $[V(r)|F]$ of operators $[V(r)\|E]$ of the group Ω_V and operators $[E\|F]$ of the group Ω_F, where F is the symmetry group of the crystal $C_s(3)$. The action of an operator pair $[V(r)\|F]$ on a spin arrangement $S(r)$ transforms $S(r)$ into the spin arrangement denoted by $[V(r')\|F]S(r)$ and defined by

$$[V(r')\|F]S(r) = S(F^{-1}r) + V(r), \tag{6}$$

where again, as in eq. (5), the action of the operator pair $[V(r)\|F]$ is position dependent. It follows from the definition of action, eq. (6), that the product of two operator pairs $[V_1(r)\|F_1]$ and $[V_2(r)\|F_2]$ is given by

$$[V_1(r)\|F_1][V_2(r)\|F_2] = [V_1(r) + V_2(F_1^{-1}r)\|F_1F_2]. \tag{7}$$

The set of all pairs $[V(r)\|F]$ of operators $[V(r)\|E]$ of Ω_V and $[E\|F]$ of Ω_F together with the product defined in eq. (7) constitutes the semi-direct product $\Omega_V Ⓢ \Omega_F$ of the group Ω_V by the group Ω_F. The identity element of this group is $[V_e(r)\|F_e]$ where F_e is the identity element of F and $V_e(r)$ is the function which maps all points r of the crystal $C_s(3)$ to the null vector of spin space. The inverse $[V(r)\|F]^{-1}$ of an element $[V(r)\|F]$ is given by $[V(r)\|F]^{-1} = [-V(Fr)\|F^{-1}]$.

This semi-direct product $\Omega_V Ⓢ \Omega_F$ is called the "wreath product" $\mathsf{V}^+ Ⓦ \Omega_F$ of spin space V^+, considered as an abelian group V^+ under vector addition, and the group Ω_F. That is $\mathsf{V}^+ Ⓦ \Omega_F \equiv \Omega_V Ⓢ \Omega_F$. A brief review of the construction of wreath products of groups is given in appendix I.

A spin arrangement $S(r)$ is said to be "invariant" under an operator $[V(r)\|F]$ of the wreath product $\mathsf{V}^+ Ⓦ \Omega_F$ if

$$[V(r')\|F]S(r) = S(r) \tag{8}$$

for all r of the crystal $C_s(3)$. We shall say in such a case that $[V(r)\|F]$ is a "symmetry element" of the spin arrangement $S(r)$. It follows from eqs. (6) and (8) that $[V(r)\|F]$ is a symmetry element if

$$S(F^{-1}r)+V(r)=S(r), \tag{9}$$

and consequently, unlike magnetic and spin group operators defined in eqs. (1) and (3), for the operator $[V(r)\|F]$ to be a symmetry element, it is not necessary for the spins $S(r)$ and $S(F^{-1}r)$ to be of the same magnitude.

The set of all symmetry elements $[V(r)\|F]$ of a spin arrangement $S(r)$ is called the "symmetry group" of the spin arrangement $S(r)$. We now define a wreath group: a subgroup of the wreath product $\mathbf{V}^{+}ⓦ\boldsymbol{\Omega}_F$ will be called a "wreath group" if it is the symmetry group of some spin arrangement.

3. The structure of wreath groups

In this section we determine the structure of wreath groups, subgroups of wreath products $\mathbf{V}^{+}ⓦ\boldsymbol{\Omega}_F$ which are symmetry groups of spin arrangements. We show that wreath groups are those subgroups of wreath products $\mathbf{V}^{+}ⓦ\boldsymbol{\Omega}_F$ which are isomorphic to $\mathbf{F}$. We first show that the symmetry groups of all spin arrangements are such subgroups, and then show that every such subgroup is the symmetry group of some spin arrangement.

Consider an arbitrary given spin arrangement $S(r)$ defined on a crystal $C_s(3)$ whose symmetry group is $\mathbf{F}$. The wreath group of this spin arrangement is the subgroup of the wreath product $\mathbf{V}^{+}ⓦ\boldsymbol{\Omega}_F$ consisting of all operators $[V(r)\|F]$ which are symmetry elements of the spin arrangement. For each element F of the symmetry group $\mathbf{F}$ of the crystal, there exists a single function $V(r)$, which we denote as $V_F(r)$, such that $[V_F(r)\|F]$ is a symmetry element of the spin arrangement. For each F, the function $V_F(r)$ is determined from eq. (9) the condition that $[V_F(r)\|F]$ is a symmetry element of the spin arrangement $S(r)$. This condition, rewritten in a form to determine the function $V_F(r)$, is:

$$V_F(r)=S(r)-S(F^{-1}r). \tag{10}$$

For a given spin arrangement $S(r)$, the function $V_F(r)$ defined in eq. (10) is unique. Consequently, for each element F of the symmetry group $\mathbf{F}$ of the crystal, there is a single operator $[V_F(r)\|F]$ of the wreath product $\mathbf{V}^{+}ⓦ\boldsymbol{\Omega}_F$ which is a symmetry element of the spin arrangement.

