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Spin line groups

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Spin line groups describe the symmetries of spin arrangements in quasi-one-dimensional systems. These groups are derived for the first family of line groups. Among them, magnetic groups are singled out as a special case. Spin arrangements generated by the derived groups are first discussed for single-orbit systems and then the conclusions are extended to multi-orbit cases. The results are illustrated by the examples of a CuO_2 zigzag chain, a ^{13}C nanotube and the hexaferrite $Ba_2Mg_2Fe_{12}O_{22}$. Applications to neutron diffraction and classical ground-state determination are indicated.

1. Introduction

The rapidly increasing interest in quasi-one-dimensional helimagnets imposes a need for the analysis of such systems by means of symmetry. Neutron diffraction measurements and other experimental techniques confirm the existence of long-range quasi-one-dimensional helimagnetic subsystems in three-dimensional crystals (Lemmens *et al.*, 2003). Such systems show exciting properties, such as multiferroicity (Tokunaga *et al.*, 2010). On the other hand, the recent synthesis (Schnack *et al.*, 2004; Seeber *et al.*, 2004; Simon *et al.*, 2005; Garlea *et al.*, 2008) of quantum spin nanotubes initiated proposals for their applications in magnetic data storage or in the field of quantum computing.

The spatial symmetries of quasi-one-dimensional systems are gathered in 13 families of line groups (Damnjanović & Milošević, 2010). However, when atoms (or ions) possess non-zero magnetic moments (spins), line groups should be extended to include them. A part of such systems can be described by magnetic line groups (Damnjanović & Vujičić, 1982), but it turned out that these groups are insufficient to describe the numerous spin arrangements in real quasi-one-dimensional systems.

In fact, the symmetry of magnetic ordering and the crystallographic lattice was firstly treated by Shubnikov's theory of black-and-white magnetic groups, assuming that spins are (axial) vectors subjected to geometrical transformation and time reversal. Later on, it was realized that this is an incomplete description of the symmetry of magnetic materials. To overcome this deficiency, the concept of spin groups was introduced by several authors (Brinkman & Elliott, 1966; Bertaut, 1971; Litvin, 1973; Litvin & Opechowski, 1974) for point, translational and space groups. This concept has been reinforced recently by fruitful applications to magnetically ordered quasicrystals (Lifshitz, 1998; Lifshitz & Even-Dar Mandel, 2004).

Here, the spin groups of the first family line groups are derived. As these groups are subgroups (of index two or four) of all other line groups, this is the most important step, inevitable in constructing all other spin line groups. The classification of the spin groups is performed using the irreducible representations of the line groups, and this technique, together with the main conclusions of the theory of spin groups derived in Litvin & Opechowski (1974), is highlighted in §2. Applying this to the line groups of the first family, we derive all their spin groups in §3, introducing suitable notation; we also consider their relation to magnetic line groups. We discuss possible spin arrangements generated by the derived spin groups, starting with two possible types of single-orbit[1] systems (§4), and then extend the conclusions to the multi-orbit ones (§5). Finally, in §6 the most important results are summarized, illustrated by realistic systems, and possible applications are outlined.

2. Spin groups

We begin with a short reminder about spin groups (Litvin & Opechowski, 1974). A spin arrangement is a vector field over atoms, *i.e.* a set of pairs $(\mathbf{r}, \mathbf{s}_\mathbf{r})$ of atomic positions and corresponding spins. Let the atomic configuration (regardless of the spins) have a symmetry group $\mathbf{G}$, which is a subgroup of the Euclidean group $E(3)$ (point, line, diperiodic or space group), with elements g [here $g = (O|\mathbf{v})$ is the Seitz symbol: O is an orthogonal transformation and $\mathbf{v}$ a translational vector]. Then the spin group $B(\mathbf{G})$ is a subgroup in $E(3) \times O(3)$, where $O(3)$ is the three-dimensional orthogonal group. Precisely, the elements of the spin group are pairs (g, b) where g and b belong, respectively, to $\mathbf{G}$ and to the subgroup $\mathbf{B}$ of $O(3)$. It was shown that derivation of the spin groups was reduced to the classification of the *nontrivial spin groups*. The spin arrangement of some system is completely defined by the nontrivial spin group. Linear and planar arrangements possess an additional *spin-only group* ($\tilde{\mathbf{B}}$, equal to $\mathbf{C}_\infty$ and $\mathbf{C}_{1h}$,

[1] An orbit is a subsystem generated by a symmetry group from a single atom (simple crystal).

respectively) completing their full symmetry (spin group); for a three-dimensional spin arrangement the spin-only group contains only an identity element. A nontrivial spin group $N(\mathbf{G})$ is determined by the isomorphism $N(\mathbf{G})/\tilde{\mathbf{G}} \cong \mathbf{B}^*$, where $\tilde{\mathbf{G}}$ is a normal subgroup of $\mathbf{G}$ ($\mathbf{G} = \tilde{\mathbf{G}} + g_2\tilde{\mathbf{G}} + \ldots$), while $\mathbf{B}^*$ is the group of coset representatives $\{e, b_2, \ldots\}$ (in the coset decomposition $\mathbf{B} = \tilde{\mathbf{B}} + b_2\tilde{\mathbf{B}} + \ldots$ with normal subgroup $\tilde{\mathbf{B}}$). The isomorphism (denoted by $\not\ell$) between the quotient group $N(\mathbf{G})/\tilde{\mathbf{G}}$ and $\mathbf{B}^*$ [which maps each coset $g_i\tilde{\mathbf{G}}$ into the element $\not\ell(g_i\tilde{\mathbf{G}}) = b_i$ from $\mathbf{B}^*$] generates the homomorphism $D^{\rm sp}(g) = \not\ell(g\tilde{\mathbf{G}})$ of $\mathbf{G}$ onto $\mathbf{B}^*$ (every element g is mapped to an orthogonal matrix). Bearing in mind that a representation is a homomorphism of $\mathbf{G}$ into a group of nonsingular matrices of some carrier space, one concludes that $D^{\rm sp}$ is a representation of $\mathbf{G}$, called the *spin representation* in $\mathbb{R}^3$. Therefore, the nontrivial spin group is completely determined by the spin representation, whose kernel is the normal subgroup $\tilde{\mathbf{G}}$.

Elements of the nontrivial spin group are $(g, D^{\rm sp}(g))$ and act on the spin field as

$$(g, D^{\rm sp}(g))(\mathbf{r}, \mathbf{s}_\mathbf{r}) = (g\mathbf{r}, D^{\rm sp}(g)\mathbf{s}_\mathbf{r}), \qquad (1)$$

assigning to the atom in $g\mathbf{r}$ the vector $\mathbf{s}_{g\mathbf{r}}$, which is the spin from $\mathbf{r}$ transformed by $D^{\rm sp}(g)$ (the lengths of spin vectors are preserved).

For some fixed group $\mathbf{G}$, different nontrivial spin groups are those with nonequivalent spin representations. In other words, nontrivial spin groups with the spin representations $D_1^{\rm sp}(\mathbf{G})$ and $D_2^{\rm sp}(\mathbf{G})$ are equivalent if there is a matrix R from SO(3) such that $RD_1^{\rm sp}(\mathbf{G})R^{-1} = D_2^{\rm sp}(\mathbf{G})$. In fact, the usual equivalence relation, *i.e.* conjugation by some nonsingular matrix X, leads to the condition that X can be taken from $O(3)$ too, as $XD_1^{\rm sp}(\mathbf{G})X^{-1}$ has to be a spin representation. This means that X can be a rotation $X = R$ or rotoinversion $X = -IR$ (here I is a three-dimensional identity matrix, thus $-I$ represents spatial inversion), but conjugation under these two gives the same spin representation.

