THE PHASE PROBLEM OF MAGNETIC STRUCTURES WITH NON SYMMETRY-RELATED PROPAGATION VECTORS

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ABSTRACT

In these notes the limitations of neutron diffraction for determining the *true magnetic structure* of some compounds are discussed. The analytical expressions linking the measurable quantities to the model of a magnetic structure do not contain a crucial parameter: the phase factor between two Fourier coefficients not related by symmetry. The impossibility to obtain this parameter by conventional methods precludes the access to the true spin arrangement in the solid. The problem is first formulated analytically and illustrated by some simple examples, secondly we shall present some real examples concerning incommensurate-to-commensurate magnetic phase transitions and, finally, some conclusions are stated

1. Introduction

It is frequent the discovery of magnetic compounds that exhibit more than one propagation vector. The typical case is the so called multi-**k** structures, observed in some intermetallic compounds of high crystallographic symmetry [1]. Multi-**k** structures refers to a magnetic structure in which more than one arm of the star of **k** participates into the actual spin arrangement *. That is, the *transition chanel*, in terms of the Izyumov's school [2], has more than one propagation vector. Symmetry relations between the Fourier coefficients of the magnetic structure, when all the propagation vectors belong to a single star, can be obtained by group theory using the *geometrical* method of Bertaut [3] or the *algebraic* straightforward expressions that have been given by Izyumov and collaborators [2]. The practical determination of the transition chanel could be difficult because the magnetic phase transition, and the concommitant domain formation, produces satellites (in a single crystal diffraction pattern) which are not distinguishable (in usual conditions) from those of a true multi-**k** structure. External fields have to be applied to decide what is the actual situation. More unusual is the case showing two propagation vectors not belonging to the same star. However, a well known case is particularly common: the conical structures. Nagamiya [4] has given the conditions for two independent propagation vectors to describe *constant moment* (CM) magnetic structures. Nagamiya treated combinations of propagation vectors of the form $\mathbf{k}_1 = 1/2\mathbf{H}$ (or $\mathbf{k}_1 = 1/4\mathbf{H}$, $\mathbf{k}_1 = 3\mathbf{q}$) and $\mathbf{k}_2 = \mathbf{q}$ at the interior of the Brillouin Zone ($\mathbf{k}_2 \in IBZ$), so that the relative orientation of the Fourier coefficients is fixed and the relative phase is irrelevant. In this paper we shall formulate the problem in its full generality in relation with the practical structure determination. For that a summary of the most important scattering formulas is first given.

2. Neutron Scattering Cross Sections and Magnetic Structure Factor

For polarized neutrons the total scattered intensity and the final polarisation of scattered neutrons for the scattering vector **h** is given by the Blume's equations [5]. The scattered intensity is:

$$I_{\mathbf{h}} = N_{\mathbf{h}} N^*_{\mathbf{h}} + N_{\mathbf{h}}\{\mathbf{P}\cdot\mathbf{M}^*_{\perp\mathbf{h}}\} + N^*_{\mathbf{h}}\{\mathbf{P}\cdot\mathbf{M}_{\perp\mathbf{h}}\} + \mathbf{M}_{\perp\mathbf{h}}\cdot\mathbf{M}^*_{\perp\mathbf{h}} + i\mathbf{P}\cdot\{\mathbf{M}_{\perp\mathbf{h}}\times\mathbf{M}^*_{\perp\mathbf{h}}\} \quad (1)$$

*In this paper we use the terms *spin* and *magnetic moment* indistinctly. The term *spin arrangement* is also used as synonymous of *magnetic structure*

The equation defining the scattered polarisation is:

$$\begin{aligned}\mathbf{P}_s I_{\mathbf{h}} &= \mathbf{P}N_{\mathbf{h}}N_{\mathbf{h}}^* + N_{\mathbf{h}}\mathbf{M}_{\perp\mathbf{h}}^* + N_{\mathbf{h}}^*\mathbf{M}_{\perp\mathbf{h}} + i\mathbf{P}\times\{\mathbf{M}_{\perp\mathbf{h}}N_{\mathbf{h}}^* - \mathbf{M}_{\perp\mathbf{h}}^*N_{\mathbf{h}}\} + \mathbf{M}_{\perp\mathbf{h}}\{\mathbf{P}\cdot\mathbf{M}_{\perp\mathbf{h}}^*\} \\ &+ \mathbf{M}_{\perp\mathbf{h}}^*\{\mathbf{P}\cdot\mathbf{M}_{\perp\mathbf{h}}\} - \mathbf{P}\{\mathbf{M}_{\perp\mathbf{h}}\cdot\mathbf{M}_{\perp\mathbf{h}}^*\} + i\{\mathbf{M}_{\perp\mathbf{h}}\times\mathbf{M}_{\perp\mathbf{h}}^*\} \qquad (2)\end{aligned}$$