The set of all such symmetry elements $[V_F(r)\|F]$ constitutes a group. To prove this we must show that operators $[V_F(r)\|F]$ with $V_F(r)$ defined by eq. (10) satisfy the product rule given in eq. (7). That is, we must show that $V_{F_1}(r)+V_{F_2}(F_1^{-1}r)=V_{F_1F_2}(r)$. Using eq. (10) we have:

$$\begin{aligned} V_{F_1}(r)+V_{F_2}(F_1^{-1}r) &= S(r)-S(F_1^{-1}r)+S(F_1^{-1}r)-S(F_2^{-1}F_1^{-1}r) \\ &= S(r)-S((F_1F_2)^{-1}r) \\ &= V_{F_1F_2}(r). \end{aligned}$$

Consequently, the wreath group of a given spin arrangement $S(r)$ consists of all operators of the form $[V_F(r)\|F]$, for all F of the symmetry group F of the crystal, and where $V_F(r)$ is defined in eq. (10). Since a single function $V_F(r)$ is coupled to each element F and the product rule eq. (7) is satisfied, the wreath group is isomorphic to F, the symmetry group of the crystal on which the spin arrangement is defined.

We shall now show that every subgroup isomorphic to F of a wreath product $\mathsf{V}^+ \textcircled{w} \boldsymbol{\Omega}_F$ is a wreath group, the symmetry group of some spin arrangement: Consider a crystal generated by the group F from a general position r_0. That is, all positions of the atoms of the crystal are obtained by applying all elements of F to the position r_0, and such that $F_1 r_0 \neq F_2 r_0$ if $F_1 \neq F_2$. Consider a subgroup isomorphic to F of the wreath product $\mathsf{V}^+ \textcircled{w} \boldsymbol{\Omega}_F$ whose elements are denoted by $[V_F(r)\|F]$ and which satisfy the product rule eq. (7). We shall now construct a spin arrangement on the crystal generated by F from the general position r_0, whose symmetry group is this subgroup of $\mathsf{V}^+ \textcircled{w} \boldsymbol{\Omega}_F$.

At r_0 we assign an arbitrary spin $S(r_0)$. We assign at $F^{-1}r_0$, for all F, the spin $S(F^{-1}r_0)$ defined by

$$S(F^{-1}r_0) = S(r_0) - V_F(r_0), \tag{11}$$

where $V_F(r_0)$ is the value of the function $V_F(r)$ of the operator $[V_F(r)\|F]$ at r_0. To show that this spin arrangement is invariant under the subgroup isomorphic to F of $\mathsf{V}^+ \textcircled{w} \boldsymbol{\Omega}_F$ one must show, see eq. (9), for all F and atomic positions r, that $S(F^{-1}r) + V_F(r) = S(r)$. From the product rule eq. (7) for arbitrary elements F and F_1 of F we can write

$$V_{F_1F}(r_0) = V_{F_1}(r_0) + V_F(F_1^{-1}r_0),$$

which can be rewritten, adding $S(r_0)$ to both sides, as

$$S(r_0) - V_{F_1F}(r_0) + V_F(F_1^{-1}r_0) = S(r_0) - V_{F_1}(r_0).$$

Using eq. (11) we can then write

$$S(F^{-1}F_1^{-1}r_0) + V_F(F_1^{-1}r_0) = S(F_1^{-1}r_0),$$

and finally by denoting the arbitrary atomic position $F_1^{-1}r_0$ by r, we have

$$S(F^{-1}r) + V_F(r) = S(r).$$

Therefore, we have shown that every subgroup isomorphic to F of a wreath product $\mathsf{V}^+ \textcircled{w} \boldsymbol{\Omega}_F$ is a wreath group, the symmetry group of a spin arrangement.

4. Classification labels of spin arrangements using wreath groups

In this section we discuss three examples of assigning a wreath group to a given spin arrangement.