The procedure for the classification of nontrivial spin groups proposed by Litvin and Opechowski assumes that one finds all normal subgroups $\tilde{\mathbf{G}}$ of the geometrical group $\mathbf{G}$ and orthogonal group $\mathbf{B}^*$ establishing the isomorphism $\not\ell$. We found spin line groups (*i.e.* $\not\ell$) directly, by construction of spin representations $D^{\rm sp}$, utilizing a convenient form of the irreducible representations of the line groups (as explained in Appendix *A*). The procedures are equivalent (as equivalent representations have the same kernels).

2.1. Magnetic groups

It is important to realize that magnetic groups are special cases of the spin groups; it is thus not possible to describe all the spin systems which are within the scope of the spin groups only by magnetic groups.

A magnetic group is isomorphic to the group of geometrical transformations of a particular system, but together with the Euclidean transformations it involves also the time reversal θ. Precisely, for a given system with the geometrical group $\mathbf{G}$ there are two types of magnetic groups (we omit here grey groups as they refer to systems with vanishing spins): besides the *ordinary* group $\mathbf{G}$, in addition one *black-and-white magnetic group* is obtained from each halving subgroup $\tilde{\mathbf{G}}$ of $\mathbf{G}$:

$$\tilde{\mathbf{G}} + \theta g'\tilde{\mathbf{G}}; \qquad (2)$$

here g' is an arbitrary element of the coset $\mathbf{G} \setminus \tilde{\mathbf{G}}$. As the time reversal changes the orientation of the spin vectors, whereas the geometrical transformations act on a spin field by the axial (pseudo) vector representation $D^{\rm av}$, it follows that the magnetic groups are nontrivial spin groups with the particular spin representation $D^{\rm sp}(g) = \delta_g D^{\rm av}(g)$, where δ_g is equal to 1 when g belongs to $\tilde{\mathbf{G}}$, and -1 otherwise.

3. First family spin line groups

Symmetry groups of the systems periodic (this includes not only translational but also helical periodicity) along one direction (the z axis by convention) are gathered into 13 infinite families of line groups. Among them there are 75 rod groups (Kopský & Litvin, 2002), subperiodic ones, with the crystallographic isogonal group principal axis of the order 1, 2, 3, 4 or 6.

The first family line groups are subgroups of index either two or four in the groups of the remaining families, making this family the most significant for understanding all the spin line groups. Accordingly, in this section we start with a brief reminder of the first family line groups and then in the next subsection the nontrivial spin groups are derived.

3.1. First family line groups

Line group $\mathbf{L}$ of the first family is an abelian group with the elements $\ell_{ts} = (C_Q|f)^t C_n^s$ ($t = 0, \pm1, \ldots$ and $s = 0, \ldots, n-1$), manifesting factorization into the direct product ($\otimes$ is omitted following the usual notation for line groups, where generalizations to semi- and weak-direct products appear in higher families) $\mathbf{L} = \mathbf{T}_Q(f)\mathbf{C}_n$ of two cyclic subgroups: the infinite helical group $\mathbf{T}_Q(f)$ and the rotational group $\mathbf{C}_n$ of order n. The generator of the helical group is $(C_Q|f)$, being the rotation C_Q for $2\pi/Q$ (Q is a real number not less than 1; for $Q = 1$ an ordinary translational group is obtained) followed by the translation for f along the z axis. The rotational group is generated by the rotation C_n for $2\pi/n$ around the z axis.

Choosing a point $\mathbf{r}_{00} = (\rho, \varphi_{00}, z_{00})$ (cylindrical coordinates), the action of the first family line group generates the set of points (orbit):

$$\mathbf{r}_{ts} = (C_Q|f)^t C_n^s \mathbf{r}_{00} = \left(\rho, \varphi_{00} + 2\pi\left(\frac{t}{Q} + \frac{s}{n}\right), z_{00} + tf\right),$$
$$t = 0, \pm1, \ldots, \quad s = 0, \ldots, n-1. \qquad (3)$$

For $\mathbf{r}_{00}$ out of the z axis (*i.e.* $\rho > 0$) this is a *generic orbit* (general-position orbit), with a trivial (identity element only, $\mathbf{C}_1$) stabilizer (site-symmetry group). In particular, when $n = 1$, the group is reduced to the helical group $\mathbf{T}_Q(f)$ and the atoms [equation (3)] are arranged on a helix. Note that for irrational Q a system with such symmetry is incommensurate

(no pure translations in **L**); otherwise, when $Q = q/r$ (q and r are coprime integers, $r < q$), it is possible to choose q to be a multiple of n and there is a translational period $a = qf/n$. In the opposite case, when the orbit representative $\mathbf{r}_{00}$ is a point of special position, *i.e.* $\mathbf{r}_{00}$ is on the z axis ($\rho = 0$), a *linear orbit* is obtained and the corresponding stabilizer is a rotational subgroup $\mathbf{C}_n$. These orbits are illustrated in Fig. 1 and will be used in realistic examples which follow. Note that the zigzag orbit, in the middle of the figure, is a general-position orbit of the helical line group which is also the rod group $\mathbf{p}2_1$.

The irreducible representations of the first family line groups are one-dimensional (as **L** is abelian). They are classified (Damnjanović & Milošević, 2010) by the pairs $(\tilde{k}, \tilde{m})$ of helical quantum numbers. To an arbitrary element ℓ_{ts} such a representation ${}_{\tilde{k}}A_{\tilde{m}}$ assigns the number:

$$ {}_{\tilde{k}}A_{\tilde{m}}(\ell_{ts}) = \exp\left(i\tilde{k}ft + \tilde{m}\frac{2\pi}{n}s\right); \quad (4)$$

here the helical quasi-momentum $\tilde{k}$ takes values from the helical Brillouin zone $(-\pi/f, \pi/f]$, while the angular momentum $\tilde{m}$ is an integer from the interval $(-n/2, n/2]$. It is obvious that these representations are complex (the third kind according to Wigner's classifications, see Appendix *A*), except

$$ {}_0A_0(\ell_{ts}) = 1, \quad {}_{\pi/f}A_0(\ell_{ts}) = (-1)^t, \quad {}_0A_{n/2}(\ell_{ts}) = (-1)^s, $$
$$ {}_{\pi/f}A_{n/2}(\ell_{ts}) = (-1)^{t+s}, \quad (5)$$

which are real (the first kind). The latter are written in the unified way as $(-1)^C$ with $C = 0, t, s, w$ where $w = t + s$. The representations with $\tilde{m} = n/2$ exist only for the groups with even n.

As the spin representations are real, it is important to classify the real (or physical) irreducible representations of the line groups. To this end we note that each pair of mutually conjugated complex representations ${}_{\tilde{k}}A_{\tilde{m}}(\ell_{ts})$ and ${}_{-\tilde{k}}A_{-\tilde{m}}(\ell_{ts})$ gives a two-dimensional real representation equivalent to their direct sum

$$ {}_{\tilde{k}}E_{\tilde{m}}(\ell_{ts}) = X({}_{\tilde{k}}A_{\tilde{m}}(\ell_{ts}) \oplus {}_{-\tilde{k}}A_{-\tilde{m}}(\ell_{ts}))X^\dagger $$
$$ = \begin{pmatrix} \cos(\tilde{k}ft + \tilde{m}\frac{2\pi}{n}s) & -\sin(\tilde{k}ft + \tilde{m}\frac{2\pi}{n}s) \\ \sin(\tilde{k}ft + \tilde{m}\frac{2\pi}{n}s) & \cos(\tilde{k}ft + \tilde{m}\frac{2\pi}{n}s) \end{pmatrix}, \quad (6)$$

where

$$ X = \frac{1}{2^{1/2}}\begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix}. $$

To count all these nonequivalent representations, $\tilde{k}$ takes the values only from the right half $[0, \pi/f]$ of the helical Brillouin zone, while the range of $\tilde{m}$ is the same as in the complex case. To recap, the real irreducible representations of **L** are one dimensional [(5)] and two dimensional [(6)].

