Central European Journal of Physics
DOI: 10.2478/s11534-007-0023-8
Research article
CEJP 5(3) 2007 377–384

On the symmetry of magnetic structures in terms of the fibre bundles

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Received 07 February 2007; accepted 10 April 2007

Abstract: The paper concerns the application of the fibre bundle approach to the description of the magnetic structures and their symmetry groups. Hence the explicit formulas describing both the variety of magnetic structures and their symmetry groups have been derived. The assumption was made that the bundle sections correspond to magnetizations of the separate crystal planes multiplied by a certain Gaussian factor defined in $\mathbb{R}^3$, the last factor making the problem continuous and more physical.

Keywords: fibre bundles, magnetic structures, symmetry groups
PACS (2006): 75.10.-b,75.10.Hk

1 Introduction

To describe the symmetry of the magnetic structures as well as of all other aperiodic structures one needs to formulate the corresponding symmetry groups whose action on these structures leaves them invariant. Several attempts in this respect have been undertaken, e.g. spin groups [1–3], generalized color groups [4–6]. The extension of the spin groups to the description of quasicrystals is presented in [7].

Let us first recall a few definitions since the fibre bundle approach will be applied here to the description of the symmetry of magnetic structures. The fibre bundles and their topological structures present a kind of a generalization of the Cartesian product of two spaces with arbitrary dimensions. Moreover this approach resembles to some extent

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the wreath groups concept introduced by Litvin [8–10], because a wreath group acts in a similar way as a structural group of the fibre bundle (see below).

A fibre bundle consists of [11]:

(1) E — total space,
(2) M — base manifold,
(3) $\mathbf{E}$ — fibre,
(4) G — a structural group which acts in the standard fibre $\mathbf{E}$,
(5) projection $\pi : E \to M$.

The system (E, π, M, G) is called a fibre bundle if the following relations are satisfied:

(1) for each open subset U_α of M there exists a diffeomorphism φ_α such that:

$$\varphi_\alpha : \pi^{-1}(U_\alpha) \simeq U_\alpha \times E_x,$$

where E_x is an isomorphic space with the fiber $\mathbf{E}$,

(2) for two subsets $U_\alpha, U_\beta \subset M$ such that $U_\alpha \cap U_\beta \neq \emptyset$ there exists a diffeomorphism $\varphi_{\alpha\beta} \equiv \varphi_\alpha \circ \varphi_\beta^{-1}$ such that:

$$\varphi_{\alpha\beta} : (U_\alpha \cap U_\beta) \times E_x \to (U_\alpha \cap U_\beta) \times E_x$$

and $\varphi_{\alpha\beta}$ has the form:

$$\varphi_{\alpha\beta}(x, e) = (x, g_{\alpha\beta}(x) \cdot e)$$

where $g_{\alpha\beta}$ is a map from $U_\alpha \cap U_\beta$ to G, and $e \in E_x$.

(3) $\mathbf{E}$ is isomorphic to fibre E_x for all x.

We say that the map $s : M \to E$ is a section of E if: $\pi \circ s = id$. On a fibre bundle there exists a structure called a connection which allows us to compare elements belonging to different fibres. The connection A is defined as an operator acting on sections:

$$Ds = As, \tag{1}$$

where D is a covariant derivative. Using coordinates the Eq. (1) can be rewritten as follows:

$$D_i s_a = A_{iab} s_b,$$

where s_a form a basis in E_x. A is a 1-form which assumes values in the algebra g of the structural group G. Two sections $s(x)$ and $\widetilde{s}(y)$ are connected by the operator $T(y, x)$ in the following way:

$$\tilde{s}(y) = T(y, x)s(x), \tag{2}$$

where x, y are connected by the curve $\gamma : [0, 1] \to M$ such that $x = \gamma(0)$, $y = \gamma(1)$.

The operator T is expressed by the connection A as follows:

$$T(y, x) = P \exp\left(\int_x^y A\right). \tag{3}$$

The aim of this paper is an attempt to apply the fiber bundle formalism to the description of the magnetic structures and their symmetry groups.

2 Magnetic structures

To describe the symmetry of a magnetic structure in terms of the fibre bundles one needs a 6-dimensional space E_6. This space is a vector bundle and is represented locally as a Cartesian product of $\mathbb{R}^3$ and a certain vector space V_3 which is spanned by the orthogonal vectors $\widehat{\mathbf{e}}_1, \widehat{\mathbf{e}}_2, \widehat{\mathbf{e}}_3$. The vector space V_3 is the fibre of E_6. Note that the crystal structure itself can be fully described in $\mathbb{R}^3$ whereas the spin structure can be fully described in V_3.

