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# Time inversion in the representation analysis of magnetic structures

Jacques Schweizer

*CEA-Grenoble, DSM/DRFMC/SPSMS/MDN, 38054 Grenoble cedex 9, France*

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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 coreprésentations ; Analyse en représentations ; Structures magnétiques

*E-mail address:* schweizer@cea.fr (J. Schweizer).

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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:

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

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 $\alpha$ and $\beta$ the axes $x$, $y$ or $z$, and where the $J_{\mathbf{l}\mathbf{l}'jj'\alpha\beta}$ 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):

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

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

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

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

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

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 $\tau_\nu$ 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 $\Theta$, both reversing the sign of the magnetic moments $\mathbf{m}_{\mathbf{l}j}$. We shall show that introducing the antilinear operator $\Theta$ 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.

[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 $\mathbf{k}\mathbf{l} \neq n\pi$, 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 $A(as) = a^*A(s)$.