Where $\mathbf{P}$ and $\mathbf{P}_s$ are the incident and scattered neutron polarisation, $N_{\mathbf{h}}$ is the nuclear structure factor and $\mathbf{M}_{\perp\mathbf{h}}$ is the magnetic interaction vector defined as:

$$\mathbf{M}_{\perp\mathbf{h}} = \mathbf{e}\times(\mathbf{M}(\mathbf{h})\times\mathbf{e}) = \mathbf{M}(\mathbf{h}) - (\mathbf{e}\cdot\mathbf{M}(\mathbf{h}))\mathbf{e} \qquad (3)$$

$\mathbf{M}(\mathbf{h})$ is the magnetic structure factor, and $\mathbf{e}$ is the unit vector along the scattering vector $\mathbf{h}$. The scattering vector is $\mathbf{h}$=$\mathbf{H}$+$\mathbf{k}$ where $\mathbf{H}$ is a reciprocal lattice vector of the crystal structure and $\mathbf{k}$ the propagation vector corresponding to the current magnetic reflection. For a pure magnetic reflection $N_{\mathbf{h}} = 0$

The magnetic structures that we are considering have a distribution of magnetic moments that can be expanded as a Fourier series:

$$\mathbf{m}_{lj} = \sum_{\{\mathbf{k}\}} \mathbf{S}_{\mathbf{k}j}\exp\{-2\pi i\mathbf{k}\mathbf{R}_l\} \qquad (4)$$

The sum is extended to all propagation vectors that could belong to different stars. The Fourier coefficients $\mathbf{S}_{\mathbf{k}j}$ are, in general, complex vectors. The magnetic structure factor can be written as:

$$\mathbf{M}(\mathbf{H}+\mathbf{k}) = p\sum_{j=1}^{n_c} f_j(\mathbf{H}+\mathbf{k})\mathbf{S}_{\mathbf{k}j}\exp\{2\pi i(\mathbf{H}+\mathbf{k})\mathbf{r}_j\} \qquad (5)$$

The sum is over *all the magnetic atoms* in the crystallographic cell. The constant $p(= r_e\gamma/2)$ is 0.2695 and allows the conversion of the Fourier components of magnetic moments, given in Bohr magnetons (μ_B) to scattering lengths units of 10^{-12}cm. $f_j(\mathbf{H}+\mathbf{k})$ is the magnetic form factor and $\mathbf{r}_j$ is the vector position of atom j. In the above expression the atoms have been considered at rest. If thermal motion is considered and if symmetry relations are established for coupling the different Fourier components, we obtain the general expression of the magnetic structure factor:

$$\mathbf{M}(\mathbf{h}) = p\sum_{j=1}^{n} O_j f_j(\mathbf{h})T_j(iso)\sum_s M_{js}\mathbf{S}_{\mathbf{k}j}T_{js}\exp\{2\pi i[(\mathbf{H}+\mathbf{k})\{S\mid\mathbf{t}\}_s\mathbf{r}_j - \psi_{\mathbf{k}js}]\} \qquad (6)$$