A magnetic structure in V_3 is represented by a pair $(\mathbf{M},p)$ where $\mathbf{M}$ is a kind of magnetization vector in V_3 and p is a point in $\mathbb{R}^3$ of the attaching of the vector $\mathbf{M}$ on a given crystal plane. Thus $\mathbf{M}$ represents the resulting magnetic moment of this plane. The position vector of the point p has coordinates: $(0, 0, na/l)$, where: $n = 0, \pm 1, \pm 2, \pm 3, ...$, l is the distance between the magnetic lattice planes and a is a certain scaling factor.

The vector $\mathbf{M}$ after a certain modification (see below), can be interpreted as a section of the vector bundle E_6. This section should have a special form because in the physical system the magnetic moments are localized on the magnetic atoms and vanish outside these atoms in the ideal crystal. The types of these sections are given below for a variety of magnetic structures:

(1) Ferromagnetic structure (f):

$$\mathbf{M}_f = M\widehat{\mathbf{e}}_1, \tag{4}$$

(2) Antiferromagnetic structure (a):

$$\mathbf{M}_a = (-1)^n \, M\widehat{\mathbf{e}}_1, \tag{5}$$

(3) Simple spiral (s):

$$\mathbf{M}_s = M\cos(n\phi)\,\widehat{\mathbf{e}}_1 + M\sin(n\phi)\,\widehat{\mathbf{e}}_2, \tag{6}$$

where ϕ is the spiral angle,

(4) Ferromagnetic spiral (fs):

$$\mathbf{M}_{fs} = M\cos(n\phi)\,\widehat{\mathbf{e}}_1 + M\sin(n\phi)\,\widehat{\mathbf{e}}_2 + M\sin\psi\widehat{\mathbf{e}}_3, \tag{7}$$

where ψ is the angle between the vector $\mathbf{M}$ and the plane $(\widehat{\mathbf{e}}_1, \widehat{\mathbf{e}}_2)$,

(5) Skew spiral (ss) :

$$\begin{aligned} \mathbf{M}_{ss} = {} & M\left[\cos^2(n\phi) + \sin^2(n\phi)\cos\theta\right]\cos(n\phi)\,\widehat{\mathbf{e}}_1 + \\ & M\left[\cos^2(n\phi) + \sin^2(n\phi)\cos\theta\right]\sin(n\phi)\,\widehat{\mathbf{e}}_2 + \\ & 2M\sin(n\phi)\sin\frac{\theta}{2}\sqrt{\cos^2\frac{\theta}{2} + \sin^2\frac{\theta}{2}\cos^2(n\phi)}\widehat{\mathbf{e}}_3, \end{aligned} \tag{8}$$

where θ is the angle between the plane $(\widehat{\mathbf{e}}_1, \widehat{\mathbf{e}}_2)$ and the plane of the spiral; in other words θ is the skew angle and $\theta < \pi/2$.

Let us consider the spin waves as the frozen waves in the crystal. Therefore, regardless of whether we deal with the commensurate or incommensurate spin waves one can represent these waves as follows:

6. Transverse spin wave (t):

$$\mathbf{M}_t = f(n)\, M\widehat{\mathbf{e}}_1, \tag{9}$$

where $f(n)$ is the periodic function with the period equal to the spin wavelength. Note that if the latter period is commensurate with the crystal periodicity one can say that the spin wave is commensurate, and vice versa the incommensurability of $f(n)$ points to the incommensurability of the spin wave. Therefore if n numerates the crystal planes, then $f(n)$ represents the values of this function on these planes. The above remarks apply also to the longitudinal spin waves:

7. Longitudinal spin wave (l):

$$\mathbf{M}_l = f(n)\, M\widehat{\mathbf{e}}_3. \tag{10}$$

Note that the general formula concerning all the three spirals mentioned above, i.e. items 3., 4. and 5., can be expressed as follows:

$$\begin{gathered}\mathbf{M}_A(\phi,\theta,\psi) = M\left[\cos^2(n\phi) + \sin^2(n\phi)\cos\theta\right]\cos(n\phi)\,\widehat{\mathbf{e}}_1 + \\ M\left[\cos^2(n\phi) + \sin^2(n\phi)\cos\theta\right]\sin(n\phi)\,\widehat{\mathbf{e}}_2 + \\ M\left(2\sin(n\phi)\sin\frac{\theta}{2}\sqrt{\cos^2\frac{\theta}{2} + \sin^2\frac{\theta}{2}\cos^2(n\phi)} + \sin\psi\right)\widehat{\mathbf{e}}_3,\end{gathered} \tag{11}$$

where $A = s, fs, ss$. Thus the three angles ϕ, θ, ψ describe in an unambiguous manner all the three spirals, namely s corresponds to $0 < \phi < \pi$, $\theta = 0$, $\psi = 0$, fs corresponds to $0 < \phi < \pi$, $\theta = 0$, $\psi < \pi/2$ and ss corresponds to $0 < \phi < \pi$, $\theta < \pi/2, \psi = 0$.

