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J. Schweizer
CEA-Grenoble, DSM/DRFMC/SPSMS/MDN

J. Villain

A. Brooks Harris
University of Pennsylvania, harris@sas.upenn.edu

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Symmetry of magnetic structures: the case of $CeAl_2$

J. Schweizer[1,a], J. Villain[1], and A.B. Harris[2]

[1] Département de Recherche Fondamentale sur la Matière Condensée D.S.M., Commissariat à l'Énergie Atomique, 17 avenue des Martyrs, 38054 Grenoble Cedex 9, France
[2] Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA, 19104, USA

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Abstract. This article presents a group-theoretical investigation of an incommensurate magnetic structure in the case where the crystal structure is centrosymmetric while the structure vector **k** is not conserved by inversion. A first method starts with the conventional group-theoretical treatment taking into account the transformations which conserve **k** and then combines the solutions to obtain a centrosymmetric and real magnetization. A second method includes inversion in the group-theoretical treatment, for instance by introducing the complex conjugation operator and corepresentations. The general theory is applied to $CeAl_2$ with the scope of improving the knowledge of its magnetic structure.

PACS. 61.12.Ld Neutron diffraction – 61.50.Ah Theory of crystal structure, crystal symmetry; calculations and modeling – 75.50.Ee Antiferromagnetics

1 Introduction

$CeAl_2$ is a face-centered, cubic Laves phase compound, with two magnetic Ce atoms in the unit cell (labelled $i = 1, 2$) at the same positions as the carbon in the diamond structure, namely (000) and $(a/4, a/4, a/4)$, where a is the side of the cubic cell. This compound orders below $T_N = 3.8$ K and a first neutron diffraction experiment [1] has shown that a particular Fourier component

$$\mathbf{m}_i(\mathbf{k}) = \frac{1}{N} \sum_R \mathbf{M}_i(\mathbf{R}) \exp(i\mathbf{k}.\mathbf{R}) \qquad (1)$$

of the magnetization becomes macroscopic. Here, **R** denotes a lattice translation vector and therefore labels the various unit cells, and $\mathbf{M}_i(\mathbf{R})$ is the magnetization of the atom of species i in the cell **R**. The propagation vector is $\mathbf{k} = (\frac{1}{2} - \delta, \frac{1}{2} + \delta, \frac{1}{2})$ in units of $2\pi/a$. This propagation vector can be decomposed in two parts: the first one, $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, represents an antiferromagnetic structure with negative coupling between adjacent (1, 1, 1) planes and the second one, $(-\delta, \delta, 0)$, corresponds to a modulation of the former structure along a direction [-1, 1, 0], perpendicular to the diagonal [1, 1, 1]. This modulation is weak, $|\delta| \ll 1$. These neutron data have also shown that the magnetic moments of the two Ce atoms are opposed one to the other and are aligned along the diagonal direction.

A further neutron experiment [2] pointed out that the structure is double **k**, with 2 (symmetrically equivalent) propagation vectors $\mathbf{k}_1 = (\frac{1}{2} - \delta, \frac{1}{2} + \delta, \frac{1}{2})$ and $\mathbf{k}_2 = (\frac{1}{2} - \delta, \frac{1}{2} + \delta, -\frac{1}{2})$, which share the modulation part $(-\delta, \delta, 0)$, but with different directions for the antiferromagnetic propagation $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ and $(\frac{1}{2}, \frac{1}{2}, -\frac{1}{2})$. Such a double **k** structure should result for the two Ce atoms in two elliptical helices with opposite chiralities. It is the subject of a separate paper by two of us [14] and will not considered here.

A more sophisticated neutron diffraction analysis, using a spherical analysis of the polarization scattered by the magnetic reflections [3] brought another piece of information: when the temperature decreases below T_N, the Fourier components of the magnetic moments are increasingly shifted from the direction of the cube diagonal, thereby reducing the ellipticity of the helices.

