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Time inversion in the representation analysis of magnetic structures

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Abstract

The representation analysis of magnetic structures (group theory) considers generally the group $G_{\mathbf{k}}$ (symmetry elements of the space group G which keep unchanged the propagation vector $\mathbf{k}$). There exists a certain confusion about the way and the usefulness of introducing time inversion, the operation which reverses the directions of the magnetic moments. We show here that we can define two 'time inversion' operators, one which is linear and one which is antilinear. While introducing the linear operator does not bring any new piece of information, introducing the antilinear operator brings more details on the possible magnetic structures. Because of this antilinearity, the corepresentations have to be used instead of the usual representations. The corepresentation theory had been introduced by Wigner for the operator 'time inversion in quantum mechanics', operator which, in quantum mechanics, must be antilinear. Finally we show that, for magnetic structures, using an antilinear operator instead of a linear operator, is connected with the reality of the magnetic moments. ***To cite this article: J. Schweizer, C. R. Physique 6 (2005).***

Résumé

L'analyse des structures magnétiques en représentations irréductibles (théorie des groupes) s'effectue en général en considérant le groupe $G_{\mathbf{k}}$ (groupe des éléments de symétrie du groupe d'espace G qui laissent le vecteur de propagation $\mathbf{k}$ inchangé). Une certaine confusion existe quant à la façon et à l'utilité d'y introduire le renversement du temps, opération qui renverse les moments magnétiques. Nous montrons qu'il est possible de définir deux opérateurs « renversement du temps », un linéaire et un antilinéaire, et que si l'introduction de l'opérateur linéaire n'apporte pas d'information nouvelle, ce n'est pas le cas de l'opérateur antilinéaire qui donne plus de précisions sur les structures magnétiques possibles. A cause de son caractère antilinéaire cet opérateur impose l'utilisation de la théorie des coreprésentations introduites par Wigner pour l'opérateur « renversement du temps en mécanique quantique », opérateur qui, pour la mécanique quantique, ne peut être qu'antilinéaire. Enfin nous montrons que, pour les structures magnétiques, le fait de pouvoir utiliser un opérateur antilinéaire est lié à la réalité des moments magnétiques de la structure. ***Pour citer cet article : J. Schweizer, C. R. Physique 6 (2005).***

Keywords: Time inversion; Antilinear operator; Corepresentation theory; Representation analysis; Magnetic structures

Mots-clés : Renversement du temps ; Opérateur antilinéaire ; Théorie des corepresentations ; Analyse en représentations ; Structures magnétiques

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1. Introduction

In a crystalline material, the magnetic moments are submitted to exchange interactions, with an energy U_0 which, developped into series at the second order, can be written as:

$$U_0 = \sum_{\mathbf{ll}'} \sum_{jj'} \sum_{\alpha\beta} J_{\mathbf{ll}'jj'\alpha\beta} m_{\mathbf{l}j\alpha} m_{\mathbf{l}'j'\beta} \tag{1}$$

where the $m_{\mathbf{l}j\alpha}$ represent the components of the magnetic moments $\mathbf{m}_{\mathbf{l}j}$, $\mathbf{l}$ and $\mathbf{l}'$ labelling the crystal cells, j and j' the magnetic atoms in the cell, and α and β the axes x, y or z, and where the $J_{\mathbf{ll}'jj'\alpha\beta}$ are the exchange interactions between the components of the magnetic atoms. At higher temperatures, in the paramagnetic state, there is no long range order of the magnetic moments, but only magnetic fluctuations, which represent a certain tendency to short range order. When cooling down the material, the range of these fluctuations increases and, below a characteristic temperature, one of them transforms into a long range order: a magnetic structure has been established. Such a structure can be described in terms of propagation vectors $\mathbf{k}$ and Fourier components $\mathbf{m}_j^{\mathbf{k}}$ (one Fourier vector $\mathbf{m}_j^{\mathbf{k}}$ per atom j in the unit cell):

$$\mathbf{m}_{\mathbf{l}j} = \sum_{\mathbf{k}} \mathbf{m}_j^{\mathbf{k}} \, \mathrm{e}^{-\mathrm{i}\mathbf{kl}} \tag{2}$$

where the sum concerns the different propagation vectors $\mathbf{k}$ which generate the structure.[1]

With the expression of $\mathbf{m}_{\mathbf{l}j}$ given by (2), the magnetic energy becomes

$$U_0 = \sum_{\mathbf{k}} \sum_{jj'} \sum_{\alpha\beta} J_{jj'\alpha\beta}(\mathbf{k}) m_{j\alpha}^{\mathbf{k}} \big(m_{j'\beta}^{\mathbf{k}}\big)^* \tag{3}$$

where $J_{jj'\alpha\beta}(\mathbf{k})$ is the Fourier transform of $J_{\mathbf{ll}'jj'\alpha\beta}$ and can be defined as:

$$J_{jj'\alpha\beta}(\mathbf{k}) = \sum_{\mathbf{l}} J_{\mathbf{ll}'jj'\alpha\beta} \, \mathrm{e}^{-\mathrm{i}\mathbf{k}(\mathbf{l}-\mathbf{l}')}. \tag{4}$$

In practice, the propagation vector $\mathbf{k}$ is determined from neutron diffraction by indexing the magnetic diagramme. Then, the magnetic structure can be determined by comparing the intensities of the magnetic reflections to those which are expected from the possible arrangements of the magnetic moments in the unit cell. The number of these possible arrangements can be considerably reduced when restricting to those which are compatible with the symmetry of the crystal [1,2]. In particular, when the magnetic order establishes from the paramagnetic state through a second order phase transition, it is very fruitful to apply the Landau theory for phase transitions [3] to the group G of the symmetry elements of the crystal. These symmetry elements act on the basis vectors $\mathbf{m}_{j\alpha}^{\mathbf{k}} = m_{j\alpha}^{\mathbf{k}} \, \mathbf{e}_\alpha$ which are the vectorial components of the $\mathbf{m}_j^{\mathbf{k}}$ vectors along the 3 axes of the crystal, the vectors $\mathbf{e}_\alpha$ being unitary.

The Landau approach classifies the magnetic fluctuations according to the symmetry of the different irreducible representations of the little group $G_{\mathbf{k}}$ (the group of vector $\mathbf{k}$). Actually, it states that, in order to keep the magnetic energy (3) invariant under all the symmetry operations of $G_{\mathbf{k}}$, the magnetic structures must be built from basis vectors $\mathbf{m}_\nu^{\mathbf{k}i}$ belonging only to one irreducible representation τ_ν of $G_{\mathbf{k}}$.

This little group $G_{\mathbf{k}}$ is composed of the symmetry elements of the space group G of the paramagnetic crystal which leave the propagation vector $\mathbf{k}$ unchanged. However, all the authors consider as relevant to add to these spatial symmetry elements a purely magnetic invariance which reverses all the magnetic moments and which is generally called invariance by time inversion. However, when the time comes to put this concept into practice in the representation analysis, a certain confusion exists in literature about the way to introduce it, and about the usefulness of this introduction.