To enable us to use the fibre bundles approach one has to assure that these sections (vectors $\mathbf{M}$) be continuous. Let us modify first a magnetic momentum $\mathbf{s}_i$ of the i-th magnetic atom in the following way:

$$\mathbf{s}(\mathbf{r}) = \mathbf{s}_i \exp\left[-\frac{(\mathbf{r} - \mathbf{r}_i)^2}{\xi^2}\right], \tag{12}$$

where $\mathbf{r}_i$ is the coordinate of the i-th magnetic atom, ξ is the characteristic scale of the atomic sizes. Such a situation seems to be more physical, because, as a matter of fact, a magnetic moment presents a field which is significant only close to the crystal positions of the magnetic atoms and decreases outside very quickly. The vector $\mathbf{M}$ itself presents a vector sum of the atomic magnetic moments on a crystal plane. Therefore according to the central theorem of the theory of probability (the Lyapunov theorem) the formula analogous to Eq. (12) is valid for the vector $\mathbf{M}$:

$$\mathbf{M}_m(\mathbf{r}) = \mathbf{M}_m \exp\left[-\frac{(\mathbf{r} - \mathbf{r}_l)^2}{d^2}\right], \tag{13}$$

where $\mathbf{r}_l$ is the coordinate of the l-th crystal plane, d is a distance between the neighbour crystal planes. The index m corresponds to the appropriate structures from points

1–7: $m = f, a, s, fs, ss, t, l$. The exponential factor here guarantees that the section **M** is continuous and has a small value outside the crystal plane.

It is well known that every arbitrary vector bundle on $\mathbb{R}^3$ is trivial. Therefore the bundle under consideration is also trivial. It means that there exists a global section of this bundle, which in our case corresponds to the vector **M**. According to formulas (4–8) the length of vector **M** is constant for a given magnetic structure. Thus in this case the fibers become spheres with the radii equal to the corresponding values of vector **M**, whereas the bundles become spherical. Triviality here means that sections do not vanish.

A total magnetic symmetry group can then be defined as a group which leaves $\mathbf{M}_m(\mathbf{r})$ invariant. This group consists of two factors: G_m, which is defined below, and G_Λ, which presents the symmetry group of the crystalline structure.

A magnetic symmetry group G_m is defined here by the invariance of the above vectors $\mathbf{M}_m$ with respect to some elements of the Euclidean group $e(3)$ of V_3.

Thus the magnetic group G_m is defined for the above structures by the condition:

$$G_m = \{g \in e(3) \,|g \cdot \mathbf{M}_m = \mathbf{M}_m\}\,, \tag{14}$$

where the dot $(\cdot)$ denotes the action of g on $\mathbf{M}_m$:

$$g \cdot \mathbf{M}_m = A\mathbf{M}_m + \mathbf{t}, \tag{15}$$

$$g = (A, \mathbf{t})\,. \tag{16}$$

A is a rotation matrix and $\mathbf{t}$ is a translation vector and is taken as the modulo lattice vector.

Let us determine the explicit forms of the symmetry groups for the above seven magnetic structures.

1. The magnetic group G_f for the ferromagnetic structure. This group has to conserve $\mathbf{M}_f{=}M\widehat{\mathbf{e}}_1$:

$$g \cdot \mathbf{M}_f = A\mathbf{M}_f + \mathbf{t}. \tag{17}$$

Thus:

$$A\widehat{\mathbf{e}}_1 = \widehat{\mathbf{e}}_1, \tag{18}$$

$$\mathbf{t} = 0. \tag{19}$$

From these conditions it follows that the matrix A has the form:

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & a & b \\ 0 & c & d \end{pmatrix} \tag{20}$$

where $ad - bc = 1$. This magnetic group in the space V_3 has the form:

$$G_f = \left\{ \left(\begin{pmatrix} 1 & 0 & 0 \\ 0 & a & b \\ 0 & c & d \end{pmatrix}, 0 \right) \text{ and } ad - bc = 1 \right\}. \tag{21}$$

The total magnetic group $\widehat{G}_f$ in the space E_6 is the tensor product of G_f and the space group G_Λ of the crystal structure:

$$\widehat{G}_f = G_f \otimes G_\Lambda. \tag{22}$$

2. For the antiferromagnetic structure one can obtain:

$$G_a = \left\{ \left(\begin{pmatrix} (-1)^n & 0 & 0 \\ 0 & a & b \\ 0 & c & d \end{pmatrix}, 0 \right) \text{ and } ad - bc = 1 \right\}. \tag{23}$$

The index n numerates the consecutive crystal lattice planes; to each such plane a corresponding vector $\mathbf{M}$ is ascribed.