A first analysis of the $CeAl_2$ symmetries, using group theory and representation analysis [5] concluded that the coupling between the two Ce atoms is either positive or negative and that the Fourier components of the magnetic moments are not necessarily along the cube diagonal. But the direction of the second moment is completely determined when the direction of the first one is fixed. However, this analysis was restricted to the symmetry elements which keep the propagation vector **k** unchanged, without taking into account the inversion symmetry which transforms **k** into **-k**. It is the aim of this paper to make a full analysis of the problem, considering all the symmetry elements which are relevant, to determine the possible magnetic structures. In Section 3, it is pointed out that the inversion symmetry can be taken into account by an appropriate manipulation of the structure determined by the standard method. An alternative method, proposed by one of us in a previous paper [11] is to apply group theory to a group larger than the group of the **k** vector,

[a] e-mail: jacques.schweizer@cea.fr

Table 1. Action of the symmetry operators of $G_{0\mathbf{k}}$ on the components of $CeAl_2$.

h_1	$m_{1x}(\mathbf{k})$	$m_{1y}(\mathbf{k})$	$m_{1z}(\mathbf{k})$	$m_{2x}(\mathbf{k})$	$m_{2y}(\mathbf{k})$	$m_{2z}(\mathbf{k})$
h_{13}	$-m_{2y}(\mathbf{k})$	$-m_{2x}(\mathbf{k})$	$-m_{2z}(\mathbf{k})$	$-m_{1y}(\mathbf{k})$	$-m_{1x}(\mathbf{k})$	$-m_{1z}(\mathbf{k})$

for instance by using a corepresentation analysis instead of the usual representation technique. It will be formulated in Section 4 of the present paper, where a mistake of the previous work will be corrected.

2 Magnetic structures and symmetries

The structure of a non-magnetic material is invariant under the symmetry operations of a group G which is one of the 230 space groups. In $CeAl_2$, the group G is Fd3m. A magnetic material has the same property in the paramagnetic region. If one considers the linear response of the local magnetization of the magnetic atoms to a field acting on the various magnetic moments in a different way, one can define a generalized susceptibility which is a $3Nn \times 3Nn$ matrix if there are N unit cells and n magnetic atoms in the unit cell (i.e. $n = 2$ in $CeAl_2$). By considering the Fourier transforms $m_{i\alpha}(\mathbf{k})$ and $h_{i\alpha}(\mathbf{k})$ of the moments and of the fields, as defined by (1), the susceptibility matrix becomes a $3n \times 3n$ matrix $\chi(\mathbf{k})$. Its elements are $\chi_{i,j,\alpha,\gamma}(\mathbf{k})$ where $i, j = 1, 2, ..., n$ label the atoms of each unit cell, and $\alpha, \gamma = x, y, z$ are the Cartesian components. That matrix is invariant under the operations of the space group. At a continuous magnetic transition, at least one eigenvalue of $\chi(\mathbf{k})$ becomes infinite for a particular value of $\mathbf{k}$ and for the values which can be generated from $\mathbf{k}$ by symmetry operations. These include the operations of the point group, but also the inversion $\mathbf{k} \rightarrow -\mathbf{k}$, whether or not spatial inversion belongs to the point group. This is because $\chi(\mathbf{k})$ is hermitian. The magnetic structure below the transition is expected to have the form

$$m_i(\mathbf{k}) = \sum_{\mathbf{k}} \sum_{p} \left[\lambda_p(\mathbf{k}) u_{i\alpha}^{(p)}(\mathbf{k}) + \lambda_p^*(\mathbf{k}) u_{i\alpha}^{(p)*}(\mathbf{k}) \right] \quad (2)$$

where the sum is over equivalent vectors $\mathbf{k}$ (which are said to constitute a "star", p is an additional index which is necessary if the infinite eigenvalue of $\chi(\mathbf{k})$ is a multiple one, $u_{i\alpha}^{(p)}(\mathbf{k})$ are the components of the corresponding normalized eigenvectors, and the coefficients $\lambda_p(\mathbf{k})$ depend on temperature. The present paper is focused on the symmetry properties of the coefficients $u_{i\alpha}^{(p)}(\mathbf{k})$ which can be derived from the crystal symmetry.