In this article, we shall explain that it is possible to define two 'time inversion' operators, a linear[2] operator R and an antilinear operator Θ, both reversing the sign of the magnetic moments $\mathbf{m}_{\mathbf{l}j}$. We shall show that introducing the antilinear operator Θ in the representation analysis is much more fruitful than introducing operator R. We shall explain that with such an antilinear operator it is necessary to employ the Wigner's corepresentations instead of the usual representations of group theory, and we shall give the recipe to do this. Finally, we shall discuss the physics which is behind the success of the antilinear time inversion operator in the magnetic structure analysis.

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[1] A structure is mono-k or multi-k according to the number of equivalent propagation vectors $\mathbf{k}$ which generate it. However, even in mono-k structures, for $\mathbf{k}$ vectors such as $\mathbf{kl} \neq n\pi$, a vector $-\mathbf{k}$ is associated to the vector $\mathbf{k}$ with $\mathbf{m}^{-\mathbf{k}} = (\mathbf{m}^{\mathbf{k}})^*$, in such a way that the magnetic moments given by expansion (2) are real.

[2] A linear operator L is such that, when applied on an observable s, it obeys $L(as) = aL(s)$ while an antilinear operator A implies $A(as) = a^*A(s)$.

2. Two possible definitions for the time inversion operator

The necessity to add the time inversion to the spatial symmetry operators has been stated for a long time. As Landau and Lifshits [3] explained, this operator reverses the direction of the electric currents, and then reverses the signs of the magnetic moments which are axial vectors. However, when applied to the Fourier decomposition of the magnetic moments as given by formula (2), there are two possibilities to define a 'time inversion' operator:

– a linear operator R such that

$$R\mathbf{m}_{\mathbf{l}j} = -\mathbf{m}_{\mathbf{l}j} = -\sum_{\mathbf{k}} \mathbf{m}_j^{\mathbf{k}}\,\mathrm{e}^{-\mathrm{i}\mathbf{kl}}; \tag{5}$$

– and an antilinear operator Θ such that

$$\Theta\mathbf{m}_{lj} = -\mathbf{m}_{lj} = -\sum_{\mathbf{k}} \big(\mathbf{m}_j^{\mathbf{k}}\big)^*\,\mathrm{e}^{+\mathrm{i}\mathbf{kl}}. \tag{6}$$

Both operators reverse the magnetic moments and leave the magnetic energy U_0, as given by formula (3), unchanged.

The linear operator R is the operator usually chosen to deal with the Shubnikov groups. It has been introduced in the representation analysis of the magnetic structures by Izyumov et al. [4,5], and these authors have concluded that such an introduction does not bring anything new in the prediction of possible magnetic structures.

The antilinear operator Θ has been defined by Wigner [6]. He has shown that, in quantum mechanics, the time inversion operator acting on the wave functions must be antilinear ($\Theta a|\Psi\rangle = a^*\Theta|\Psi\rangle$), and he has developped a generalisation of the representation theory (the theory of corepresentations), valid for antilinear operators. As early as 1971, Bertaut [7] has used the antilinear operator Θ to represent the time inversion in the representation analysis of magnetic structures. He gave an example where the symmetry of the little group $G_{\mathbf{k}}$ is too low to connect all the magnetic positions of a magnetic site, but where the introduction of the antilinear operator Θ permitted to connect all these atoms, reducing that way the number of possible magnetic structures. One year later, Bradley and Cracknell [8] published a complete mathematical theory of symmetry in solids where the corepresentations resulting from the presence of the antilinear operator Θ are thoroughly analyzed. Other authors, as, for example, Rossat Mignod [9], have followed Bertaut's procedure, but without applying the rigorous treatment outlined by [8]. It is the purpose of this article to do this and to show how useful it is.

3. Conjugation and chirality

A part of the confusion which exists about the use of the time inversion in the representation analysis of the magnetic structures is due to the presence in literature of the two operators, linear and antilinear. One reads sometimes that the time inversion changes $\mathbf{k}$ in $-\mathbf{k}$, but does not conjugate the Fourier components $\mathbf{m}_j^{\mathbf{k}}$ because they are not quantum objects. This is not a right procedure as it would define a third 'time inversion' operator T which would transform $\mathbf{m}_j^{\mathbf{k}}\,\mathrm{e}^{-\mathrm{i}\mathbf{kl}}$ in $-\mathbf{m}_j^{\mathbf{k}}\,\mathrm{e}^{+\mathrm{i}\mathbf{kl}}$, an operator which would be neither linear nor antilinear.

To illustrate the differences between these operators, let us look at their action on an helix. A simple helix is generated by a Fourier component $\mathbf{m}_j^{\mathbf{k}} = \mathbf{U} + \mathrm{i}\mathbf{V}$, with $\mathbf{U}$ and $\mathbf{V}$ noncollinear

$$\mathbf{m}_{\mathbf{l}j} = \mathbf{m}_j^{\mathbf{k}}\,\mathrm{e}^{-\mathrm{i}\mathbf{kl}} + \big(\mathbf{m}_j^{\mathbf{k}}\big)^*\,\mathrm{e}^{+\mathrm{i}\mathbf{kl}} = 2[\mathbf{U}\cos\mathbf{kl} + \mathbf{V}\sin\mathbf{kl}]. \tag{7}$$

The actions of operators R and Θ on such an helix are:

$$R\mathbf{m}_{\mathbf{l}j} = -\big[\mathbf{m}_j^{\mathbf{k}}\,\mathrm{e}^{-\mathrm{i}\mathbf{kl}} + \big(\mathbf{m}_j^{\mathbf{k}}\big)^*\,\mathrm{e}^{+\mathrm{i}\mathbf{kl}}\big] = -2[\mathbf{U}\cos\mathbf{kl} + \mathbf{V}\sin\mathbf{kl}], \tag{8}$$

$$\Theta\mathbf{m}_{\mathbf{l}j} = -\big[\big(\mathbf{m}_j^{\mathbf{k}}\big)^*\,\mathrm{e}^{+\mathrm{i}\mathbf{kl}} + \mathbf{m}_j^{\mathbf{k}}\,\mathrm{e}^{-\mathrm{i}\mathbf{kl}}\big] = -2[\mathbf{U}\cos\mathbf{kl} + \mathbf{V}\sin\mathbf{kl}] \tag{9}$$

that are two helices, with all the moments reversed, but with the same chirality. On the other hand, the action of the third operator T would change the helix into an helix of the opposed chirality, which is not expected from a time inversion operator:

$$T\mathbf{m}_{\mathbf{l}j} = -\big[\mathbf{m}_j^{\mathbf{k}}\,\mathrm{e}^{+\mathrm{i}\mathbf{kl}} + \big(\mathbf{m}_j^{\mathbf{k}}\big)^*\,\mathrm{e}^{-\mathrm{i}\mathbf{kl}}\big] = -2[\mathbf{U}\cos\mathbf{kl} - \mathbf{V}\sin\mathbf{kl}]. \tag{10}$$

Furthermore, it is easy to see that, while the magnetic energy U_0, as defined by formulae (3) and (4), is invariant under the application of R and Θ, it is not invariant under the application of T, the two points being closely connected.