3.2. Spin groups

As shown in §2, the classification of the nontrivial spin line groups $N(\mathbf{L})$ corresponding to a group of geometrical transformations **L** is reduced to the classification of the nonequivalent spin representations $D^{\rm sp}(\mathbf{L})$, using physically irreducible representations of **L**. This implies that one has to form three-dimensional real representations combining (making the direct sum of) the representations (5) and (6). There are only two ways to do this (Appendix *A*, the first two cases).

Firstly, any two-dimensional representation ${}_{\tilde{k}}E_{\tilde{m}}$ can be combined only with one of the representations (5); in this way, four different *classes* of spin representations are obtained:

$$ {}_{\tilde{k}}D^C_{\tilde{m}}(\ell_{ts}) = \begin{pmatrix} \cos(\tilde{k}ft + \tilde{m}\frac{2\pi}{n}s) & -\sin(\tilde{k}ft + \tilde{m}\frac{2\pi}{n}s) & 0 \\ \sin(\tilde{k}ft + \tilde{m}\frac{2\pi}{n}s) & \cos(\tilde{k}ft + \tilde{m}\frac{2\pi}{n}s) & 0 \\ 0 & 0 & (-1)^C \end{pmatrix}, $$
$$ C = 0, t, s, w, \quad \begin{matrix} \tilde{k} \in [0, \frac{\pi}{f}] \\ \tilde{m} \in (-\frac{n}{2}, \frac{n}{2}] \end{matrix}. \quad (7)$$

Within the given class C, the choice of the pairs $(\tilde{k}, \tilde{m})$ gives a particular spin representation.

Note that in (7) the upper-left two-by-two block corresponds to the rotation in the xy plane. It follows that, for the class $C = 0$, the spin representation of the group element ℓ_{ts} is the rotation $R_{\mathbf{z}}(\varphi_{ts})$ for $\varphi_{ts} = \tilde{k}ft + \tilde{m}(2\pi/n)s$ around the z axis. In the remaining three classes, $C = t, s, w$, the halving subgroup containing elements with C even is represented by the rotations $R_{\mathbf{z}}(\varphi_{ts})$, while the other elements, with C odd (the remaining coset), are reflections $-R_{\mathbf{z}}(\varphi_{ts} + \pi)$.

The second way to build a spin representation is to combine three representations (5). However, note that the classes (7) include for $\tilde{k} = 0$ or π and $\tilde{m} = 0$ or $n/2$, 12 cases $D^{\rm sp}(\ell_{ts}) = {\rm diag}[(-1)^C, (-1)^C, (-1)^{C'}]$ and four $D^{\rm sp}(\ell_{ts}) = {\rm diag}[(-1)^C, (-1)^C, (-1)^C]$. Hence, only the representations $D^{\rm sp}(\ell_{ts}) = {\rm diag}[(-1)^{C_1}, (-1)^{C_2}, (-1)^{C_3}]$ with three different representations (5) are not included in the classes (7). This

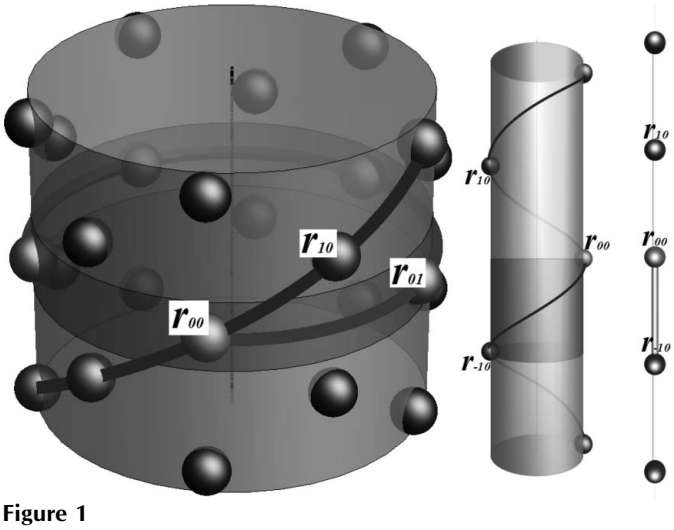

Figure 1
Orbit types for the first family line groups: general-position orbit for the groups $\mathbf{T}_{10}(1.23\ \text{Å})\mathbf{C}_5$ with $\mathbf{r}_{00} = (3.392\ \text{Å}, 2\pi/15, 0)$ and translational period $a = 2.46$ Å (left), $\mathbf{T}_2(1.43\ \text{Å})\mathbf{C}_1$ with $\mathbf{r}_{00} = (0.715\ \text{Å}, 0, 0)$ and $a = 2.86$ Å (middle) and linear orbit for the family of the groups $\mathbf{T}_Q(f)\mathbf{C}_n$ (right) with $\mathbf{r}_{00}$ on the system axis and $a = f$. $\mathbf{r}_{10}$ and $\mathbf{r}_{01}$ are the atoms obtained by the action of the helical generator and the generator of rotations on $\mathbf{r}_{00}$, respectively. The height of the dark grey area on the cylinder corresponds to the fractional translation f.

makes four *exceptional* spin representations, denoted by $\hat{C}$, where C is one of 0, t, s or w, which are omitted in the construction. Conveniently, the remaining three representations are arranged as in the set $\{t, s, w, 0\}$ before one of the symbols is taken out:

$$\begin{aligned} D^{\hat{0}}(\ell_{ts}) &= \mathrm{diag}[(-1)^t, (-1)^s, (-1)^w], \\ D^{\hat{t}}(\ell_{ts}) &= \mathrm{diag}[(-1)^s, (-1)^w, 1], \\ D^{\hat{s}}(\ell_{ts}) &= \mathrm{diag}[(-1)^t, (-1)^w, 1], \\ D^{\hat{w}}(\ell_{ts}) &= \mathrm{diag}[(-1)^t, (-1)^s, 1]. \end{aligned} \tag{8}$$

Thus, in all four exceptional groups the identity matrix is associated with the elements of $\mathbf{L}$ with even t and s simultaneously. This means that the kernel of these representations is an index-four subgroup of $\mathbf{L}$ and its three cosets correspond to the remaining three different matrices of $D^{\hat{C}}$. These matrices are involutions (their square is the identity matrix) and they describe the rotations or the reflections in the spin space (a detailed specification is given at the bottom of Table 2).

Recall that all equivalent spin representations are $RD^{\mathrm{sp}}(\mathbf{L})R^{-1}$, for arbitrary rotation R; these matrices have the same form as (7) or (8), but in the coordinate system $x'y'z'$ obtained by the rotation R from the original one xyz. The rotation R is usually given by three Euler angles α, β and γ ($R(\alpha, \beta, \gamma)$), making ${}^{(\alpha,\beta,\gamma)}_{\tilde{k}}D^{C}_{\tilde{m}}$, *i.e.* ${}^{(\alpha,\beta,\gamma)}D^{\hat{C}}$ the complete label of a spin representation.

To summarize, there are four classes and four exceptional spin representations of the line groups of the first family $\mathbf{L} = \mathbf{T}_Q(f)\mathbf{C}_n$ with even n. When n is odd, there are only two classes $C = 0, t$ of the spin representations (no exceptional representations and classes $C = s, w$).