The point group G_0 of $CeAl_2$ contains 48 elements. However, according to the usual view [4,5,7], a symmetry can only be exploited if it conserves the propagation vector $\mathbf{k} = (\frac{1}{2} - \delta, \frac{1}{2} + \delta, \frac{1}{2})$. Apart from the unity, a single operation of G_0 has this property. It is the two-fold rotation $(x, y, z) \rightarrow (1/4 - y, 1/4 - x, 1/4 - z)$, called h_{13} by Kovalev [8]. Indeed it transforms $\mathbf{k} = (\frac{1}{2} - \delta, \frac{1}{2} + \delta, \frac{1}{2})$ into $(-\frac{1}{2} - \delta, -\frac{1}{2} + \delta, -\frac{1}{2})$, which can be made equal to $(\frac{1}{2} - \delta, \frac{1}{2} + \delta, \frac{1}{2})$ by addition of (1,1,1), which is a reciprocal lattice vector. The operation h_{13}, together with the unity (called h_1 by Kovalev), forms a subgroup $G_{0\mathbf{k}}$ of G_0 which may be called the point group of the $\mathbf{k}$ vector. The operations of the space group G which contain h_1 and h_{13} as rotation parts form the so-called group of the $\mathbf{k}$ vector or little group G_k. Generally, they have the form $\{h_1|\mathbf{R}\}$ and $\{h_{13}|\mathbf{t}_{13} + \mathbf{R}\}$. The case of $CeAl_2$ is particularly simple because its space group is symmorphic, which means that G_0 is a subgroup of G. It results that $G_{0\mathbf{k}}$ is a subgroup of G_k and $t_{13} = 0$. If the operations $h_1 = \{h_1|0\}$ and $h_{13} = \{h_{13}|0\}$ of $G_{0\mathbf{k}}$ act on the 6 components of the Fourier transform (1), their effect is displayed by Table 1.

Table 1 defines a transformation matrix $\Gamma(h_{13})$ which commutes with $\chi(\mathbf{k})$, i.e.

$$\Gamma^{-1}(h_{13})\chi(\mathbf{k})\Gamma(h_{13}) = \chi(\mathbf{k}). \quad (3)$$

This symmetry property may be used to simplify the diagonalization of the 6×6 matrix $\chi(\mathbf{k})$. The standard group-theoretical method [5,7] proceeds as follows. The matrix $\Gamma(h_{13})$, together with $\Gamma(h_1)$ which is just the unit matrix of dimension 6, constitutes a representation $\{\Gamma\}$ of $G_{0\mathbf{k}}$, which may be called 'natural' and is reducible. The reduction of this representation reduces the diagonalization of $\chi(\mathbf{k})$ to the diagonalization of two 3×3 submatrices. More explicitly, one has to find (and one can find!) new coordinates, i.e. new basis vectors in the 6-dimensional space, such that $\chi(\mathbf{k})$ reduces to two diagonal blocks, plus two off-diagonal blocks all of whose elements are 0. The new basis vectors are particularly easy to find in the present case of a group which contains only two elements, the unity and h_{13}. It is indeed sufficient to take the eigenvectors of $\Gamma(h_{13})$ as basis vectors. Since $\Gamma^2(h_{13}) = \Gamma(h_{13}^2) = 1$, the eigenvalues are obviously 1 and -1. Thus, the irreducible representations are of dimension 1 and given by Table 2 (which holds for any group of two elements).

The basis vectors of the representation λ can alternatively be found by using the projection operator P_λ given, for a one-dimensional representation, by the formula [5,7]

$$P_\lambda = \sum_g \gamma_\lambda^*(g)\Gamma(g) \quad (4)$$

where a normalization factor has been omitted, g designates the operations of the group (two in the present case), $\Gamma(g)$ is the matrix associated to g in the natural representation of Table 1, and $\gamma_\lambda(g)$ is the number associated to g in the representation λ according to Table 2. To help the inexperienced reader, it will be seen how eigenvectors of h_{13} can be found by inspection of Table 1. For instance, if $m_{1x}(\mathbf{k}) = \pm m_{2y}(\mathbf{k}) = \epsilon m_{2y}(\mathbf{k})$ and all other components are 0, one obtains an eigenvector for the eigenvalue $-\epsilon$. In

Table 2. Irreducible representations of $G_{0\mathbf{k}}$.

	h_1	h_{13}
τ_1	1	1
τ_2	1	−1

terms of the old basis vectors $\mathbf{e}_{i\alpha}$, the new basis vectors may be written as $\mathbf{e}_{1x} + \epsilon\mathbf{e}_{2y}$. The 3 eigenvectors for the eigenvalue 1, i.e. the 3 basis vectors for the representation $\tau_1 = (1, 1)$, are (omitting the normalization factor $2^{-1/2}$)

$$\begin{aligned}\mathbf{u}_1^+ &= \mathbf{e}_{1x}(\mathbf{k}) - \mathbf{e}_{2y}(\mathbf{k}),\\ \mathbf{u}_2^+ &= \mathbf{e}_{1y}(\mathbf{k}) - \mathbf{e}_{2x}(\mathbf{k}),\\ \mathbf{u}_3^+ &= \mathbf{e}_{1z}(\mathbf{k}) - \mathbf{e}_{2z}(\mathbf{k})\end{aligned} \tag{5}$$