To conclude with the choice of a 'time inversion operator' in the representation analysis of the magnetic structures, the first point to consider is not the quantum or not quantum of the vectors $\mathbf{m}_j^{\mathbf{k}}$, but whether or not it keeps invariant the magnetic energy, which is the case of both operators R and Θ. And then, one has to ask how useful it is to introduce it in the representation analysis.

For the linear operator R, Refs. [4] and [5] have already investigated its impact in the representation analysis and shown that it does not bring any new element of information. Each irreducible representation τ_ν of the little group $G_{\mathbf{k}}$ splits, with the time inversion operator, into two new irreducible representations τ_ν^+ and τ_ν^-: the τ_ν^+ representation being unable to yield a magnetic structure, and the τ_ν^- representation giving exactly the same magnetic structure as representation τ_ν, without the time inversion.

For the antilinear operator Θ, the usual group theory cannot be applied and we shall see in the next section how to handle a group containing both linear and antilinear operators.

4. The magnetic little group $M_{\mathbf{k}} = G_{\mathbf{k}}^{\Theta}$

In the paramagnetic state, the magnetic group M is now composed of all the elements of the space group G and also of all the elements of G associated with Θ. The construction of the magnetic little group $M_{\mathbf{k}}$ is thoroughly explained by Bradley and Cracknell [8]. It consists of all the spatial operators which keep $\mathbf{k}$ and all the spatial operators which reverse $\mathbf{k}$, these last ones being associated with Θ.

Practically, we can have 3 different cases:

(i) There is no symmetry operator in the group G which reverses the vector $\mathbf{k}$ ($-\mathbf{k}$ does not belong to the star $\{\mathbf{k}\}$). We have then:

$$M_{\mathbf{k}} = G_{\mathbf{k}}^{\Theta} = G_{\mathbf{k}} \quad \text{(Fedorov group)}. \tag{11}$$

(ii) $-\mathbf{k}$ is equivalent to $\mathbf{k}$, which means that either $\mathbf{k} = 0$ or $\mathbf{k} = -\mathbf{k} + \mathbf{K}$, where $\mathbf{K}$ is a reciprocal lattice vector. This leads to:

$$M_{\mathbf{k}} = G_{\mathbf{k}}^{\Theta} + \Theta G_{\mathbf{k}} \quad \text{(grey group)}, \tag{12}$$

which, compared to $G_{\mathbf{k}}$, doubles the number of operators.

(iii) $-\mathbf{k}$ belongs to the star $\{\mathbf{k}\}$ but is not equivalent to $\mathbf{k}$. There exists in G an element h_0 which reverses $\mathbf{k}$ and, associated to Θ, it constitutes the reversing element a_0:

$$a_0 = \Theta h_0 = h_0 \Theta \quad \text{and} \tag{13}$$

$$M_{\mathbf{k}} = G_{\mathbf{k}}^{\Theta} = G_{\mathbf{k}} + a_0 G_{\mathbf{k}} \quad \text{(black and white group)}. \tag{14}$$

Here also, compared to $G_{\mathbf{k}}$, the number of operators is doubled.

In the following, we shall treat together grey groups and black and white groups, writing $M_{\mathbf{k}} = G_{\mathbf{k}} + a_0 G_{\mathbf{k}}$ for both of them, with $a_0 = \Theta$ for grey groups and $a_0 = \Theta h_0$ for black and white groups.

As the time reversal operator Θ is not a linear but an antilinear operator, it is not possible to use the theory of representations as it stands. One is obliged to use the theory of corepresentations.

5. The Wigner corepresentations of the magnetic little group $M_{\mathbf{k}}$

The theory of corepresentations has been developped by Wigner [6] for groups including both linear operators h_i and antilinear operators a_j. The main difference between representations (Γ) and corepresentations ($c\Gamma$) concerns the rules of multiplication of the matrices representing the operators. Whereas, for usual representations, they are:

$$\Gamma(h_i)\Gamma(h_j) = \Gamma(h_i h_j) \tag{15}$$

for the corepresentations, the matrices representing the linear operators h_i and the antilinear operators a_j multiply in the following way:

$$c\Gamma(h_i)c\Gamma(h_j) = c\Gamma(h_i h_j), \tag{16}$$

$$c\Gamma(h_i)c\Gamma(a_j) = c\Gamma(h_i a_j), \tag{17}$$

$$c\Gamma(a_i)c\Gamma^*(h_j) = c\Gamma(a_i h_j), \tag{18}$$

$$c\Gamma(a_i)c\Gamma^*(a_j) = c\Gamma(a_i a_j). \tag{19}$$

The magnetic little group $G_{\mathbf{k}}^{\Theta} = G_{\mathbf{k}} + a_0 G_{\mathbf{k}}$ contains both linear operators h_i and antilinear operators $a_j = a_0 h_j$. The basis vectors on which operators h_i and a_j apply are all the Fourier components $\mathbf{m}_{j\alpha}^{\mathbf{k}}$ and $(\mathbf{m}_{j\alpha}^{\mathbf{k}})^* = \mathbf{m}_{j\alpha}^{-\mathbf{k}}$:

– h_i transforms a vector $\mathbf{m}^{\mathbf{k}}_{j\alpha}$ in a sum of vectors $\mathbf{m}^{\mathbf{k}}_{j'\beta}$ and a vector $(\mathbf{m}^{\mathbf{k}}_{j\alpha})^*$ in a sum of vectors $(\mathbf{m}^{\mathbf{k}}_{j'\beta})^*$;
– a_i transforms a vector $\mathbf{m}^{\mathbf{k}}_{j\alpha}$ in a sum of vectors $(\mathbf{m}^{\mathbf{k}}_{j'\beta})^*$ and a vector $(\mathbf{m}^{\mathbf{k}}_{j\alpha})^*$ in a sum of vectors $\mathbf{m}^{\mathbf{k}}_{j'\beta}$.

The number of basis vectors on which the operators act is then twice larger for $G^{\Theta}_{\mathbf{k}}$ than for $G_{\mathbf{k}}$. However, when it happens that the magnetic corepresentation and the irreducible corepresentations are real, we can choose basis vectors which are real and this restrict their number by a factor two.