3.3. Magnetic groups

According to the structure of the magnetic groups (2) discussed above, besides the ordinary first family line group $\mathbf{T}_Q(f)\mathbf{C}_n$, there are three corresponding black-and-white magnetic groups if n is even:

$$\mathbf{T}_{Q'}(2f)\mathbf{C}_n + \theta(C_Q|f)\mathbf{T}_{Q'}(2f)\mathbf{C}_n : \quad Q' = \begin{cases} Q/2, & \text{if } Q \geq 2n; \\ nQ/(2n + Q + Q[-\frac{2n}{Q}]), & \text{otherwise}; \end{cases} \tag{9a}$$

$$\mathbf{T}_Q(f)\mathbf{C}_{n/2} + \theta C_n \mathbf{T}_Q(f)\mathbf{C}_{n/2}; \tag{9b}$$

$$\mathbf{T}_{Q'}(f)\mathbf{C}_{n/2} + \theta(C_Q|f)C_n\mathbf{T}_{Q'}(f)\mathbf{C}_{n/2} : \quad Q' = \frac{Qn}{Q+n}. \tag{9c}$$

For n odd only the group in (9*a*) exists.

These groups are spin groups with the particular spin representations (7). Namely: ${}_{2\pi/Qf}D^0_1(\ell_{ts})$ corresponds to the ordinary magnetic group, while ${}^{(0,\pi,0)}_{\pi/f-2\pi/Qf}D^t_{-1}(\ell_{ts})$, ${}_{2\pi/Qf}D^s_{-n/2+1}(\ell_{ts})$ and ${}^{(0,\pi,0)}_{\pi/f-2\pi/Qf}D^w_{n/2-1}(\ell_{ts})$ correspond to (9*a*), (9*b*) and (9*c*), respectively.

4. Spin arrangements

In this section we briefly analyse spin arrangements obtained by the action of the derived spin groups. First, we consider single-orbit systems. For the orbit representative $\mathbf{r}_{00}$ placed at a general position, with the spin vector $\mathbf{s}_{00}$, the spin group distributes spins to other atoms according to (1):

$$(\ell_{ts}\mathbf{r}_{00}, D^{\mathrm{sp}}(\ell_{ts})\mathbf{s}_{00}) = (\mathbf{r}_{ts}\mathbf{s}_{ts}). \tag{10}$$

Before proceeding further, let us comment on the choice of the coordinate system $x'y'z'$ (directed along the unit vectors $\mathbf{x}'$, $\mathbf{y}'$ and $\mathbf{z}'$). It will be called a *spin* system (precisely: global spin system), as it is related to the spin space only. In this system matrices of D^{sp} are exactly those given by (7) and (8), and further general discussion will be made in this frame. However, the geometry of the atomic configuration usually introduces some other natural coordinates xyz, to be called *global* coordinates (in particular, the axis of the quasi-one-dimensional system is taken to be the z axis). As a simple illustration, let us take a look at the spin representations (7) from the class $C = 0$. As these are rotations around the z axis, conjugation by rotation R intertwining the global and the spin frames changes the axis of rotation but not the angle, and this new rotation is the spin representation in the global frame.

For further discussion it is useful to introduce the convention that the angle χ between the z' axis and $\mathbf{s}_{00}$ is not greater than $\pi/2$, which is enabled by the freedom in the choice of spin system; in particular, the choice of the orientation of z' suffices to obey this convention.

The components of the spin vector $\mathbf{s}_{ts}$ of the atom $\mathbf{r}_{ts}$ in the spin frame are for the classes and exceptional groups:

$$\mathbf{s}_{ts} = |\mathbf{s}_{00}|(\sin\chi\cos(\varphi_{ts} + \varphi_{00}), \sin\chi\sin(\varphi_{ts} + \varphi_{00}), (-1)^C\cos\chi), \tag{11a}$$

$$\mathbf{s}_{ts} = |\mathbf{s}_{00}|((-1)^{C_1}\sin\chi\cos\varphi_{00}, (-1)^{C_2}\sin\chi\sin\varphi_{00}, (-1)^{C_3}\cos\chi), \tag{11b}$$

where φ_{00} is the angle between the projection of $\mathbf{s}_{00}$ onto the $x'y'$ plane and the x' axis. In the case of the classes, for C even, $\mathbf{s}_{ts}$ is the vector obtained from $\mathbf{s}_{00}$ by the rotation around z' for the angle $\varphi_{ts} = \tilde{k}ft + \tilde{m}(2\pi/n)s$ (and positioned in $\mathbf{r}_{ts}$), while for C odd z' projection of $\mathbf{s}_{ts}$ is in addition reversed. Obviously, for C even the spin vector belongs to the cone obtained by the rotation of $\mathbf{s}_{00}$ around the z' axis, and to the reversed cone when C is odd. This conclusion is valid for the exceptional groups, too, as in this case x', y', z' coordinates of $\mathbf{s}_{ts}$ are simply multiplied by ±1 with respect to $\mathbf{s}_{00}$, and lie on the same or on the opposite cone with $\mathbf{s}_{00}$, depending on the parity of C_3. Thus, we showed that for quasi-one-dimensional systems spin arrangements are necessarily *conical*.

Special cases are $\chi = 0$ and $\chi = \pi/2$, when these cones degenerate in the one-dimensional (ferromagnetic and antiferromagnetic) or two-dimensional (planar, flat) spin arrangements, respectively. Precisely, if $\chi = 0$ all the spins are along the z' direction, making ferromagnetic spin order for class $C = 0$ and exceptional groups $\hat{t}$, $\hat{s}$ and $\hat{w}$, and antiferromagnetic in the remaining cases. For $\chi = \pi/2$ all spins are

Table 1
Description of the spin arrangements.

In the first column the cone angle χ is given. Then the types of spin arrangements are listed: in the upper part for the classes C with spin groups singled out by $(\tilde{k}, \tilde{m})$, and in the lower part for exceptional spin groups $\hat{C}$. Types are characterized by F (ferromagnet), A (antiferromagnet), P (planar) or C (conical). (*) stands for the conditions $\tilde{k} \neq 0, \pi/f$ or $\tilde{m} \neq 0, n/2$.

χ	C	$\tilde{k}$	$\tilde{m}$	Type
0	0	$\forall\tilde{k}$	$\forall\tilde{m}$	F
	t, s, w	$\forall\tilde{k}$	$\forall\tilde{m}$	A
$0 < \chi < \pi/2$	$0, t, s, w$	(*)		C
	0	0	0	F
	t, s, w	0	0	A
	$0, t, s, w$	π/f	0	P
	$0, t, s, w$	0	$n/2$;	P
	$0, t, s, w$	π/f	$n/2$;	P
$\pi/2$	$0, t, s, w$	(*)		P
	$0, t, s, w$	0	0	F
	$0, t, s, w$	π/f	0	A
	$0, t, s, w$	0	$n/2$;	A
	$0, t, s, w$	π/f	$n/2$;	A

χ	$\hat{C}$	Type
0	$\hat{\boldsymbol{t}}, \hat{\boldsymbol{s}}, \hat{\boldsymbol{w}}$	F
	$\hat{\mathbf{0}}$	A
$0 < \chi < \pi/2$	$\hat{\mathbf{0}}, \hat{\boldsymbol{t}}, \hat{\boldsymbol{s}}, \hat{\boldsymbol{w}}$	P for $\varphi_{00} = 0, \pm\pi/2$
	$\hat{\mathbf{0}}, \hat{\boldsymbol{t}}, \hat{\boldsymbol{s}}, \hat{\boldsymbol{w}}$	C for $\varphi_{00} \neq 0, \pm\pi/2$
$\pi/2$	$\hat{\mathbf{0}}, \hat{\boldsymbol{t}}, \hat{\boldsymbol{s}}, \hat{\boldsymbol{w}}$	A for $\varphi_{00} = 0, \pm\pi/2$
	$\hat{\mathbf{0}}, \hat{\boldsymbol{t}}, \hat{\boldsymbol{s}}, \hat{\boldsymbol{w}}$	P for $\varphi_{00} \neq 0, \pm\pi/2$

in the $x'y'$ plane (planar helimagnet); note that for a few particular groups such a spin arrangement degenerates to a linear one, but not along the z' axis. Again, there are particular groups with $0 < \chi < \pi/2$ for which a conical spatial arrangement reduces to a planar or linear case. The dimensionality of spin arrangements for all classes and all exceptions is given in Table 1. Finally, because of the freedom in the choice of z', some groups give ferromagnetic or antiferromagnetic spin arrangement as in the case $\chi = 0$ but not along the z' axis; in fact, the class $C = 0$ always corresponds to ferromagnets, while the remaining three classes $C = t, s, w$ determine three different types of antiferromagnets.