The sum over j concerns the atoms of the magnetic asymmetric unit for the wavevector $\mathbf{k}$ (the Fourier component with index $\mathbf{k}$ contributes only to the $\mathbf{k}$-satellite). So that j labels different sites. The anisotropic temperature factor, T_{js}, is not generally necessary to be used in magnetic refinements($T_{js} = 1$). The sum over s concerns the different symmetry operators of the crystal space group that belong to the wave vector group. The matrix M_{js} transform the components of the Fourier term $\mathbf{S}_{\mathbf{k}j} = \mathbf{S}_{\mathbf{k}j1}$ of the starting atom $j1$ to that numbered as js in the orbit of j. The phase factor $\psi_{\mathbf{k}js}$ has two components:

$$\psi_{\mathbf{k}js} = \Phi_{\mathbf{k}j} + \phi_{\mathbf{k}js} \qquad (7)$$

$\Phi_{\mathbf{k}j}$ is a phase factor which is not determined by symmetry. It is a refinable parameter and it is significant only for an independent set of magnetic atoms (one orbit) which respect to another one. $\phi_{\mathbf{k}js}$ is a phase factor determined by symmetry. The Fourier component $\mathbf{k}$ of the magnetic moment of atom $j1$, $\mathbf{S}_{\mathbf{k}j}$, is transformed to

$$\mathbf{S}_{\mathbf{k}js} = M_{js}\mathbf{S}_{\mathbf{k}j}\exp\{-2\pi i\phi_{\mathbf{k}js}\} \qquad (8)$$

The matrices M_{js} and phases $\phi_{\mathbf{k}js}$ can be deduced from the atomic basis functions, obtained by applying projection operator formulas, corresponding to the active representation(s) participating in the definition of the actual magnetic structure. The sign of $\phi_{\mathbf{k}js}$ changes for -**k**.

In the general case $\mathbf{S}_{\mathbf{k}j}$ is a complex vector with six components. These six components per magnetic orbit constitute the parameters that have to be refined from the diffraction data. Symmetry reduces the number of free parameters per orbit to be refined. An alternative expression of the magnetic structure factor can be written as a function of *mixing coefficients* (parameters to be refined) and the atomic components of the basis functions of the relevant representation(s) [2]. In the case of a commensurate magnetic structure one can calculate the magnetic structure factor in the magnetic unit cell. In such a case $\mathbf{S}_{\mathbf{k}j}$ are real vectors corresponding to the magnetic moment of the atom j, the matrices M_{js} are real and all phases verify $\phi_{\mathbf{k}js} = 0$. The crystallographic magnetic groups theory can be fully applied in such a case [6].

If the magnetic structure represents an helical order the Fourier coefficients are of the form:

$$\mathbf{S}_{\mathbf{k}j} = \frac{1}{2}[m_{1j}\mathbf{u}_j + im_{2j}\mathbf{v}_j]\exp\{-2\pi i\phi_{\mathbf{k}j}\} \tag{9}$$

where $\mathbf{u}_j$ and $\mathbf{v}_j$ are orthogonal unit vectors. If $m_{1j} = m_{2j} = m_0$ the magnetic structure for the sublattice j corresponds to a classical helix (or spiral) of cylindrical envelope. All j atoms have a magnetic moment equal to m_0. If $m_{1j} \neq m_{2j}$ the helix has an elliptical envelope and the moments have values between $\min(m_{1j}, m_{2j})$ and $\max(m_{1j}, m_{2j})$. If $m_{2j} = 0$ the magnetic structure corresponds to a modulated sinusoid of amplitude m_{1j}.

3. The phase between independent k-vectors

When more than two independent propagation vectors appears in the diffraction pattern, the analysis of the data is unable to give a unique answer to the problem of the magnetic structure. In general is not possible to discriminate between the presence of two magnetic phases co-existing in the crystal and a coherent superposition of these two magnetic structures. We shall be concerned only with the latter picture. Even from this hypothesis it is not possible to get uniqueness. This can be seen adding a phase factor, depending only on **k**, to the Fourier series equation (4):

$$\mathbf{m}_{lj} = \sum_{\{\mathbf{k}\}} \mathbf{S}_{\mathbf{k}j}\exp\{-2\pi i(\mathbf{k}\mathbf{R}_l + \Psi_{\mathbf{k}})\} \tag{10}$$

The magnetic structure factor [equation (5)] transforms to:

$$\mathbf{M}(\mathbf{H}+\mathbf{k}) = p\exp\{2\pi i\Psi_{\mathbf{k}}\}\sum_{j=1}^{n_c} f_j(\mathbf{H}+\mathbf{k})\mathbf{S}_{\mathbf{k}j}\exp\{2\pi i(\mathbf{H}+\mathbf{k})\mathbf{r}_j\} \tag{11}$$

The phase $\Psi_{\mathbf{k}}$ appears in the expresion of the magnetic structure factor as a multiplicative phase factor that does not change the intensity of equation (1) or the scattered polarisation of (2) for a pure magnetic reflection. The phases $\Psi_{\mathbf{k}}$ are not accesible experimentally, so the real magnetic structure cannot be obtained from diffraction measurements alone.