Example 1. We consider the incommensurate linear transverse-wave spin arrangement defined on the terbium atoms of α-$TbAu_2$[5]). The symmetry group of the terbium atom arrangement is the space group $\mathbf{F} = \mathrm{I}4/mmm$ (D_{4h}^{17}) and the atom arrangement is generated by $\mathbf{F}$ from $r_0 = (0, 0, 0)$. The spin arrangement on the terbium atoms is given by $S(r) = zS\cos(Q \cdot r)$ where S is a constant, $Q = Q(x+y)/\sqrt{2}$ and the wavelength $\lambda = 2\pi/Q$ of this linear transverse-wave spin arrangement is incommensurate with the atom arrangement, see fig. 1. In terms of magnetic groups, this spin arrangement is specified by the "C1′ classification label", in the sense of Opechowski and Dreyfus[6]), as follows:

$$[\mathrm{I}4/mmm;\, c_{x\bar{y}}m_z m'_{x\bar{y}};\, S(r_0) = (0, 0, S),\quad S((n, n, 0)r_0) = (0, 0, S\cos(nQ))].$$

This label indicates that while the symmetry group of the terbium atom arrangement is the three-dimensional space group I4/mmm, the magnetic symmetry group of the spin arrangement is the two-dimensional magnetic group cmm'. This three-dimensional spin arrangement is generated by the

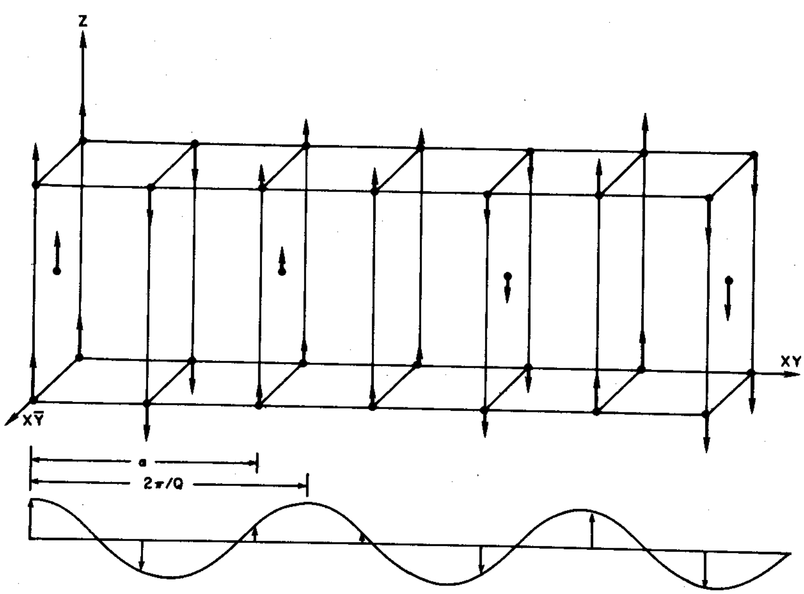

Fig. 1. The incommensurate linear transverse-wave spin arrangement of α-$TbAu_2$. Only the terbium atoms are shown.

two-dimensional magnetic group from the spin $S(r_0)$ and the infinity of spins on the xy-axis which are specified by the additional condition $S((n, n, 0)r_0) = (0, 0, S\cos(nQ)$.

In terms of wreath groups, the corresponding label specifying this spin arrangement is

$$[\mathrm{I}4/mmm; [V_F(r)\|F]; \quad S(r_0) = (0, 0, S)],$$

where the wreath group consists of all elements $[V_F(r)\|F]$, for all F of the symmetry group $\mathbf{F} = \mathrm{I}4/mmm$ of the terbium atom arrangement, and where $V_F(r) = zS(\cos(Q \cdot r) - \cos(Q \cdot F^{-1}r))$. The functions $V_F(r)$ have been defined using eq. (10). This spin arrangement is generated by the wreath group from a single spin $S(r_0)$.

Example 2. This is the case of the incommensurate linear transverse-wave spin arrangement on the dysprosium atom arrangement in DyC_2[7]). The symmetry group of the dysprosium atom arrangement is $\mathbf{F} = \mathrm{I}4/mmm$ (D_{4h}^{17}) and the atom arrangement is generated by $\mathbf{F}$ from $r_0 = (0, 0, 0)$. The spin arrangement on the dysprosium atoms is given by $S(r) = zS\cos(Q \cdot r)$ where $Q = Qx$ In terms of magnetic groups, the classification label of this spin arrangement is

$$[\mathrm{I}4/mmm; p_{yz}m'_x m'_y m_z; S(r_0) = (0, 0, S),$$
$$S((n, 0, 0)r_0) = (0, 0, S\cos(nQ))],$$

where $pm'm'm$ is the two-dimensional magnetic symmetry group of this spin arrangement. In terms of wreath groups, the classification label of this spin arrangement is the same as that in example 1, except that the functions $V_F(r)$ differ here in that $Q = Qx$.