Expressions (11*a*) and (11*b*) completely describe the spin arrangement, provided the orbit representative spin $\mathbf{s}_{00}$ is known. So, it remains to find this vector. In general, it cannot be arbitrarily chosen, but obeys the condition of being invariant under the action of the stabilizer. This means that for each element ℓ from the stabilizer the relations

$$D^{\mathrm{sp}}(\ell)\mathbf{s}_{00} = \mathbf{s}_{00} \tag{12}$$

must be fulfilled. Of course, for the generic orbit, with trivial stabilizer, $\mathbf{s}_{00}$ is arbitrary. On the contrary, in the case of the linear orbit (and $n > 1$), there are severe restrictions. Let us thoroughly consider these restrictions on the components of vector $\mathbf{s}_{00} = (s^1_{00}, s^2_{00}, s^3_{00})$ for the class $C = 0$ from (7) and the linear orbit. As the linear orbit corresponds to elements ℓ_{0s} ($s = 0, \ldots, n-1$), fixing a point $\mathbf{r}_{00}$; from (12) it follows that

$$\begin{pmatrix} \cos(\tilde{m}\frac{2\pi}{n}s) & -\sin(\tilde{m}\frac{2\pi}{n}s) & 0 \\ \sin(\tilde{m}\frac{2\pi}{n}s) & \cos(\tilde{m}\frac{2\pi}{n}s) & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} s^1_{00} \\ s^2_{00} \\ s^3_{00} \end{pmatrix} = \begin{pmatrix} s^1_{00} \\ s^2_{00} \\ s^3_{00} \end{pmatrix}.$$

It is obvious that s^3_{00} remains the same; thus any spin vector along the z' axis is allowed and then the spin arrangement generated by the spin representation ${}_{\tilde{k}}D^0_{\tilde{m}}(\mathbf{L})$ is ferromagnetic. The components in the $x'y'$ plane s^1_{00} and s^2_{00} are invariant if $(\tilde{m}s)/n$ (for all s) is an integer number. Taking into account that $\tilde{m}$ is defined to be an integer from the interval $(-n/2, n/2]$, this can be only for $\tilde{m} = 0$, which means that for the spin representations ${}_{\tilde{k}}D^0_0(\mathbf{L})$ all directions for spin vector $\mathbf{s}_{00}$ are allowed (conical helimagnet).

Similarly, for the class $C = t$ vector $\mathbf{s}_{00}$ is parallel to z' ($\chi = 0$), generating antiferromagnetic order, except for $\tilde{m} = 0$, when all directions are allowed. For the remaining two classes $C = s, w$, for $\tilde{m} \neq 0$ there is no allowed direction, while for $\tilde{m} = 0$ all the directions perpendicular to z' ($\chi = \pi/2$) are allowed and generate planar helimagnetic order. This is summarized in the upper part of Table 2, while examples of spin arrangements for one group from each class and exceptional groups are illustrated in Fig. 2. Note that many of the arrangements obtained by the spin groups, in particular those incommensurate with the lattice, cannot be described by the magnetic groups.

Analogous analysis for the exceptional representations gives the results summarized in Table 2 (bottom part). The condition (12) for the linear orbit leaves only $\mathbf{s}_{00}$ along x' for $\hat{\mathbf{0}}$ (antiferromagnet) and along z' for $\hat{\boldsymbol{t}}$ (ferromagnet). The other two groups, $\hat{\boldsymbol{s}}$ and $\hat{\boldsymbol{w}}$, for the linear orbit give the same spin arrangement, with spins in a plane containing the z' axis.

As for the magnetic groups, from Table 2 one finds that for $n > 1$ the ordinary group generates ferromagnetic and the group in (9*a*) antiferromagnetic spin ordering along the system axis. Further, for the groups in (9*b*) and (9*c*) there are no allowed directions for $n > 2$, while for $n = 2$ spins are in the plane perpendicular to the system axis forming the planar helimagnet.

Table 2
Classification of the spin arrangements for a linear orbit.

In the upper part groups from the classes $C = 0, s, t, w$ (column 1) are given by the quantum numbers $\tilde{k}$ and $\tilde{m}$ (columns 2 and 3); in the bottom part exceptional groups $\hat{C}$ are specified in column 1, while their elements are explained in the following four columns. In the last two columns are the allowed vector $\mathbf{s}_{00}$ and the type of spin arrangement (characterized as in Table 1).

C	$\tilde{k}$	$\tilde{m}$	$\mathbf{s}_{00}$	Type
0	$\forall\tilde{k}$	$\tilde{m} \neq 0$	z'	F
t	$\forall\tilde{k}$	$\tilde{m} \neq 0$	z'	A
$0, t$	$\forall\tilde{k}$	$\tilde{m} = 0$	All	C
s, w	$\forall\tilde{k}$	$\tilde{m} \neq 0$	None	/
s, w	$\forall\tilde{k}$	$\tilde{m} = 0$	$x'y'$ plane	P

$\hat{C}$	t even s even	t even s even	t odd s odd	t odd s odd	$\mathbf{s}_{00}$	Type
$\hat{\mathbf{0}}$	I	$C_{2x'}$	$C_{2y'}$	$C_{2z'}$	x'	A
$\hat{\boldsymbol{t}}$	I	$C_{2z'}$	$-C_{2y'}$	$-C_{2x'}$	z'	F
$\hat{\boldsymbol{s}}$	I	$-C_{2y'}$	$C_{2z'}$	$-C_{2x'}$	$x'z'$ plane	H
$\hat{\boldsymbol{w}}$	I	$-C_{2y'}$	$-C_{2x'}$	$C_{2z'}$	$x'z'$ plane	H