while the 3 basis vectors for the representation $\tau_2 = (1, -1)$ are

$$\begin{aligned}\mathbf{u}_1^- &= \mathbf{e}_{1x}(\mathbf{k}) + \mathbf{e}_{2y}(\mathbf{k}),\\ \mathbf{u}_2^- &= \mathbf{e}_{1y}(\mathbf{k}) + \mathbf{e}_{2x}(\mathbf{k}),\\ \mathbf{u}_3^- &= \mathbf{e}_{1z}(\mathbf{k}) + \mathbf{e}_{2z}(\mathbf{k}).\end{aligned} \tag{6}$$

The eigenvectors of $\chi(\mathbf{k})$ have either the form

$$\mathbf{v}^+ = \lambda\mathbf{u}_1^+ + \mu\mathbf{u}_2^+ + \nu\mathbf{u}_3^+ \tag{7}$$

or the form

$$\mathbf{v}^- = \lambda\mathbf{u}_1^- + \mu\mathbf{u}_2^- + \nu\mathbf{u}_3^-. \tag{8}$$

The corresponding expression in the real space is the Fourier transform of (8), i.e.

$$\mathbf{v}_1(\mathbf{R}) = \begin{bmatrix}\lambda\\ \mu\\ \nu\end{bmatrix} \exp(-i\mathbf{k}.\mathbf{R}),\ \mathbf{v}_2(\mathbf{R}) = -\epsilon \begin{bmatrix}\mu\\ \lambda\\ \nu\end{bmatrix} \exp(-i\mathbf{k}.\mathbf{R}). \tag{9}$$

These formulae also restrict the possible form of the Fourier transform of propagation vector $\mathbf{k}$ of the magnetic structure near the transition. The magnetization *must* have a Fourier component of propagation vector $-\mathbf{k}$, so that it is real in the direct space. It *may* have additional Fourier components whose propagation vectors are equivalent to $\mathbf{k}$, and it does have them in $CeAl_2$ as said in the introduction. For each propagation vector, the coefficients λ, μ, ν can in principle be determined experimentally. Thanks to group theory, there are only 3 complex parameters, i.e. 6 real ones. One of these parameters is the phase of the helix. For an incommensurate structure it has no effect on the energy. For a commensurate structure with a long period (i.e. if $\mathbf{k}$ is not equal to 0 or half a reciprocal lattice vector) the phase of the helix does affect the energy if it contains higher order terms, but not in the linear theory presented here, where only the eigenvectors of the susceptibility matrix are considered.

Five parameters are still too much. In the next section the number of parameters will be reduced to 3 by considering symmetry operations which are not in the group of the $\mathbf{k}$ vector, but transform $\mathbf{k}$ into $-\mathbf{k}$.

3 Inversion

In $CeAl_2$, the inversion I $(x, y, z \to 1/8-x, 1/8-y, 1/8-z)$ is an element of the space group and therefore transforms any eigenvector of the $3Nn \times 3Nn$ susceptibility matrix χ into another eigenvector for the same eigenvalue. This property has not been taken into account in the preceding argument because the inversion transforms $\mathbf{k}$ into $-\mathbf{k}$. Thus it is not an element of G_k and transforms an eigenvector of $\chi(\mathbf{k})$ into an eigenvector of $\chi(-\mathbf{k})$. However, it is possible to exploit invariance under inversion. One has to consider the 12×12 matrix

The inversion operator I conserves globally the crystal structure but modifies the magnetic structure. It transforms a state with magnetization $\mathbf{M}_1(\mathbf{R})$ at site 1 in the cell $\mathbf{R}$ into a state with the same magnetization (because the magnetization is an axial vector and not a polar vector!) at site 2 in the cell $-\mathbf{R}$. Thus the transformed magnetization is $\mathbf{M}_1'(\mathbf{R}) = \mathbf{M}_2(-\mathbf{R})$, and conversely $\mathbf{M}_2'(\mathbf{R}) = \mathbf{M}_1(-\mathbf{R})$. Introducing the column matrix $|\,M\rangle$ of $3Nn$ elements $M_{i\alpha}(\mathbf{R})$, where $i = 1$ or 2 and $\alpha = x, y, z$, this relation can be written $|\,M'\rangle = \Gamma(I)\,|\,M\rangle$, where the $3Nn \times 3Nn$ permutation matrix $\Gamma(I)$ satisfies the relations