The way to construct the irreducible corepresentations $c\tau_\nu$ of the magnetic little group $G^{\Theta}_{\mathbf{k}}$ from the irreducible representations τ_ν of the little group $G_{\mathbf{k}}$ is explained in [6,8,10]. There are 3 different cases according to the value taken by the sum $\sum_{a_j}\chi(a_j^2)$, sum over all the antilinear operators a_j, noticing that the operators a_j^2 are of type h, which means linear operators. Let us note that this criterion is often called reality criterion because it is used to know whether the irreducible representations of the little groups $G_{\mathbf{k}}$ are real, pseudoreal or complex.

Case (a): $\sum_{a_j}\chi(a_j^2)=g$, where g is the order of the little group $G_{\mathbf{k}}$.

From the irreducible representation τ_ν, one can build 2 irreducible corepresentations $c\tau_\nu^+$ and $c\tau_\nu^-$, in a way which is similar to the procedure followed with the operator R:

$$c\tau_\nu^+(h_i)=\tau_\nu(h_i),\qquad c\tau_\nu^+(a_j)=\tau_\nu\bigl(a_j a_0^{-1}\bigr)\beta, \tag{20}$$

$$c\tau_\nu^-(h_i)=\tau_\nu(h_i),\qquad c\tau_\nu^-(a_j)=-\tau_\nu\bigl(a_j a_0^{-1}\bigr)\beta. \tag{21}$$

As $a_j a_0^{-1}$ is a linear operator (of type h), $\tau_\nu(a_j a_0^{-1})$ is well defined. β is an auxiliary matrix and such matrices are tabulated in Ref. [10].

In the case of wave functions, as well as in the general case of complex basis vectors, the two irreducible corepresentations $c\tau_\nu^+$ and $c\tau_\nu^-$, are equivalent and the corresponding magnetic structures are the same. This is illustrated later, for the corepresentations $c\tau_1^+$ and $c\tau_1^-$ of the second example. However, if it is possible, as in the third example, to restrict the basis vector set $\mathbf{m}^{\mathbf{k}i}_\nu$ to real vectors only, and the two irreducible corepresentations may be no longer equivalent.

Case (b): $\sum_{a_j}\chi(a_j^2)=-g$.

The irreducible representation τ_ν is transformed in an irreducible corepresentation with an order which is twice larger:

$$c\tau_\nu(h_i)=\begin{pmatrix}\tau_\nu(h_i) & 0\\ 0 & \tau_\nu(h_i)\end{pmatrix},\qquad c\tau_\nu(a_j)=\begin{pmatrix}0 & -\tau_\nu(a_j a_0^{-1})\beta\\ \tau_\nu(a_j a_0^{-1})\beta & 0\end{pmatrix} \tag{22}$$

also with an auxiliary matrix β tabulated in [10].

Case (c): $\sum_{a_j}\chi(a_j^2)=0$.

In this case, it exists another irreducible representation of $G_{\mathbf{k}}$: $\bar\tau_\nu$ distinct from τ_ν ($\bar\tau_\nu=\tau_{\nu'}$, with $\nu'\neq\nu$), such as:

$$\bar\tau_\nu(h_i)=\tau_{\nu'}(h_i)=\bigl[\tau_\nu\bigl(a_0^{-1}h_i a_0\bigr)\bigr]^*. \tag{23}$$

These two representations, τ_ν and $\tau_{\nu'}$ of the little group $G_{\mathbf{k}}$, are joined together by the time inversion operator, to give an irreducible corepresentation $\tau_{\nu+\nu'}$ of the magnetic little group $G^{\Theta}_{\mathbf{k}}$, with an order which is, here also, twice larger.

$$c\tau_{\nu+\nu'}(h_i)=\begin{pmatrix}\tau_\nu(h_i) & 0\\ 0 & \tau_{\nu'}(h_i)\end{pmatrix},\qquad c\tau_{\nu+\nu'}(a_j)=\begin{pmatrix}0 & \tau_\nu(a_j a_0)\\ \tau_{\nu'}(a_j a_0^{-1}) & 0\end{pmatrix}. \tag{24}$$

The situation where the magnetic group is equivalent to the Fedorov group ($M_{\mathbf{k}}=G^{\Theta}_{\mathbf{k}}=G_{\mathbf{k}}$), when there is no symmetry operator in the group G which reverses the vector $\mathbf{k}$, implies also, in a trivial way, the relation $\sum_{a_j}\chi(a_j^2)=0$, as the magnetic little group contains no antilinear operators of type a_j. The vector $-\mathbf{k}$, although it does not belong to the star{$\mathbf{k}$}, is associated to vector $\mathbf{k}$ by the time inversion: there is no additional degeneracy inside the group $G_{\mathbf{k}}$, but an extra degeneracy exists which associates, with the same magnetic energy, the Fourier components $\mathbf{m}^{-\mathbf{k}}_j$ and $\mathbf{m}^{\mathbf{k}}_j$, as already mentioned above:

$$\mathbf{m}_{\mathbf{l}j}=\mathbf{m}^{\mathbf{k}}_j\,\mathrm{e}^{-\mathrm{i}\mathbf{kl}}+\bigl(\mathbf{m}^{\mathbf{k}}_j\bigr)^*\,\mathrm{e}^{\mathrm{i}\mathbf{kl}}. \tag{25}$$

This degeneracy is labelled (x) [8].

In practice, for all little groups $G_{\mathbf{k}}$, that is for the 230 space groups and all the possible symmetries of the propagation vector $\mathbf{k}$, Bradley and Cracknell [8] on the one hand and Kovalev [10] on the other hand indicate whether $G_{\mathbf{k}}$ belongs to case (a), (b), (c) or (x). Furthermore, Kovalev gives also the auxiliary matrix β when it is different from unitary.

6. The usefulness of introducing the time inversion symmetry

In the following examples, we shall show that the introduction of the antilinear time inversion invariance in the representation analysis may bring more specifications to the possible magnetic structures than the spatial symmetries alone.