The most simple case in which the phase plays an important role is the sinusoidally modulated structure in a simple Bravais lattice (a single magnetic atom per primitive cell) when the propagation vector takes special values. The Fourier coefficient and the corresponding magnetic moment at cell l are:

$$\mathbf{S}_{\mathbf{k}} = \frac{1}{2}m_o\mathbf{u}\exp\{-2\pi i\Psi_{\mathbf{k}}\} \qquad \mathbf{m}_l = m_o\mathbf{u}\cos 2\pi(\mathbf{k}\mathbf{R}_l + \Psi_{\mathbf{k}})$$

The phase $\Psi_{\mathbf{k}}$ plays no role when $\mathbf{k} \in IBZ$ and has no rational components. A change in the phase has the same effect as a change of the origin in the whole crystal. All magnetic moments between $-m_o\mathbf{u}$ and $m_o\mathbf{u}$ are realized somewhere in the lattice. However, if $\mathbf{k} = 1/4\mathbf{H}$ and $\Psi_{\mathbf{k}} = 1/8$ the magnetic structure is a CM-structure with the sequence $\{++--++--...\}$. This structure is indistinguishable of the sinusoidally modulated structure obtained with an arbitrary value of $\Psi_{\mathbf{k}}$. If all the components of $\mathbf{k}$ are rational the selection of the phase can have important consequences for the spin arrangement. This is the simplest case in which the physical picture depends on the election of a parameter ($\Psi_{\mathbf{k}}$) that is not accessible by diffraction methods. Physical considerations lead us to prefer one model among several other. For instance, CM-structures are normally expected at vey low temperatures when magnetic atoms have an intrinsic magnetic moment. This condition reduces the number of ways to combine non symmetry-related propagation vectors to several specific cases that have been discussed by Nagamiya [4]. Let us discuss some unusual simple cases that will be illustrated with real examples.

4. Fluctuating magnetic structures

The magnetic structures with more than one pair ($\mathbf{k}$,-$\mathbf{k}$) of propagation vectors not satisfying the Nagamiya's conditions are, as is the sinusoidally modulated magnetic structure, general non-constant moment structures. We shall call these spin configurations: *fluctuating structures* †

Fluctuating Structures with irrelevant phase-factors

This case corresponds to the combination of $\mathbf{k} = 1/2\mathbf{H}$ and $\mathbf{q} \in IBZ$ vectors. To simplify the notation we shall treat only one of the atoms of a particular Wyckoff site and we drop the reference index. The propagation vector $\mathbf{q}$ describes a helical configuration, and $\mathbf{k}$ corresponds to a uniaxial antiferromagnetic configuration, so that the Fourier coefficients of the atom are:

$$\mathbf{S}_{\mathbf{q}} = \frac{1}{2} m_1 [\mathbf{u} + i\mathbf{v}] \exp\{-2\pi i \Psi_{\mathbf{q}}\} \qquad \mathbf{S}_{\mathbf{k}} = m_2 \mathbf{n}$$

where, as above, $\mathbf{u}$ and $\mathbf{v}$ are orthogonal unit vectors defining the plane of the spiral of axis $\mathbf{w} = \mathbf{u} \times \mathbf{v}$, and $\mathbf{n}$ is a unit vector defining the axis of the spin configuration related to propagation vector $\mathbf{k} = 1/2\mathbf{H}$. The director cosines of $\mathbf{n}$ with respect to the axes ($\mathbf{u}, \mathbf{v}, \mathbf{w}$) are (n_1, n_2, n_3). The magnetic moment distribution of a coherent superposition of the two types of Fourier coefficients is given by the following formula (notice that $\Phi_l = 2\pi(\mathbf{q}\mathbf{R}_l + \Psi_{\mathbf{q}})$ and $l_h = \mathbf{H}\mathbf{R}_l$):