$$I^2 = 1$$

and

$$\Gamma^{-1}(I)\chi\Gamma(I) = \chi. \tag{10}$$

The last formula looks like (3). This suggests to include I in a group-theoretical method. This will be done in Section 4. In the present section, the particularly simple properties of I and $\Gamma(I)$ will be exploited. The matrix $\Gamma(I)$ is indeed real, symmetric, and its square is the unit matrix. Therefore it has $3Nn$ eigenvectors, but only two eigenvalues, 1 and −1. The commutation relation (10) implies that χ and $\Gamma(I)$ can be diagonalized simultaneously. Therefore the eigenvectors $|\,M\rangle$ of χ can be chosen such that they satisfy either $\Gamma(I)\,|\,M\rangle = |\,M\rangle$ or $\Gamma(I)\,|\,M\rangle = -|\,M\rangle$. Moreover, all eigenvectors $|\,M\rangle$ can be chosen real, in agreement with the physical condition that $M_{i\alpha}(\mathbf{R})$ is real.

In the case of $CeAl_2$, $|\,M\rangle$ is given by (9). That expression does not generally satisfy $\Gamma(I)\,|\,M\rangle = \pm|\,M\rangle$. However the action of $\Gamma(I)$ transforms (9) into another eigenvector of χ for the same eigenvalue. Multiplying this transformed eigenvector by $\epsilon' = \pm 1$ and adding the result to (9), the following expression is obtained, which does satisfy $\Gamma(I)\,|\,M\rangle = \epsilon\epsilon'\,|\,M\rangle$.

$$\mathbf{W}_1(\mathbf{R}) = \begin{bmatrix}\lambda\\ \mu\\ \nu\end{bmatrix} \exp(-i\mathbf{k}.\mathbf{R}) - \epsilon\epsilon' \begin{bmatrix}\mu\\ \lambda\\ \nu\end{bmatrix} \exp(i\mathbf{k}.\mathbf{R}) \tag{11}$$

and

$$\mathbf{W}_2(\mathbf{R}) = -\epsilon \begin{bmatrix}\mu\\ \lambda\\ \nu\end{bmatrix} \exp(-i\mathbf{k}.\mathbf{R}) + \epsilon' \begin{bmatrix}\lambda\\ \mu\\ \nu\end{bmatrix} \exp(i\mathbf{k}.\mathbf{R}). \tag{12}$$

A real eigenvector of the susceptibility matrix, and therefore an acceptable expression of the magnetization, is obtained by adding these expressions and their complex conjugates, namely

$$\mathbf{M}_1(\mathbf{R}) = \begin{bmatrix} \lambda - \mu^* \epsilon\epsilon' \\ \mu - \lambda^* \epsilon\epsilon' \\ \nu - \nu^* \epsilon\epsilon' \end{bmatrix} \times \exp(-i\mathbf{k}.\mathbf{R}) + \begin{bmatrix} \lambda^* - \mu\epsilon\epsilon' \\ \mu^* - \lambda\epsilon\epsilon' \\ \nu^* - \nu\epsilon\epsilon' \end{bmatrix} \exp(i\mathbf{k}.\mathbf{R}) \quad (13)$$

and

$$\mathbf{M}_2(\mathbf{R}) = -\epsilon \begin{bmatrix} \mu - \lambda^* \epsilon\epsilon' \\ \lambda - \mu^* \epsilon\epsilon' \\ \nu - \nu^* \epsilon\epsilon' \end{bmatrix} \times \exp(-i\mathbf{k}.\mathbf{R}) - \epsilon \begin{bmatrix} \mu^* - \lambda\epsilon\epsilon' \\ \lambda^* - \mu\epsilon\epsilon' \\ \nu^* - \nu\epsilon\epsilon' \end{bmatrix} \exp(i\mathbf{k}.\mathbf{R}). \quad (14)$$