6.1. 1st example: a triangular structure in an acentric trigonal group (Fedorov magnetic little group, degeneracy (x))

Let us consider one magnetic atom at the origin of the cell of space group P3 (space group n$^{\text{o}}$ 143), with a propagation vector $\mathbf{k} = (1/3, 1/3, 0)$. The space group contains 3 symmetry elements: $h_1(x, y, z)$, $h_3(-y, x-y, z)$ and $h_5(-x+y, -x, z)$ according to Kovalev's notations [10]. As there is no vector $-\mathbf{k}$ in the star $\{\mathbf{k}\}$ (acentric structure), the magnetic little group is the Fedorov group (degeneracy x): vectors $\mathbf{m}^{-\mathbf{k}}$ and $\mathbf{m}^{\mathbf{k}}$ are associated together by the time inversion, but the search for basis vectors in $M_{\mathbf{k}} = G_{\mathbf{k}}^{\Theta} = G_{\mathbf{k}}$ does not imply the operator Θ and is therefore done with the ordinary representations. Table 1 gives the action of the 3 operators h_1, h_3 and h_5 of the magnetic little group $M_{\mathbf{k}} = G_{\mathbf{k}}$ on the vectorial components of the magnetic moment of the unique magnetic atom of the cell, as well as the character of the representation Γ based on these components. Table 2 reproduces the irreducible representations as listed in [8] or [10]. According to the usual rules of decomposition:

$$\Gamma = \tau_1 + \tau_2 + \tau_3.$$

The application of the projection operators on the 3 subspaces spanned by 3 irreducible representations yields the 3 basis vectors:

for τ_1 $\mathbf{m}_1^{\mathbf{k}} = \mathbf{m}_z^{\mathbf{k}}$,
for τ_2 $\mathbf{m}_2^{\mathbf{k}} = \mathbf{m}_x^{\mathbf{k}} + \mathrm{i}\sqrt{3}(\mathbf{m}_x^{\mathbf{k}} + 2\mathbf{m}_y^{\mathbf{k}}) = \mathbf{U} + \mathrm{i}\mathbf{V}$,
for τ_3 $\mathbf{m}_3^{\mathbf{k}} = \mathbf{m}_x^{\mathbf{k}} - \mathrm{i}\sqrt{3}(\mathbf{m}_x^{\mathbf{k}} + 2\mathbf{m}_y^{\mathbf{k}}) = \mathbf{U} - \mathrm{i}\mathbf{V}$

the two vectors $\mathbf{U}$ and $\mathbf{V}$ being orthogonal.

Coming back to the magnetic moments $\mathbf{m_l}$ in all the crystal, using Eq. (27), there are 3 structures compatible with the spatial and time inversion symmetries:

for τ_1, a modulated structure $\mathbf{m_l} = 2\mathbf{m}_z^{\mathbf{k}} \cos \mathbf{kl}$,
for τ_2, an helicoidal (here triangular structure) $\mathbf{m_l} = 2[\mathbf{U} \cos \mathbf{kl} + \mathbf{V} \sin \mathbf{kl}]$,
for τ_3, an helicoidal (here triangular) structure, but with an opposed chirality $\mathbf{m_l} = 2[\mathbf{U} \cos \mathbf{kl} - \mathbf{V} \sin \mathbf{kl}]$.

These three structures, and particularly the two helices, corresponding to different irreducible representations, are not supposed to have the same magnetic energy. In this case of degeneracy (x), the time inversion plays its role, but not inside the little group $G_{\mathbf{k}}$. It allows us to combine $\mathbf{m}^{\mathbf{k}}$ and $\mathbf{m}^{-\mathbf{k}}$ in retrieving the magnetic moments $\mathbf{m_l}$ even when $-\mathbf{k}$ is not in the star $\{\mathbf{k}\}$.

6.2. 2nd example: a triangular structure in a centric trigonal group (black and white magnetic little group, cases (a) and (c))

We consider now the same magnetic atom at the origin of the cell but in the space group P$\bar{3}$ (space group n$^{\text{o}}$ 147), with the same propagation vector $\mathbf{k} = (1/3, 1/3, 0)$. The space group contains now 6 symmetry elements: as before $h_1(x, y, z)$, $h_3(-y, x-y, z)$ and $h_5(-x+y, -x, z)$, but also the 3 operators resulting from the inversion: $h_{13}(-x, -y, -z)$, $h_{15}(y, -x+y, -z)$ and $h_{17}(x-y, x, -z)$. Here, the structure is centric: $-\mathbf{k}$ belongs to the star $\{\mathbf{k}\}$. The little group $G_{\mathbf{k}}$ is restricted to the 3 operators h_1, h_3 and h_5 as in the former case for the acentric structure. Its irreducible representations are given in Table 2. However, when including the time inversion, the magnetic little group $M_{\mathbf{k}} = G_{\mathbf{k}}^{\Theta} = G_{\mathbf{k}} + a_0 G_{\mathbf{k}}$ is black and white. It contains

Table 1
Space group P3: action of the operators of $G_{\mathbf{k}=(1/3,1/3,0)}$ on the components $\mathbf{m}_{\alpha}^{\mathbf{k}}$

	h_1	h_3	h_5
	$\mathbf{m}_x^{\mathbf{k}}$	$\mathbf{m}_y^{\mathbf{k}}$	$-\mathbf{m}_x^{\mathbf{k}} - \mathbf{m}_y^{\mathbf{k}}$
	$\mathbf{m}_y^{\mathbf{k}}$	$-\mathbf{m}_x^{\mathbf{k}} - \mathbf{m}_y^{\mathbf{k}}$	$\mathbf{m}_x^{\mathbf{k}}$
	$\mathbf{m}_z^{\mathbf{k}}$	$\mathbf{m}_z^{\mathbf{k}}$	$\mathbf{m}_z^{\mathbf{k}}$
χ	3	0	0

Table 2
Space group P3: irreducible representations of the little group $G_{\mathbf{k}=(1/3,1/3,0)}$, $\varepsilon = \exp(2\pi \mathrm{i}/3)$

	h_1	h_3	h_5
τ_1	1	1	1
τ_2	1	ε	ε^2
τ_3	1	ε^2	ε

Table 3
Space group P$\bar{3}$: action of the operators of $G_{\mathbf{k}=(1/3,1/3,0)}$ on the components $\mathbf{m}_\alpha^\mathbf{k}$

	h_1	h_3	h_5	Θh_{13}	Θh_{15}	Θh_{17}
	$\mathbf{m}_x^\mathbf{k}$	$\mathbf{m}_y^\mathbf{k}$	$-\mathbf{m}_x^\mathbf{k}-\mathbf{m}_y^\mathbf{k}$	$-\mathbf{m}_x^{-\mathbf{k}}$	$-\mathbf{m}_y^{-\mathbf{k}}$	$\mathbf{m}_x^{-\mathbf{k}}+\mathbf{m}_y^{-\mathbf{k}}$
	$\mathbf{m}_y^\mathbf{k}$	$-\mathbf{m}_x^\mathbf{k}-\mathbf{m}_y^\mathbf{k}$	$\mathbf{m}_x^\mathbf{k}$	$-\mathbf{m}_y^{-\mathbf{k}}$	$\mathbf{m}_x^{-\mathbf{k}}+\mathbf{m}_y^{-\mathbf{k}}$	$-\mathbf{m}_x^{-\mathbf{k}}$
	$\mathbf{m}_z^\mathbf{k}$	$\mathbf{m}_z^\mathbf{k}$	$\mathbf{m}_z^\mathbf{k}$	$-\mathbf{m}_z^{-\mathbf{k}}$	$-\mathbf{m}_z^{-\mathbf{k}}$	$-\mathbf{m}_z^{-\mathbf{k}}$
	$\mathbf{m}_x^{-\mathbf{k}}$	$\mathbf{m}_y^{-\mathbf{k}}$	$-\mathbf{m}_x^{-\mathbf{k}}-\mathbf{m}_y^{-\mathbf{k}}$	$-\mathbf{m}_x^\mathbf{k}$	$-\mathbf{m}_y^\mathbf{k}$	$\mathbf{m}_x^\mathbf{k}+\mathbf{m}_y^\mathbf{k}$
	$\mathbf{m}_y^{-\mathbf{k}}$	$-\mathbf{m}_x^{-\mathbf{k}}-\mathbf{m}_y^{-\mathbf{k}}$	$\mathbf{m}_x^{-\mathbf{k}}$	$-\mathbf{m}_y^\mathbf{k}$	$\mathbf{m}_x^\mathbf{k}+\mathbf{m}_y^\mathbf{k}$	$-\mathbf{m}_x^\mathbf{k}$
	$\mathbf{m}_z^{-\mathbf{k}}$	$\mathbf{m}_z^{-\mathbf{k}}$	$\mathbf{m}_z^{-\mathbf{k}}$	$-\mathbf{m}_z^\mathbf{k}$	$-\mathbf{m}_z^\mathbf{k}$	$-\mathbf{m}_z^\mathbf{k}$
χ	6	0	0	0	0	0