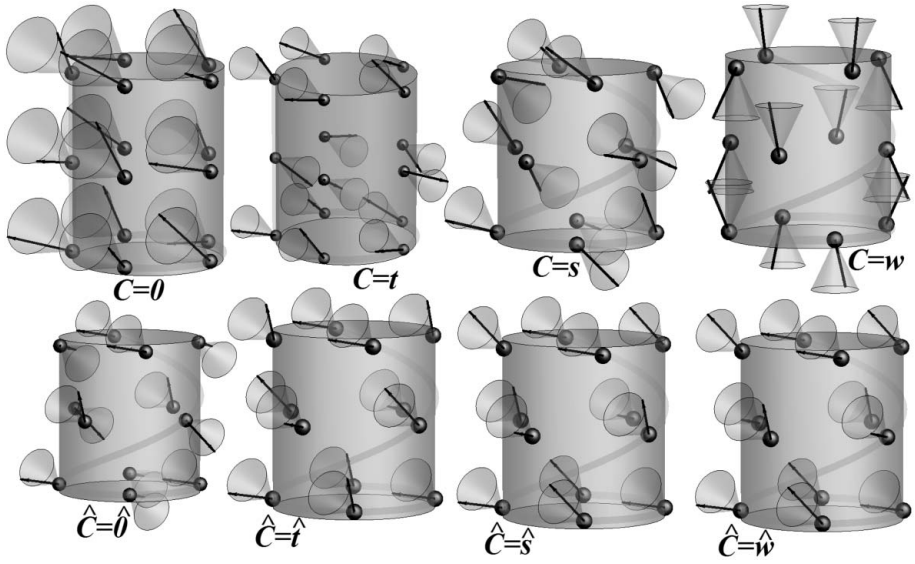

Figure 2
Spin arrangements for various spin groups. The top row shows spin representations belonging to the following classes: commensurate are ${}^{(0,\pi/3,\pi/5)}_{\pi/2f}D^{0}_{2}(\mathbf{T}_5(f)\mathbf{C}_5)$ and ${}^{(0,\pi/3,\pi/5)}_{\pi/2f}D^{t}_{-2}(\mathbf{T}_5(f)\mathbf{C}_5)$, with opposite quantum number $\tilde{m}$ resulting in the opposite sense of rotation of spin within the monomer; ${}^{(0,\pi/3,\pi/5)}_{1}D^{s}_{1}(\mathbf{T}_7(f)\mathbf{C}_4)$ is incommensurate, and ${}^{(0,\pi,0)}_{5\pi/7f}D^{w}_{1}(\mathbf{T}_7(f)\mathbf{C}_4)$ is a magnetic group. The bottom row shows the arrangements generated by the four exceptional spin representations ${}^{(0,\pi/3,\pi/5)}D^{\hat{0}}(\mathbf{T}_7(f)\mathbf{C}_4)$, ${}^{(0,\pi/3,\pi/5)}D^{\hat{t}}(\mathbf{T}_7(f)\mathbf{C}_4)$, ${}^{(0,\pi/3,\pi/5)}D^{\hat{s}}(\mathbf{T}_7(f)\mathbf{C}_4)$ and ${}^{(0,\pi/3,\pi/5)}D^{\hat{w}}(\mathbf{T}_7(f)\mathbf{C}_4)$.

5. Generalization to multi-orbit systems

So far single-orbit systems have been analysed (this implies that all the spins have the same magnitude). Let us now consider a system consisting of M orbits. Each of them is either a general-position or special-position orbit. Denoting the orbit representative positions by $\mathbf{r}_{i;0}$ $(i = 1, \ldots, M)$, the whole system is generated by the action of symmetry group $\mathbf{G}$ on the set of these orbit representatives (called symcell, or asymmetric unit), *i.e.* on the $3M$-dimensional vector $\mathbf{r}_0^{\rm sym} = (\mathbf{r}_{1;0}, \ldots, \mathbf{r}_{M;0})$ of their positions. Analogously, a multi-orbit magnetic system is generated by the action of the nontrivial spin-group elements $(g, D^{\rm sp}(g))$ for each $g \in \mathbf{G}$ on the pair $(\mathbf{r}_0^{\rm sym}, \mathbf{s}_0^{\rm sym})$, where $\mathbf{s}_0^{\rm sym}$ is the set of spin vectors $\mathbf{s}_{i;0}$ in the ith orbit representative:

$$(g, D^{\rm sp}(g))(\mathbf{r}_0^{\rm sym}, \mathbf{s}_0^{\rm sym}) = ((g\mathbf{r}_{1;0}, \ldots, g\mathbf{r}_{M;0}), (D_1^{\rm sp}(g)\mathbf{s}_{1;0}, \ldots, D_M^{\rm sp}(g)\mathbf{s}_{M;0})). \quad (13)$$

Clearly, the total spin space of the symcell is the direct sum $\oplus_{i=1}^{M}\mathcal{S}_i$ of the spin spaces $\mathcal{S}_i = \mathbb{R}^3$ of the orbit representatives. Thus, for multi-orbit systems the spin part of a spin-group element is the direct sum of the orbital spin representations:

$$D^{\rm sp}(g) = \oplus_{i=1}^{M} D_i^{\rm sp}(g). \quad (14)$$

For the first family line groups $D_i^{\rm sp}$ are spin representations derived in §3. Of course, for each special orbit the restrictions (12) must be satisfied independently.

Finally, note that the magnitude of spin of various orbits can be different.

6. Discussion

It is shown that orthogonal three-dimensional representations $D^{\rm sp}(\mathbf{G})$ of the group of geometrical transformations $\mathbf{G}$ give nontrivial spin groups $(\mathbf{G}, D^{\rm sp}(\mathbf{G}))$ of $\mathbf{G}$, with elements $(g, D^{\rm sp}(g))$ which describe spin arrangements of a single-orbit system. Accordingly, the classification of the nontrivial spin groups of $\mathbf{G}$ reduces to determination of all such non-equivalent three-dimensional representations, which can be performed by combining real irreducible representations into the direct sums. After the standard form is obtained this way, all equivalent representations ${}^{R}D^{\rm sp}(\mathbf{G})$ are obtained as $RD^{\rm sp}(\mathbf{G})R^{-1}$, where R is a rotation relating the global coordinate to the global spin frame. Note that the position of the projection of the spin vector onto the $x'y'$ plane is parameterized both by the azimuthal angle φ_{00} and the Euler angle γ. Therefore, these two angles are related and one of them is superfluous. The spin representations derived for single-orbit systems are directly summed in the case of multi-orbit systems to give the total spin representation.

As an illustration, we find the spin group for the proposed spin structure of a 'triangular' two-leg ladder (Fig. 3, left) in the cuprate compound $LiCu_2O_2$ (Masuda *et al.*, 2004). $LiCu_2O_2$ crystallizes in the orthorhombic lattice with unit-cell parameters $a = 5.73$, $b = 2.86$ and $c = 12.42$ Å. Magnetic divalent cations Cu^{2+}, with spin 1/2, form 'triangular' two-leg ladders (or zigzag chains) along the crystallographic b axis. As these zigzag chains are mutually weakly coupled, each can be viewed as a quasi-one-dimensional system. It was experimentally verified that below the critical temperature $T_{\rm c} \simeq 22$ K this system has incommensurate helimagnetic long-range order: the spins rotate in the crystallographic ab plane with the angle $\pi(1 - \zeta)$ where $\zeta = 0.1738$ (2). The angle between this plane and the plane of the ladder is 45°; also, the axis around which spins rotate makes the same angle with the ladder plane.

Determination of spin groups should be performed in two steps: first one finds the geometrical symmetry group and orbit, then the corresponding spin representation. The zigzag chain can be seen as a single (general-position) orbit with the symmetry being the first family line group $\mathbf{T}_2(f)\mathbf{C}_1$ (Fig. 3, left). Therefore it is natural to choose the z axis to be along the crystallographic b axis. From the data for the unit cell, one immediately reads that the translational period is b, giving the fractional translation $f = b/2$. Further, let the ladder be in the xz plane with the orbit representative at $\mathbf{r}_{00} = (w/2, 0, 0)$, where $w = 1.43$ Å is the ladder width. The spin frame (Fig. 3, bottom left) is determined by coincidence of the z' axis with the axis of spin rotation (thus spins rotate in the $x'y'$ plane),

giving the Euler angles $\alpha = \pi/2$, $\beta = \pi/2$ and $\gamma = \pi/4$. As the system is a general-position orbit, there are no restrictions on the orbit representative spin vector $\mathbf{s}_{00}$ and one can take $\varphi_{00} = 0$; $\chi = \pi/2$ (planar arrangements) and $|\mathbf{s}_{00}| = 1/2$ (magnitude of spins). Finally, the period of the magnetic lattice is incommensurate with the period of the geometrical lattice; among the spin representations this is realized for those from the classes (for helical groups $\tilde{m} = 0$). Relation (11*a*) gives the spin arrangement of the zigzag chain (the atoms are counted by t, $s = 0$) that was sought, by noting that the experimental value of the angle of rotation of the spins is actually the angle between spin vectors of the t-th and $t+1$-th atom, *i.e.* $\varphi_{10} = \pi(1 - \zeta)$. To conclude, the geometry of the zigzag chain is obtained by the action of the group $\mathbf{T}_2(b/2)\mathbf{C}_1$ on the atom in the position $\mathbf{r}_{00} = (0.715\ \text{Å}, 0, 0)$, while the corresponding spin arrangement is obtained by the action of the spin representation ${}^{(\pi/2,\pi/2,\pi/4)}_{2\pi(1-\zeta)/b}D^C_0$ on the vector $R(\pi/2, \pi/2, \pi/4)\mathbf{s}_{00}$ [$\mathbf{s}_{00} = (1/2, 0, 0)$ in Cartesian coordinates]. Note, in this way all relevant quantities of the magnetic system may be given in the coordinate frame xyz.