It is convenient to rewrite these formulae in another form, introducing the real quantities m_0^z, u, α and θ defined by

$$\nu - \nu^* \epsilon\epsilon' = m_0^z \exp(i\alpha)$$

and

$$\lambda - \mu^* \epsilon\epsilon' = u m_0^z \exp(i\theta + i\alpha)$$

where the phase α is equal to 0 (if $\epsilon\epsilon' = -1$) or $\pi/2$ (if $\epsilon\epsilon' = 1$). The parameter ϵ' can be eliminated because $\epsilon\epsilon' = -\exp(2i\alpha)$, so that

$$\mu - \lambda^* \epsilon\epsilon' = \epsilon\epsilon' u m_0^z \exp(i\theta + i\alpha) = -u m_0^z \exp(i\theta - i\alpha).$$

Using these relations, formulae (13) and (14) read

$$\mathbf{M}_1(\mathbf{R}) = m_0^z \begin{bmatrix} u\cos(\mathbf{k}.\mathbf{R} - \theta - \alpha) \\ u\cos(\mathbf{k}.\mathbf{R} + \theta - \alpha) \\ \cos(\mathbf{k}.\mathbf{R} - \alpha) \end{bmatrix},$$

$$\mathbf{M}_2(\mathbf{R}) = \epsilon m_0^z \begin{bmatrix} -u\cos(\mathbf{k}.\mathbf{R} + \theta - \alpha) \\ -u\cos(\mathbf{k}.\mathbf{R} - \theta - \alpha) \\ -\cos(\mathbf{k}.\mathbf{R} - \alpha) \end{bmatrix}. \quad (15)$$

The phase α was defined as being 0 and $\pi/2$. However, this restriction can be dropped in the case of an incommensurate structure. Indeed, the two structures $\alpha = 0$ and $\pi/2$ differ only by a shift of the helix and should have the same energy, and correspond to the same eigenvalue of the susceptibility matrix. They can therefore be added after multiplication by $\cos\beta$ and $\sin\beta$ respectively. The final result has still the form (15), but now α can take any value and full translational invariance is restored.

4 Group-theoretical approach

In the previous section, space inversion has been treated by linear algebra rather than group theory. This is possible because we decided to investigate the eigenvectors of the susceptibility matrix, which is a linear algebra problem. This approach is not strictly justified below the transition (which is precisely the region of interest) and a group-theoretical approach may be more general. It will be presented in the present section.

The method is an extension of Bertaut's original method. One looks for magnetic structures which transform as irreducible representations of a group $G_{\mathbf{k}}^{(2)}$ which is not the group of the $\mathbf{k}$ vector, but is larger, twice as large as a matter of fact. This group can be chosen in different ways.

Choice A. The group $G_{\mathbf{k}}^{(2)}$ may be defined as the group generated by $G_{\mathbf{k}}$ and the space inversion I. This group would contain the elements g of $G_{\mathbf{k}}$, and the products gI. In an irreducible representation where a translation of vector $\mathbf{T}$ is represented by $\exp(-i\mathbf{k}.\mathbf{T})$, the product of this translation by I is represented by $\exp(i\mathbf{k}.\mathbf{T})$ as will be seen below.

Choice B. The choice which will be made here avoids mixing $\mathbf{k}$ and $-\mathbf{k}$. It makes use of the complex conjugation operator C, which transforms a number x into $Cx = x^*$. This operator commute with I and with the $3Nn \times 3Nn$ susceptibility matrix since it is real.

Instead of considering the space inversion operator I as before, it is appropriate to use the product CI, or more generally $C\{I|T\} = \{I|T\}C$ rather than $\{I|T\}$ itself. These operations are not linear, but antilinear, i.e. they anticommute with i while they commute with real numbers.

The advantage of choice B can be seen if one looks for a solution of the form $\mathbf{M}_i(\mathbf{R}) = \mathbf{m}_i \exp(-i\mathbf{k}.\mathbf{R})$. The operation $\{h_{25}|T\}$ transforms this into $\mathbf{M}_i'(\mathbf{R}) = \mathbf{m}_j \exp(i\mathbf{k}.\mathbf{R}) \exp(i\mathbf{k}.\mathbf{T}))$, with $j \neq i$, (i.e. $j = 2$ if $i = 1$) and the action of C yields

$$\mathbf{M}_i''(\mathbf{R}) = C\mathbf{M}_i'(\mathbf{R}) = \mathbf{m}_j^* \exp(-i\mathbf{k}.\mathbf{R}) \exp(-i\mathbf{k}.\mathbf{T}). \quad (16)$$

Thus, the transformed function has the same form $\mathbf{M}_i''(\mathbf{R}) = \mathbf{m}_i'' \exp(-i\mathbf{k}.\mathbf{R})$ as the initial one, while the exponential $\exp(i\mathbf{k}.\mathbf{R})$ appears when C or $\{I|T\}$ are separately used.