3. For the simple spiral the symmetry group G_s in V_3 has to conserve:

$$g \cdot \mathbf{M}_s = A\mathbf{M}_s + \mathbf{t}. \tag{24}$$

This condition leads to the group G_s:

$$G_s = \left\{ \left(\begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}, 0 \right) \text{ and } \alpha = \phi \right\}. \tag{25}$$

Thus:

$$\widehat{G}_s = G_s \otimes G_\Lambda. \tag{26}$$

4. In the case of the ferromagnetic spiral the symmetry group G_{fs} in V_3 presents a product of the corresponding symmetry matrices for both the simple spiral and the ferromagnetic structure taking into account that this time the ferromagnetic component points in the direction $\widehat{\mathbf{e}}_3$:

$$G_{fs} = \left\{ \left(\begin{pmatrix} a\cos\alpha + b\sin\alpha & -a\sin\alpha + b\cos\alpha & 0 \\ c\sin\alpha + d\sin\alpha & -c\sin\alpha + d\cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}, 0 \right) \text{ and } \alpha = \phi,\ ad - bc = 1 \right\}. \tag{27}$$

Note that the value of ψ is related to the values of a, b, c, d. Thus

$$\widehat{G}_{fs} = G_{fs} \otimes G_{\Lambda}. \tag{28}$$

5. In the case of the skew spiral the symmetry group G_{ss} in V_3 presents a product of the corresponding symmetry matrices for both the simple spiral and the rotation of this simple spiral about the $\widehat{\mathbf{e}}_1$ axis by the angle θ:

$$G_{ss} = \left\{ \left(\left(\begin{array}{ccc} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha\cos\theta & \cos\alpha\cos\theta & -\sin\theta \\ \sin\alpha\sin\theta & \cos\alpha\sin\theta & \cos\theta \end{array} \right), 0 \right) \text{ and } \alpha = \phi \right\}. \tag{29}$$

$$\widehat{G}_{ss} = G_{ss} \otimes G_{\Lambda}.$$

6. and **7.** Spin waves:

$$G_{t,l} = \{(0, \mathbf{h}), \text{ where } \mathbf{h} \text{ is the periodicity vector of the function } f \text{ in 6 or 7}\}.$$

Thus:

$$\widehat{G}_{t,l} = G_{t,l} \otimes G_{\Lambda}. \tag{30}$$

Usually in the structures with a magnetic ordering an additional type of symmetry operation can be introduced. This operation is represented by the time reversal operator r, which changes the sign of either the magnetic moment or spin. The time reversal operator here is represented by the Z_2 group with two elements only: $-1, +1$. This operator then acts as follows:

$$r \otimes G_{\Lambda} = G'_{\Lambda} = \{(r, \lambda)\},$$

where λ belongs to G_{Λ}. In this description a general point in the four-dimensional space, where G'_{Λ} acts, is represented by x, y, z, s, and s is equal to either -1 or $+1$. In our approach the time reversal operator is already included into the groups G_m, where $m = f, a, s, fs, ss, t, l$, as one of their elements.

3 Discussion

Proposed in the present paper is a description of the magnetic structures in terms of fibre bundles. Such an approach turns out to be the most general, because it is based on the most general product of two arbitrary spaces, namely the Cartesian product, which is very suitable to the combination of two "worlds", e.g. the "world of positions" ($\mathbb{R}^3$) and the "world of spins" (V_3). Thus the description of crystal structures is to be carried out in $\mathbb{R}^3$, whereas the description of spin structures is to be carried out in V_3. This approach equates the symmetry analysis of magnetic structures with the method of the higher dimensional embeddings of the modulated structures. The symmetry groups appearing in the symmetry analysis become structural groups of the bundles. From the other side, a higher dimensional space needed for the description of a modulated structure makes here the total space of the bundle. Thus these three methods, namely the symmetry analysis, the higher dimensional embeddings and the fibre bundles are equivalent. Note that the Gaussian factor introduced here plays a double role: it makes the vector **M** a field and simultaneously makes the description of the magnetic structures more physical. The total magnetic group $\widehat{G}_m$ in the space E_6 is the tensor product of the magnetic group G_m and the space group G_Λ of the crystal structure, where $m = f, a, s, fs, ss, t, l$. It is worthwhile to mention here that these different magnetic structures have been found by the authors to be related to the values of certain topological invariants [12]. It seems that the above approach could serve also for the description of the symmetry groups of all the other aperiodic structures, such as, e.g. the modulated nonmagnetic structures, quasicrystals (nonmagnetic and magnetic) etc. The latter will be subject of a future publication.

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