Example 3. This is the case of the ferromagnetic spin arrangement of nickel[8]). The symmetry group of the crystal is $\mathbf{F} = \mathrm{F}m3m$ (O_h^5) and the crystal is generated by $\mathbf{F}$ from $r_0 = (0, 0, 0)$. The magnetic group classification label of this spin arrangement is

$$[\mathrm{F}m3m; \mathrm{I}4/mm'm'; \quad S(r_0) = (0, 0, S)].$$

while the atom arrangement is of cubic symmetry, the magnetic symmetry group is of a lower symmetry class, i.e. tetragonal.

In terms of wreath groups, the classification label of this ferromagnetic spin arrangement is:

$$[\mathrm{F}m3m; [V_e(r)\|F]; S(r_0) = (0, 0, S)].$$

The wreath group of this spin arrangement is cubic, consisting of elements

$[V_e(r)\|F]$ for all F of the cubic symmetry group of the atom arrangement. Characteristic of all ferromagnetic spin arrangements, the function $V_e(r)$, which is coupled to all elements F of $\mathbf{F}$, is the function that maps all points of the atom arrangement to the null vector of spin space.

5. Wreath groups and magnetic scattering of neutrons

In this section we briefly indicate how the wreath group symmetry of a spin arrangement $S(r)$ manifests itself in elastic magnetic scattering of unpolarized neutrons by a magnetic single crystal. For simplicity we consider the case of a spin arrangement where all spins have the same magnetic structure factor f. The cross section for such a scattering process is usually taken to be

$$\sigma(k) = |P(k)|^2 - |k \cdot P(k)/k|^2,$$

where k is the scattering vector and k its magnitude. The scattering amplitude $P(k)$ is given by

$$P(k) = f \sum_r e^{ik \cdot r} S(r),$$

where the sum is over all atomic positions of the crystal on which the spin arrangement $S(r)$ is defined.

The scattering amplitude can be rewritten as

$$P(k) = f \sum_{r_i, t} e^{ik \cdot (r_i - t)} S(r_i - t),$$

where the sum is over all atomic positions in the primitive unit cell of the crystal and over all translations of the translational subgroup of the symmetry group $\mathbf{F}$ of the crystal. We use eq. (10), in the case of $F = (E \mid t)$ to replace $S(r_i - t)$ in the above equation by $S(r_i) - V_t(r_i)$, and rewrite the scattering amplitude as

$$P(k) = f \sum_{r_i, t} e^{ik \cdot (r_i - t)} S(r_i) - f \sum_{r_i} e^{ik \cdot r_i} \sum_t e^{-ik \cdot t} V_t(r_j).$$

The wreath group symmetry of a spin arrangement manifests itself in the elastic magnetic scattering of unpolarized neutrons via the sum $\Sigma_t\, e^{-ik \cdot t} V_t(r)$.

Considering the case of the linear transverse-wave spin arrangement defined on the terbium atoms of α-$TbAu_2$, discussed in the preceeding section, the sum $\Sigma_t\, e^{-ik \cdot t} V_t(r)$ can be calculated using the functions $V_t(r)$ given in the classification label of this spin arrangement. One obtains pairs of non-vanishing values of this sum, which infers pairs of non-vanishing values for the scattering amplitude, and in turn, of the cross section, for values of the scattering vector $\boldsymbol{k}$ such that $\boldsymbol{k} = \boldsymbol{K} \pm \boldsymbol{Q}$. $\boldsymbol{K}$ is a reciprocal lattice vector and $\boldsymbol{Q}$ is the constant vector in the definition of the functions $V_t(\boldsymbol{r})$. Such pairs of satellite reflections have been experimentally determined in α-$TbAu_2$[5]).

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Appendix I

Wreath products of groups

The construction of wreath products of groups can be divided into three steps[9,10]):

First, let P be a finite or infinite group, and H a set of order $|H|$. We define

$$\mathsf{P}^H = \mathsf{P} \times \mathsf{P} \times \cdots \times \mathsf{P},$$

the direct product of P taken H times. Elements of P^H are $|H|$-tuples of elements of P, i.e. each element of P^H is a set $\{P_h \mid h \in H\}$ of H elements of P indexed by the elements of H. In other words, each element of P^H is a function on H whose values are in P. We shall denote each element of P^H by f, a function on H whose values $f(h) = P_h$ are in P. P^H is the set of all functions on H with values in P.