$$\begin{aligned} \mathbf{m}_l &= m_1 \cos 2\pi(\mathbf{q}\mathbf{R}_l + \Psi_{\mathbf{q}})\mathbf{u} + m_1 \sin 2\pi(\mathbf{q}\mathbf{R}_l + \Psi_{\mathbf{q}})\mathbf{v} + m_2 \exp\{-\pi i \mathbf{H}\mathbf{R}_l\}\mathbf{n} \\ &= m_1 \cos \Phi_l \mathbf{u} + m_1 \sin \Phi_l \mathbf{v} + m_2 (-1)^{l_h} \mathbf{n} \\ &= (m_1 \cos \Phi_l + (-1)^{l_h} m_2 n_1)\mathbf{u} + (m_1 \sin \Phi_l + (-1)^{l_h} m_2 n_2)\mathbf{v} + (-1)^{l_h} m_2 n_3 \mathbf{w} \quad (12) \end{aligned}$$

The modulus of the magnetic moment can be calculated by taking the square of equation (12):

$$\begin{aligned} m_l^2 &= m_1^2 + m_2^2 + 2m_1 m_2 (-1)^{l_h} (n_1 \cos \Phi_l + n_2 \sin \Phi_l) \\ &= m_1^2 + m_2^2 + 2m_1 m_2 (-1)^{l_h} \cos \alpha_l \quad (13) \end{aligned}$$

If $\mathbf{n}$ is parallel to $\mathbf{w}$ the moment is constant and we obtain an antiferromagnetic conical structure (if $\mathbf{H}$= 0, we obtain the classical ferromagnetic conical structure). For the

† The term *fluctuating* has no dynamic content in the present context

general orientation of **n** (non vanishing components in the **u-v** plane) the modulus of this distribution is not constant. The amplitude varies between the two extreme values $\sqrt{m_1^2 + m_2^2 + 2m_1 m_2 \sin\theta}$ and $\sqrt{m_1^2 + m_2^2 - 2m_1 m_2 \sin\theta}$, being θ the angle of **n** with **w**. A real system in which this behaviour seems to take place is the compound $CsMnF_4$ [7]. Another interesting system is $TbMn_6Ge_6$ [8] ‡ The second wave vector, in this case, is $\mathbf{k} = 0$ and the associated magnetic moment lies within the **u-v** plane defining the spiral plane of the first propagation vector. This gives rise to a distorted spiral structure.
In all these cases, the selection of the phase factor $\Psi_{\mathbf{q}}$ is completely irrelevant. That is, the physical picture obtained after using the equation (10) is not changed by varying the phase factor.

Fluctuating Structures Approaching CM-structures

We shall now consider the case of two pairs of propagation vectors (**k**,-**k**) and (**q**,-**q**) verifying $\mathbf{k}, \mathbf{q} \in IBZ$. Such a magnetic structure has as Fourier coefficients:

$$\mathbf{S_k} = \frac{1}{2}(\mathbf{R_k} + i\mathbf{I_k}) \qquad \mathbf{S_q} = \frac{1}{2}(\mathbf{R_q} + i\mathbf{I_q})\exp\{-i\Psi\}$$

Using the notation $\Phi_{\mathbf{k}l} = 2\pi\mathbf{k}\mathbf{R}_l$ the magnetic moment distribution is given by:

$$\mathbf{m}_l = \mathbf{R_k}\cos\Phi_{\mathbf{k}l} + \mathbf{I_k}\sin\Phi_{\mathbf{k}l} + \mathbf{R_q}\cos(\Phi_{\mathbf{q}l} + \Psi) + \mathbf{I_q}\sin(\Phi_{\mathbf{q}l} + \Psi) \qquad (14)$$

This moment distribution is generally a non-CM structure and the change of the phase factor Ψ can modify the physical picture if both vectors **k** and **q** have rational components. This last case is interesting when the components are simple integer fractions because one can treat the problem using the magnetic cell and search for a magnetic space group that fix automatically the phase. The finding of such a commensurate magnetic structure does not eliminate the problem of uniqueness of the magnetic moment distribution compatible with the experimental results. However, the possibility to have a simple spin arrangement with magnetic moments of atoms approaching the expected intrinsic moment is more satisfying form the physical point of view.