Table 4
Space group P$\bar{3}$: irreducible corepresentations of the little group $G_{\mathbf{k}=(1/3,1/3,0)}$, $\varepsilon=\exp(2\pi\mathrm{i}/3)$

	h_1	h_3	h_5	Θh_{13}	Θh_{15}	Θh_{17}
$c\tau_1^+$	1	1	1	1	1	1
$c\tau_1^-$	1	1	1	−1	−1	−1
$c\tau_{2+3}$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\varepsilon&0\\0&\varepsilon^2\end{pmatrix}$	$\begin{pmatrix}\varepsilon^2&0\\0&\varepsilon\end{pmatrix}$	$\begin{pmatrix}0&1\\1&0\end{pmatrix}$	$\begin{pmatrix}0&\varepsilon\\\varepsilon^2&0\end{pmatrix}$	$\begin{pmatrix}0&\varepsilon^2\\\varepsilon&0\end{pmatrix}$

now 6 elements, with the reversing element $a_0=\Theta h_{13}$. Table 3 shows the action of its 6 elements h_1, h_3, h_5, Θh_{13}, Θh_{15} and Θh_{17} on the magnetic Fourier components $\mathbf{m}_\alpha^\mathbf{k}$ and $(\mathbf{m}_\alpha^\mathbf{k})^*$, as well as the character of the corepresentation $c\Gamma$ based on these components. Table 4 reproduces the irreducible corepresentations as indicated in [8] or [10]: τ_1 being of type (a) gives two irreducible corepresentations $c\tau_1^+$ and $c\tau_1^-$, τ_2 and τ_3 being of type (c), join together to give the irreducible corepresentation $c\tau_{2+3}$. The decomposition of corepresentation $c\Gamma$ into irreducible corepresentations is the following:

$$c\Gamma = c\tau_1^+ + c\tau_1^- + 2c\tau_{2+3}.$$

In the space of complex vectors $\mathbf{m}_\alpha^\mathbf{k}$ and $(\mathbf{m}_\alpha^\mathbf{k})^*$, the application of the projection operators on the 3 subspaces spanned by 3 irreducible representations yields the 3 basis vectors:

- for $c\tau_1^+$ $\mathbf{m}_{1+}^\mathbf{k}=\mathbf{m}_z^\mathbf{k}+(\mathbf{m}_z^\mathbf{k})^*$,
- for $c\tau_1^-$ $\mathbf{m}_{1-}^\mathbf{k}=\mathbf{m}_z^\mathbf{k}-(\mathbf{m}_z^\mathbf{k})^*$,
- for $c\tau_{2+3}$ $\mathbf{m}_{2+3}^{\mathbf{k}1}=\mathbf{m}_x^\mathbf{k}+\mathrm{i}\sqrt{3}(\mathbf{m}_x^\mathbf{k}+2\mathbf{m}_y^\mathbf{k})=\mathbf{U}+\mathrm{i}\mathbf{V}$,
  $\mathbf{m}_{2+3}^{\mathbf{k}2}=\mathbf{m}_x^\mathbf{k}-\mathrm{i}\sqrt{3}(\mathbf{m}_x^\mathbf{k}+2\mathbf{m}_y^\mathbf{k})=\mathbf{U}-\mathrm{i}\mathbf{V}$,
  $\mathbf{m}_{2+3}^{\mathbf{k}3}=(\mathbf{m}_{2+3}^{\mathbf{k}1})^*=\mathbf{m}_x^{-\mathbf{k}}-\mathrm{i}\sqrt{3}(\mathbf{m}_x^{-\mathbf{k}}+2\mathbf{m}_y^{-\mathbf{k}})$,
  $\mathbf{m}_{2+3}^{\mathbf{k}4}=(\mathbf{m}_{2+3}^{\mathbf{k}2})^*=\mathbf{m}_x^{-\mathbf{k}}+\mathrm{i}\sqrt{3}(\mathbf{m}_x^{-\mathbf{k}}+2\mathbf{m}_y^{-\mathbf{k}})$,

$c\tau_1^+$ and $c\tau_1^-$ give two solutions which just differ by a coefficient i, and which provide the same modulated magnetic structure along Oz. Corepresentation $c\tau_{2+3}$ gives two basis vectors for $\mathbf{m}^\mathbf{k}$ and two for $(\mathbf{m}^\mathbf{k})^*$ Each pair contains the 2 chiralities $\mathbf{U}-\mathrm{i}\mathbf{V}$ and $\mathbf{U}+\mathrm{i}\mathbf{V}$ in the basal plane. As in the first example, both helices are compatible with the symmetries. But in this centric case, the two helices (here triangles) correspond to the same irreducible corepresentation: they have the same energy and can be mixed in the crystal. The pair $\mathbf{m}_{2+3}^{\mathbf{k}3}=(\mathbf{m}_{2+3}^{\mathbf{k}1})^*$ and $\mathbf{m}_{2+3}^{\mathbf{k}4}=(\mathbf{m}_{2+3}^{\mathbf{k}2})^*$ which appears as basis vectors gives the same magnetic structure as the pair $\mathbf{m}_{2+3}^{\mathbf{k}1}, \mathbf{m}_{2+3}^{\mathbf{k}2}$. This reflects that, as a consequence of the time inversion, when looking at basis vectors corresponding to $\mathbf{k}$, we find also their conjugates which are the basis vectors corresponding to $-\mathbf{k}$.