The set P^H of all functions f can be promoted to a group by defining the product of two elements of P^H, i.e. of two functions f_1 and f_2, as follows:

$$f_1 f_2(h) = f_1(h) f_2(h). \tag{A.1}$$

The identity function f_e is defined by $f_e(h) = P_e$ for all h of H, where P_e is the identity element of P. The inverse function f^{-1} of f is defined by $f^{-1}(h) = [f(h)]^{-1}$ for all h of H.

Second, let $\boldsymbol{\theta}$ denote the group of all permutations of H, and let F be a group homomorphic onto a subgroup $\boldsymbol{\theta}_F$ of $\boldsymbol{\theta}$. The group F is also homomorphic onto a group $\boldsymbol{\phi}_F$ of automorphisms of the group P^H, the automorphisms $\boldsymbol{\phi}_F$ being defined, for all h of H, by

$$\phi_F f(h) = f(\theta_{F^{-1}} h). \tag{A.2}$$

Finally, we define the set

$$\{(f \| F) \mid f \in \mathbf{P}^H, F \in \mathbf{F}\}$$

of all pairs $(f \mid F)$ of elements, f belonging to the group $\mathbf{P}^H$ and F belonging to $\mathbf{F}$. This set of pairs is promoted to a group by defining the product of two pairs of elements $(f_1 \mid F_1)$ and $(f_2 \mid F_2)$ as

$$(f_1 \mid F_1)(f_2 \mid F_2) = (f_1 \cdot \phi_{F_1} f_2 \| F_1 F_2), \tag{A.3}$$

where $\phi_{F_1} f_2$ is defined by eq. (A.2) and the product of functions $f_1 \cdot \phi_{F_1} f_2$ by eq. (A.1). The identity element of this group is $(f_e \mid F_e)$ where f_e is the identity element of $\mathbf{P}^H$ and F_e the identity element of $\mathbf{F}$. The inverse $(f \mid F)^{-1}$ of $(f \mid F)$ is given by $(f \mid F)^{-1} = (\phi_{F^{-1}} f^{-1} \mid F^{-1})$.

The set of all pairs $(f \mid F)$ together with the product defined in eq. (A.3) constitutes the semi-direct product $\mathbf{P}^H \circledS_\phi \mathbf{F}$ of the group $\mathbf{P}^H$ by the group $\mathbf{F}$ determined by the homomorphism of $\mathbf{F}$ onto the group of automorphisms ϕ_F. It is this semi-direct product which is called the "wreath product" $\mathbf{P} ⓦ \mathbf{F}$ of $\mathbf{P}$ by $\mathbf{F}$, that is $\mathbf{P} ⓦ \mathbf{F} = \mathbf{P}^H \circledS_\phi \mathbf{F}$.

In this paper we are interested in wreath products $\mathbf{P} ⓦ \mathbf{F} = \mathbf{P}^H \circledS_\phi \mathbf{F}$ where $\mathbf{P}$ is the three-dimensional vector space V^+, i.e. spin space, considered as an abelian group under vector addition. H is the set of all points $\boldsymbol{r}$ in $E_s(3)$ of a crystal $C_s(3)$, and $\mathbf{F}$ is the symmetry group of the crystal. Denoting the functions $f(\boldsymbol{h})$ of $\mathbf{P}^H$ by $\boldsymbol{V}(\boldsymbol{r})$, and defining the action of permutations of $\boldsymbol{\theta}_F$ as $\boldsymbol{\theta}_F \boldsymbol{r} = F\boldsymbol{r}$, eq. (A.2) becomes $\phi_F \boldsymbol{V}(\boldsymbol{r}) = \boldsymbol{V}(F^{-1}\boldsymbol{r})$. Finally, rewriting the product, eq. (A.1), of two functions $\boldsymbol{V}_1(\boldsymbol{r})$ and $\boldsymbol{V}_2(\boldsymbol{r})$ in additive notation as $\{\boldsymbol{V}_1 + \boldsymbol{V}_2\}(\boldsymbol{r}) = \boldsymbol{V}_1(\boldsymbol{r}) + \boldsymbol{V}_2(\boldsymbol{r})$, the product given in eq. (A.3) of two elements of the wreath product takes on the form of eq. (7) given in the text.

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