If a CM-structure can be found refining the magnetic structure using the magnetic cell, a particular set of equations (14) can be established for atoms inside the magnetic cell and the phase factor Ψ can be obtained solving these equations. Of course, to get a set of compatible equations the vectors **R** and **I** cannot be arbitrary. An example can be readily shown if we consider only *real* Fourier coefficients in equation (14). We can write for the α-component:

$$R^\alpha_{\mathbf{q}}\cos(\Phi_{\mathbf{q}l} + \Psi) = m^\alpha_l - R^\alpha_{\mathbf{k}}\cos\Phi_{\mathbf{k}l} \quad \Longrightarrow \quad \Psi = \cos^{-1}\frac{m^\alpha_l - R^\alpha_{\mathbf{k}}\cos\Phi_{\mathbf{k}l}}{R^\alpha_{\mathbf{q}}} - \Phi_{\mathbf{q}l}$$

The above equations must be verified for the set of points l inside the magnetic cell and for all components simultaneously. This indicates that only very special relationships between Fourier coefficients must be verified to have a single Ψ to connect the two descriptions.

An interesting example is the magnetic ordering of $TbGe_3$ [9]. This compound crystallizes in the space group $Cmcm$, ($a = 4.07, b = 20.8, c = 3.92$ Å), with Tb-atoms in positions $(4c)$ $\pm(0, y, 1/4)$. Below the Néel temperature ($T_N = 40$K) the magnetic order is characterized by two independent propagations vectors $\mathbf{k} = (k_x, 0, 0)$ and $\mathbf{q} = (q_x, 0, q_z)$ with $k_x \approx q_x \approx \frac{1}{2}$ and $q_z \approx \frac{1}{3}$. Below $T_{ic} = 24$K the propagation vectors lock-in to commensurate values. Both vectors verify $\mathbf{k}, \mathbf{q} \in IBZ$ with a two-arm star for **k**

‡See also the article: *Magnetic Spiral Structures in the Hexagonal RMn_6Ge_6 Compounds*, by P. Schobinger-Papamantellos, J. Rodríguez-Carvajal, G. André and K.H.J. Buschow, in these proceedings

($G_{\mathbf{k}} = C2cm$) and a four-arm star for $\mathbf{q}$ ($G_{\mathbf{q}} = Cc$). The refinement of the magnetic structure at low temperature in the magnetic unit cell using powder diffraction data provides a quasi-collinear structure with two types of Tb-atoms having similar moments ($m(Tb_1) = 9.2\mu_B, m(Tb_2) = 8.8\mu_B$). The refinement using real Fourier coefficients for all propagation vectors (including the second pair of the star of $\mathbf{q}$) gave similar agreement. A systematic search of the phase factors using a computer program [10] allows the finding of a consistent set of phases that produces fluctuations of $m(Tb)$ between $9.4\mu_B$ and $7.0\mu_B$. The spin arrangement is similar to that observed in the magnetic cell refinement. For the incommensurate phase we suppose that the spin arrangement does not change dramatically, so that the phases found for the lock-in phase are still valid.
Symmetry analysis can be applied to each wave vector separately. There is no interference terms between reflections belonging to different sets of satellites, so that we can proceed as if two magnetic different phases co-exist and only at the end of the analysis we can think in the coherent superposition of both phases. The computer program [10] we have written can be used as a general tool for searching phase factors between Fourier coefficients belonging to non-symmetry related wave vectors giving the lowest fluctuation between m_{min} and m_{max}.

5. Conclusions

The physical origin of the stabilization of two propagation vectors belonging to different stars is not yet clear in the absence of external fields. In Bravais lattices we have to think in the action of higher order terms (biquadratic) in the spin hamiltonian to stabilize two propagation vectors. In complex crystal structures the nature of the ground state is not known in the general case and, probably, it is not necessary to invoke higher order terms to stabilize two non-related propagation vectors. Only the case of conical structures ($\mathbf{k} = 0$ and $\mathbf{q} \in IBZ$) has been studied with some detail [11] for the spinel lattice. We can conclude that only a physical model based in the microscopic spin-spin interactions is able to fix completely the phases appearing in the Fourier expansion of the magnetic moment distribution in the solid. Experimentally, other techniques (like Mössbauer spectroscopy, neutron or X-ray topography, μ-SR, etc...) may help, in some cases, to distinguish between several models. Unfortunately there is no general method to overcome this *phase problem.*

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