Another example of a planar helimagnet is that of single-wall carbon nanotubes grown entirely from ^{13}C (Rummeli *et al.*, 2007; Churchill *et al.*, 2009). It was shown theoretically that a weak hyperfine interaction can lead to such magnetic order of the nuclear spins (magnitude is 1/2) in armchair nanotubes (Braunecker *et al.*, 2009). In fact, spins on a cross section of the nanotube are ferromagnetically oriented, while along the nanotube axis they rotate with the period π/k_F (Fig. 3, middle), where k_F is the Fermi-level quasi-momentum. Obviously, the spin frame coincides with the system frame. In terms of the first family line groups each nanotube is composed of two general-position orbits, both being of the same type. All group parameters q, r, n and f are known functions of the chiral indexes (n_1, n_2) of the nanotube, as well as $k_F = 2\pi/3f$ (Damnjanović & Milošević, 2010). Let us mention that, despite the fact that the translational period a of the armchair nanotubes is equal to the period of the graphene hexagonal lattice $a_0 = 2.46$ Å, this and other nanotubes cannot be described by rod groups.

To illustrate the determination of spin group, a (5,5) nanotube is utilized here. The whole nanotube is generated by the action of the first family line group $\mathbf{T}_{10}(1.23\ \text{Å})\mathbf{C}_4$ on two orbit representative atoms ($M = 2$) in the positions $\mathbf{r}_{1;00}$ = (3.392 Å, $2\pi/15$, 0) (this orbit is given in Fig. 1, left) and $\mathbf{r}_{2;00}$ = (3.392 Å, $-2\pi/15$, 0) (the same type of orbit as before), both being on the same cross section. The dimension of the spin space of the symcell is two times greater than for single-orbit systems; thus the total spin vector $\mathbf{s}^{\text{sym}}_{00}$ is six-dimensional, as well as the total spin representation. As in the previous illustration of planar helimagnets, both spin vectors $\mathbf{s}_{1;00}$ and $\mathbf{s}_{2;00}$ belong to the $x'y'$ plane ($\chi = \pi/2$) where they can be selected arbitrarily, but to reproduce a ferromagnet they must be mutually parallel. The angle of rotation of spins between adjacent cross sections that contain atoms is $2k_Ff = 4\pi/3$, meaning that the spin representations D^{sp}_1 and D^{sp}_2 are from the classes with $\tilde{m} = 0$ (ferromagnetic cross sections). Thus, the total spin representation is ${}_{2k_F}D^C_0 \oplus_{2k_F} D^C_0$, and acting on the column $\mathbf{s}^{\text{sym}} = 1/2(1, 0, 0, 1, 0, 0)$ (Cartesian coordinates) gives the spin arrangement.

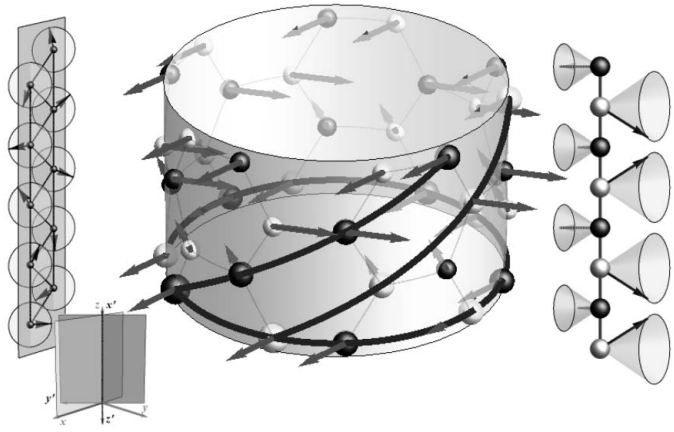

Figure 3
Spin arrangements for CuO_2 chains in $LiCu_2O_2$ (left), a (5,5) ^{13}C nanotube (middle) and $Ba_2Mg_2Fe_{12}O_{22}$ (right). Different colours of atoms indicate different orbits.

In order to describe multi-orbit systems with conically arranged spins of different magnitudes, we mention here the multiferroic Y-type hexaferrite $Ba_2Mg_2Fe_{12}O_{22}$. Neutron diffraction studies have confirmed the coexistence of several conical spin phases (Ishiwata *et al.*, 2010). The spins are ferrimagnetically ordered within two kinds of blocks (black and white balls in Fig. 3, right panel), each carrying the net magnetic moments with mutually different magnitude. Each of these blocks can be viewed as one linear orbit, thus being described by $\mathbf{T}(f)\mathbf{C}_1$ where f is translational period (the total length of both blocks). For example, the magnetic symmetry of the phase FE2 (Ishiwata *et al.*, 2010, p. 2) is described by the spin representation ${}^{(\pi/2,\pi/2,0)}_{\pi/f}D^0_0(\mathbf{L}) \oplus^{(\pi/2,\pi/2,0)}_{\pi/f} D^0_0(\mathbf{L})$, from the class $C = 0$, with quantum numbers $(\tilde{k}, \tilde{m}) = (\pi/f, 0)$. The cone angle χ is about 70° at 10 K.

One of the known applications of symmetry is reduction of the number of independent parameters describing the system. This can be of great importance in the prediction of optimal spin arrangements, and here we outline a general method illustrating the efficiency of a symmetry-based approach in determination of the classical ground state.

The most important fact is that there is a minimal set of the atoms generating the whole system by the action of the symmetry group $\mathbf{L}$; then, in the minimization one can use the energy per symcell:

$$E_{\text{sym}}[\mathbf{s}_{1;0}, \mathbf{s}_{1;1}, \ldots] = \sum_{ij}^{M} \sum_{\ell \in \mathbf{L}} \mathbf{s}_{i;0} h(\mathbf{r}_{i;0}, \mathbf{r}_{j;\ell}) \mathbf{s}_{j;\ell}. \qquad (15)$$

Here the indexes i and j count the orbits of a system, and h is an interaction tensor (its elements are coupling coefficients) between spins, being a function of atomic positions in the general case. Simultaneously, the spin vectors are arranged over the atoms by the action of the corresponding spin representations on the spins $\mathbf{s}_{i;0}$ of the symcell. Thus, to minimize the classical energy one has to vary over the symcell

spins (parameters χ_i and $\varphi_{i;0}$) and the spin representations which include classes (parameterized by the continual parameter $\tilde{k}$ and the discrete one $\tilde{m}$), as well as the finite set of exceptional representations. In the case of quasi-one-dimensional systems, with high-order helical axes (including incommensurate systems) resulting in translational elementary cells with a huge number of atoms, this can tremendously reduce the number of variational parameters.

We performed numerical minimization of the energy (15) for the isolated zigzag chain described above. For single-orbit systems sums over i and j in the energy expression vanish, and spin vectors are given by (11a), (11b) (with $s = 0$). The interaction tensor between an atom $\mathbf{r}_{00}$ and its relevant neighbours $\mathbf{r}_{t0}$ can be written

$$h(\mathbf{r}_{00}, \mathbf{r}_{t0}) = \mathrm{diag}[J_t, J_t + D_t^{\mathrm{ex}}, J_t], \tag{16}$$

where only exchange coupling coefficients $J_1 = 6.4$, $J_2 = -11.9$, $J_4 = 7.6$ meV and exchange anisotropy $D_1^{\mathrm{ex}} = D^{\mathrm{ex}} = 0.083$ meV are non-vanishing (Masuda *et al.*, 2005; Mihaly *et al.*, 2006). We found that the minimum of the energy corresponds to the ground-state arrangement given by $\chi = \pi/2$, $\varphi_{00} = \pi/2$ and $\tilde{k} = 2.58$ Å^{-1}, being in agreement with experimental values.