Let us note that, in this example, the procedure followed by Lyubarskii [11] which associates to a nonreal representation τ_ν its conjugate τ_ν^*, to create a 'physically irreducible representation' $\tau_\nu+\tau_\nu^*$, would give the same result as does the irreducible corepresentation $c\tau_{2+3}$. However, the rigorous treatment proposed here is more general as it can be applied in all the cases, even when the spatial operators h_i of the little group do not connect all the positions of the magnetic site.

6.3. 3rd example: $CeAl_2$, a modulation in a centric cubic group (black and white magnetic little group, case a with real corepresentations)

$CeAl_2$ is a face centred cubic compound, centric space group Fd3m, with 2 Ce atoms in the unit cell: $(0, 0, 0)$ and $(1/4, 1/4, 1/4)$. Neutron diffraction experiments [12] have shown that the propagation vector is $\mathbf{k} = (1/2 - \delta, 1/2 + \delta, 1/2)$. From the 48 operators which are in the group G, only 2 of them keep the vector $\mathbf{k}$ unchanged and form the little group $G_{\mathbf{k}}$: $h_1(x, y, z)$ and $h_{13}(1/4 - y, 1/4 - x, 1/4 - z)$.

We first apply the representation theory, without the time inversion symmetry. The action of the 2 operators on the components $\mathbf{m}^{\mathbf{k}}_{j\alpha}$ is represented in Table 5. The magnetic representation Γ is of order 6. Its characters are also reported in Table 5. The irreducible representations of the little group $G_{\mathbf{k}}$, as displayed in Refs. [8,10] are reported in Table 6. The representation Γ is reduced into irreducible representations as following:

$$\Gamma = 3\tau_1 + 3\tau_2.$$

The basis vectors for these irreducible representations are obtained with the help of the projection operators, which leads to:

- For representation τ_1, a structure based on the 3 following basis vectors:

$$\begin{cases} \mathbf{m}^{\mathbf{k}1}_1 = \mathbf{m}^{\mathbf{k}}_{1x} - \mathbf{m}^{\mathbf{k}}_{2y}, \\ \mathbf{m}^{\mathbf{k}2}_1 = \mathbf{m}^{\mathbf{k}}_{1y} - \mathbf{m}^{\mathbf{k}}_{2x}, \\ \mathbf{m}^{\mathbf{k}3}_1 = \mathbf{m}^{\mathbf{k}}_{1z} - \mathbf{m}^{\mathbf{k}}_{2z} \end{cases}$$

  which corresponds to an antiferromagnetic structure with the following relations between the components:

$$\begin{cases} m^k_{2y} = -m^k_{1x}, \\ m^k_{2x} = -m^k_{1y}, \\ m^k_{2z} = -m^k_{1z}. \end{cases}$$

- For representation τ_2, a structure based on the 3 following basis vectors:

$$\begin{cases} \mathbf{m}^{\mathbf{k}1}_2 = \mathbf{m}^{\mathbf{k}}_{1x} + \mathbf{m}^{\mathbf{k}}_{2y}, \\ \mathbf{m}^{\mathbf{k}2}_2 = \mathbf{m}^{\mathbf{k}}_{1y} + \mathbf{m}^{\mathbf{k}}_{2x}, \\ \mathbf{m}^{\mathbf{k}3}_2 = \mathbf{m}^{\mathbf{k}}_{1z} + \mathbf{m}^{\mathbf{k}}_{2z} \end{cases}$$

  which corresponds to a ferromagnetic structure with

$$\begin{cases} m^k_{2y} = m^k_{1x}, \\ m^k_{2x} = m^k_{1y}, \\ m^k_{2z} = m^k_{1z}. \end{cases}$$

Table 5
Action of the operators of $G_{\mathbf{k}}$ on the components $\mathbf{m}^{\mathbf{k}}_{j\alpha}$ of $CeAl_2$

	h_1	h_{13}
	$\mathbf{m}^{\mathbf{k}}_{1x}$	$-\mathbf{m}^{\mathbf{k}}_{2y}$
	$\mathbf{m}^{\mathbf{k}}_{1y}$	$-\mathbf{m}^{\mathbf{k}}_{2x}$
	$\mathbf{m}^{\mathbf{k}}_{1z}$	$-\mathbf{m}^{\mathbf{k}}_{2z}$
	$\mathbf{m}^{\mathbf{k}}_{2x}$	$-\mathbf{m}^{\mathbf{k}}_{1y}$
	$\mathbf{m}^{\mathbf{k}}_{2y}$	$-\mathbf{m}^{\mathbf{k}}_{1x}$
	$\mathbf{m}^{\mathbf{k}}_{2z}$	$-\mathbf{m}^{\mathbf{k}}_{1z}$
χ	6	0

Table 6
Irreducible representations of the little group $G_{\mathbf{k}}$ of $CeAl_2$

	h_1	h_{13}
τ_1	1	1
τ_2	1	−1

Table 7
Irreducible corepresentations of the magnetic little group $G_{\mathbf{k}}^{\Theta}$ of $CeAl_2$

	h_1	h_{13}	Θh_{25}	Θh_{37}
$c\tau_1^+$	1	1	1	1
$c\tau_1^-$	1	1	−1	−1
$c\tau_2^+$	1	−1	1	−1
$c\tau_2^-$	1	−1	−1	1

Table 8
Action of the operators of $G_{\mathbf{k}}^{\Theta}$ on the real components $\mathbf{m}_{j\alpha}^{\mathbf{k}} = (\mathbf{m}_{j\alpha}^{\mathbf{k}})^*$ of $CeAl_2$

	h_1	h_{13}	Θh_{25}	Θh_{37}
	$\mathbf{m}_{1x}^{\mathbf{k}}$	$-\mathbf{m}_{2y}^{\mathbf{k}}$	$-\mathbf{m}_{2x}^{\mathbf{k}}$	$\mathbf{m}_{1y}^{\mathbf{k}}$
	$\mathbf{m}_{1y}^{\mathbf{k}}$	$-\mathbf{m}_{2x}^{\mathbf{k}}$	$-\mathbf{m}_{2y}^{\mathbf{k}}$	$\mathbf{m}_{1x}^{\mathbf{k}}$
	$\mathbf{m}_{1z}^{\mathbf{k}}$	$-\mathbf{m}_{2z}^{\mathbf{k}}$	$-\mathbf{m}_{2z}^{\mathbf{k}}$	$\mathbf{m}_{1z}^{\mathbf{k}}$
	$\mathbf{m}_{2x}^{\mathbf{k}}$	$-\mathbf{m}_{1y}^{\mathbf{k}}$	$-\mathbf{m}_{1x}^{\mathbf{k}}$	$\mathbf{m}_{2y}^{\mathbf{k}}$
	$\mathbf{m}_{2y}^{\mathbf{k}}$	$-\mathbf{m}_{1x}^{\mathbf{k}}$	$-\mathbf{m}_{1y}^{\mathbf{k}}$	$\mathbf{m}_{2x}^{\mathbf{k}}$
	$\mathbf{m}_{2z}^{\mathbf{k}}$	$-\mathbf{m}_{1z}^{\mathbf{k}}$	$-\mathbf{m}_{1z}^{\mathbf{k}}$	$\mathbf{m}_{2z}^{\mathbf{k}}$
χ	6	0	0	2

For both cases, there are 3 parameters to be determined from the experiment: m_{1x}^k, m_{1y}^k and m_{1z}^k. Actually, what was found in refining the neutron data [12–14] is that the structure is antiferromagnetic as expected from representation τ_1, with a component m_{1z}^k which is different from the two others, but with the unpredicted equality: $m_{1x}^k = m_{1y}^k$.

We shall now introduce the time inversion Θ in the representation analysis. The magnetic little group is black and white: $G_{\mathbf{k}}^{\Theta} = G_{\mathbf{k}} + a_0 G_{\mathbf{k}}$, with the reversing element $a_0 = \Theta h_{25}$ where h_{25} is the inversion operator $(-x, -y, -z)$. With this magnetic little group, $\sum_{a_j} \chi(a_j^2) = 2$, which means that $G_{\mathbf{k}}^{\Theta}$ corresponds to case (a). There are 4 irreducible corepresentations of order 1, which are all real. They are reported in Table 7.

With the components $\mathbf{m}_{j\alpha}^{\mathbf{k}}$ and $\mathbf{m}_{j\alpha}^{-\mathbf{k}}$, the magnetic corepresentation Γ would be of order 12. However, as this corepresentation is real and we have to decompose it into irreducible corepresentations which are also real, we can restrict our investigation to real basis vectors and state:

$$\mathbf{m}_{j\alpha}^{\mathbf{k}} = \mathbf{m}_{j\alpha}^{-\mathbf{k}}.$$

The action of the operators of the little group $G_{\mathbf{k}}^{\Theta} = G_{\mathbf{k}} + a_0 G_{\mathbf{k}}$ on such real basis vectors $\mathbf{m}_{j\alpha}^{\mathbf{k}}$ are reported in Table 8, as well as the characters of the magnetic corepresentation $c\Gamma$ which is now of order 6. The decomposition of this corepresentation into the irreducible corepresentations becomes:

$$c\Gamma = 2c\tau_1^+ + c\tau_1^- + c\tau_2^+ + 2c\tau_2^-.$$

The basis vectors for each irreducible corepresentation are obtained with the projection operators, which gives:

- For representation $c\tau_1^+$ a structure based on the 2 following basis vectors:

$$\mathbf{m}_{1+}^{\mathbf{k}1} = (\mathbf{m}_{1x}^{\mathbf{k}} - \mathbf{m}_{2y}^{\mathbf{k}}) + (\mathbf{m}_{1y}^{\mathbf{k}} - \mathbf{m}_{2x}^{\mathbf{k}}), \qquad \mathbf{m}_{1+}^{\mathbf{k}2} = \mathbf{m}_{1z}^{\mathbf{k}} - \mathbf{m}_{2z}^{\mathbf{k}}.$$

- For representation $c\tau_1^-$ a structure based on only one basis vectors:

$$\mathbf{m}_{1-}^{\mathbf{k}} = (\mathbf{m}_{1x}^{\mathbf{k}} - \mathbf{m}_{2y}^{\mathbf{k}}) - (\mathbf{m}_{1y}^{\mathbf{k}} - \mathbf{m}_{2x}^{\mathbf{k}}).$$

- For representation $c\tau_2^+$ a structure based also on one basis vectors:

$$\mathbf{m}_{2+}^{\mathbf{k}} = (\mathbf{m}_{1x}^{\mathbf{k}} + \mathbf{m}_{2y}^{\mathbf{k}}) - (\mathbf{m}_{1y}^{\mathbf{k}} + \mathbf{m}_{2x}^{\mathbf{k}}).$$

- For representation $c\tau_2^-$ a structure based on the 2 following basis vectors:

$$\mathbf{m}_{2-}^{\mathbf{k}1} = (\mathbf{m}_{1x}^{\mathbf{k}} + \mathbf{m}_{2y}^{\mathbf{k}}) + (\mathbf{m}_{1y}^{\mathbf{k}} + \mathbf{m}_{2x}^{\mathbf{k}}), \qquad \mathbf{m}_{2-}^{\mathbf{k}2} = \mathbf{m}_{1z}^{\mathbf{k}} + \mathbf{m}_{2z}^{\mathbf{k}}.$$

The magnetic structure, as deduced from the experiment, corresponds to corepresentation $c\tau_1^+$. It is antiferromagnetic with the following relations:

$$\begin{cases} m_{2y}^k = -m_{1x}^k, \\ m_{2x}^k = -m_{1y}^k, \\ m_{2z}^k = -m_{1z}^k \end{cases}$$

and also with $m_{1y}^k = m_{1x}^k$.

Introducing the fact that basis vectors can be chosen real has brought a new constraint to the representation analysis, and it results that corepresentations $c\tau_1^+$ and $c\tau_1^-$ are no more equivalent (as well as corepresentations $c\tau_2^+$ and $c\tau_2^-$). Relation $m_{1y}^{\mathbf{k}} = m_{1x}^{\mathbf{k}}$ is a consequence of this nonequivalence. It is exactly what was found experimentally, but it was not expected from theory without taking into account the time inversion in the representation analysis.

7. Conclusion: invariance by conjugation and reality of the magnetic moments are the key points

The antilinear time inversion operator Θ, as it has been defined here in formula (6), consists in a change of sign and a conjugation of the Fourier development of the magnetic moments. While the change of sign does not bring any new information in the representation analysis of the magnetic structures, the conjugation is the fruitful operation as it obliges to use the Wigner corepresentations which associate the operators which keeps **k** and those which reverse **k**. Exactly the same results could have been obtained if, instead of the 'time inversion' operator Θ, we would have used the operator 'conjugation' K. It is obviously an antilinear operator which keep invariant the magnetic energy U_0 and which requires also the use of the group theory algebra developed by Wigner for the time inversion of the wave functions in quantum mechanics. The physical reason of the invariance of the magnetic energy under the action of the 'conjugation' operator is that the magnetic moments themselves are invariant under K because they are real vectorial quantities. We join here the ideas developed by Lyubarskii [11] when he produced 'physically irreducible representations', associating a non real representation to its conjugate. However, our procedure is more general as it associates, from the beginning, **k** and $-\mathbf{k}$ in the corepresentations.

To summarize, we can say that, whether operator Θ or operator K is considered, we have shown that introducing such an antilinear operator in the representation (corepresentation) analysis of the magnetic structures brings new pieces of information and is all the more important since the symmetry of the system is low. Nowadays, for applications in solid state, all the corepresentations are tabulated in text books and within the reach of everyone. It would then be a pity to neglect an element of information which may be important.

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