The intensity in elastic magnetic scattering of unpolarized neutrons by a single-orbit magnetic system [set of pairs $(\mathbf{r}_{ts}, \mathbf{s}_{ts})$], whose symmetry is the first family spin line group, is determined by the scattering amplitude,

$$\mathbf{P}(\mathbf{k}) = p \sum_{t=-\infty}^{\infty} \sum_{s=0}^{n-1} \exp(i\mathbf{k}\mathbf{r}_{ts})\mathbf{s}_{ts}, \tag{17}$$

where $\mathbf{k}$ is the scattering vector and p the magnetic structure factor. Invariance of the scattering amplitude under the elements of the first family spin line groups $(\ell_{ts}, D^{\mathrm{sp}}(\ell_{ts}))$ leads to the relations $\mathbf{P}(\mathbf{k}) = \exp(ik_z f)D^{\mathrm{sp}}(\ell_{ts})\mathbf{P}(\mathbf{C}_{Qn}^{2nQ-tn-sQ}\mathbf{k})$.

As a simple illustration we calculate the scattering amplitude for the zigzag chain discussed in §3. In the spin frame, substituting the obtained data in (17), one gets

$$\begin{pmatrix} P_{x'}(\mathbf{k}) \\ P_{y'}(\mathbf{k}) \\ P_{z'}(\mathbf{k}) \end{pmatrix} = \frac{p}{2} \sum_{t=-\infty}^{\infty} \exp\left[i(-1)^t \frac{w}{2(2^{1/2})}(k_{y'} + k_{z'}) \right] \exp\left(i\frac{b}{2}k_{x'}t \right) \times \begin{pmatrix} \cos\frac{b}{2}\tilde{k}t \\ \sin\frac{b}{2}\tilde{k}t \\ 0 \end{pmatrix}. \tag{18}$$

Separating the sum into odd and even terms yields

$$\begin{pmatrix} P_{x'}(\mathbf{k}) \\ P_{y'}(\mathbf{k}) \\ P_{z'}(\mathbf{k}) \end{pmatrix} \propto \sum_{\xi} \cos\frac{w}{2(2^{1/2})}k_{\perp} \times \begin{pmatrix} \delta(k_{x'}^{+} - \xi\frac{2\pi}{b}) + \delta(k_{x'}^{-} - \xi\frac{2\pi}{b}) \\ -i\delta(k_{x'}^{+} - \xi\frac{2\pi}{b}) + i\delta(k_{x'}^{-} - \xi\frac{2\pi}{b}) \\ 0 \end{pmatrix}, \tag{19}$$

where $k_{\perp} = k_{y'} + k_{z'}$, $k_{x'}^{\pm} = k_{x'} \pm \tilde{k}$ and ξ is an integer. Obviously, this gives sharp peaks (determining the angle of rotation between the t-th and $t+1$-th spin vectors) along the $k_{x'}$ axis (recall that the zigzag chain is along x') and some modulation in the perpendicular plane.

7. Conclusions

Spin representations for any system with geometrical symmetry described by the first family line group $\mathbf{L} = \mathbf{T}_Q(f)\mathbf{C}_n$ are found. Each of them is either from class C or exceptional $\hat{C}$. Precisely, for n even there are four classes ($C = 0, t, s, w$) of the nonequivalent spin representations and the particular spin representation of a class is determined by the pair of quantum numbers $(\tilde{k}, \tilde{m})$ in the form of (7); in addition there are four exceptional representations $\hat{C} = \hat{0}, \hat{s}, \hat{t}, \hat{w}$ given by (8). For n odd, only the representations from the two classes $C = 0, t$ describe possible magnetic symmetries.

Each line group $\mathbf{L}^F$ ($F = 2, \ldots, 13$) has one line group $\mathbf{L}$ from the first family as a subgroup of index two (in the families 2–8) or index four (in the families 9–13). Therefore, any orbit of $\mathbf{L}^F$ is either also an orbit of $\mathbf{L}$, or can be decomposed into two or four orbits of $\mathbf{L}$. This enables us to treat the systems with higher line-group symmetries with the help of the derived spin representations of the first family. A powerful method of interpretation of experimental results can be established, providing a unified classification of all spin arrangements that appear in regular quasi-one-dimensional systems.

APPENDIX *A*
Classification of real spin representations

According to Wigner's classification, a representation $D(\mathbf{G})$ of the group $\mathbf{G}$ can be [$D_1(\mathbf{G}) \sim D_2(\mathbf{G})$ means $D_1(\mathbf{G}) = XD_2(\mathbf{G})X^{-1}$ for nonsingular operator X]:

(i) of *the first kind* if $D(\mathbf{G}) \sim D^*(\mathbf{G})$ and there is an equivalent real representation;

(ii) of *the second kind* if $D(\mathbf{G}) \sim D^*(\mathbf{G})$, but there is no equivalent real representation;

(iii) of *the third kind* if $D(\mathbf{G}) \not\sim D^*(\mathbf{G})$.

Starting from the irreducible representations D^{μ} (the Greek superscript counts the irreducible representations) of dimension $|\mu|$ (of relevance are one-, two- and three-dimensional), three-dimensional real representations (spin representations) $D^{\mathrm{sp}}(\mathbf{G})$ could be constructed as one of the following:

(i) $D^{\mu}(\mathbf{G})$, $D^{\nu}(\mathbf{G})$, $D^{\lambda}(\mathbf{G})$ are the representations of the first kind and $|\mu| = |\nu| = |\lambda| = 1$, then:

(*a*) $D^{\mathrm{sp}}(\mathbf{G}) = 3D^{\mu}(\mathbf{G})$ (the same form for ν and λ),

(*b*) $D^{\mathrm{sp}}(\mathbf{G}) = 2D^{\mu}(\mathbf{G}) \oplus D^{\nu}(\mathbf{G})$ (the same $2+1$ form for the other combinations),

(*c*) $D^{\mathrm{sp}}(\mathbf{G}) = D^{\mu}(\mathbf{G}) \oplus D^{\nu}(\mathbf{G}) \oplus D^{\lambda}(\mathbf{G})$.

(ii) $D^{\mu}(\mathbf{G})$ is of the second or third kind and $D^{\nu}(\mathbf{G})$ is of the first kind, and $|\mu| = |\nu| = 1$, then $D^{\mathrm{sp}}(\mathbf{G}) = X(D^{\mu}(\mathbf{G}) \oplus D^{\mu *}(\mathbf{G}))X^{-1} \oplus D^{\nu}(\mathbf{G})$, where

$$X = \frac{1}{2^{1/2}} \begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix},$$

as $D^{\mu}(\mathbf{G}) \oplus D^{\mu *}(\mathbf{G})$ is of the first kind.

(iii) $D^{\mu}(\mathbf{G})$, $D^{\nu}(\mathbf{G})$ are of the first kind and $|\mu| = 2$, $|\nu| = 1$, then $D^{sp}(\mathbf{G}) = D^{\mu}(\mathbf{G}) \oplus D^{\nu}(\mathbf{G})$.

(iv) $D^{\mu}(\mathbf{G})$ is of the first kind and $|\mu| = 3$, then $D^{sp}(\mathbf{G}) = D^{\mu}(\mathbf{G})$.

Note that nonequivalent forms are given here. For example, the spin representation $D^{\mu}(\mathbf{G}) \oplus D^{\nu}(\mathbf{G}) \oplus D^{\lambda}(\mathbf{G})$ is equivalent to any spin representation of the same form obtained by permuting μ, ν, λ; similarly $2D^{\mu}(\mathbf{G}) \oplus D^{\nu}(\mathbf{G}) \sim D^{\nu}(\mathbf{G}) \oplus 2D^{\mu}(\mathbf{G})$.

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