Formula (16) shows that it is necessary to introduce both $\mathbf{M}(\mathbf{R})$ and its complex conjugate $\mathbf{M}^*(\mathbf{R})$, forgetting for some time that in a real magnetic structure, both should be equal. Alternatively, one can introduce the Fourier transforms $m_{i\alpha}(\mathbf{k})$ and $m_{i\alpha}^*(\mathbf{k})$, which can be considered the $6n$ components of a column matrix

Table 3. Action of the symmetry operators of $G^{(2)}_{0\mathbf{k}}$ on the magnetization of $CeAl_2$. Lines 1 and 2 correspond to the elements of $G_{0\mathbf{k}}$. Lines 3 and 4 correspond to choice A. Lines 5 and 6 correspond to choice B made in the text.

h_1	$m_{1x}(\mathbf{k})$	$m_{1y}(\mathbf{k})$	$m_{1z}(\mathbf{k})$	$m_{2x}(\mathbf{k})$	$m_{2y}(\mathbf{k})$	$m_{2z}(\mathbf{k})$
h_{13}	$-m_{2y}(\mathbf{k})$	$-m_{2x}(\mathbf{k})$	$-m_{2z}(\mathbf{k})$	$-m_{1y}(\mathbf{k})$	$-m_{1x}(\mathbf{k})$	$-m_{1z}(\mathbf{k})$
h_{25}	$m_{2x}(-\mathbf{k})$	$m_{2y}(-\mathbf{k})$	$m_{2z}(-\mathbf{k})$	$m_{1x}(-\mathbf{k})$	$m_{1y}(-\mathbf{k})$	$m_{1z}(-\mathbf{k})$
h_{37}	$-m_{1y}(-\mathbf{k})$	$-m_{1x}(-\mathbf{k})$	$-m_{1z}(-\mathbf{k})$	$-m_{2y}(-\mathbf{k})$	$-m_{2x}(-\mathbf{k})$	$-m_{2z}(-\mathbf{k})$
Ch_{25}	$m^*_{2x}(\mathbf{k})$	$m^*_{2y}(\mathbf{k})$	$m^*_{2z}(\mathbf{k})$	$m^*_{1x}(\mathbf{k})$	$m^*_{1y}(\mathbf{k})$	$m_{1z}(\mathbf{k})$
Ch_{37}	$-m^*_{1y}(\mathbf{k})$	$-m^*_{1x}(\mathbf{k})$	$-m^*_{1z}(\mathbf{k})$	$-m^*_{2y}(\mathbf{k})$	$-m^*_{2x}(\mathbf{k})$	$-m_{2z}(\mathbf{k})$

$|\, m(\mathbf{k}), m^*(\mathbf{k})\rangle$. As follows from Section 2, we are looking for such column matrices which are eigenvectors of the $6n \times 6n$ matrix

$$\tilde{\chi}(\mathbf{k}) = \begin{bmatrix} \chi(\mathbf{k}) & 0 \\ 0 & \chi^*(\mathbf{k}) \end{bmatrix}. \tag{17}$$

The search of the eigenvectors can be simplified by taking the symmetries into account. The symmetry operations $\tilde{g}$ of interest are (i) the operations g of $G_{\mathbf{k}}$ and (ii) the products CIg.

These operations form a group of $G^{(2)}_{\mathbf{k}}$. Any symmetry operations $\tilde{g}$ of this group transforms $|\, m(\mathbf{k}), m^*(\mathbf{k})\rangle$ into another column matrix $\tilde{\Gamma}_{\mathbf{k}}(\tilde{g})\,|\, m(\mathbf{k}), m^*(\mathbf{k})\rangle$, where the the $6n \times 6n$ matrices $\tilde{\Gamma}_{\mathbf{k}}(\tilde{g})$ will be explicitly given below in the case of $CeAl_2$. The crystal symmetry implies that

$$\tilde{\Gamma}^{-1}_{\mathbf{k}}(\tilde{g})\tilde{\chi}(\mathbf{k})\tilde{\Gamma}_{\mathbf{k}}(\tilde{g}) = \tilde{\chi}(\mathbf{k}). \tag{18}$$

Bertauts standard theory [4] would continue with the reduction of the natural representation, which one might expect to be constituted by the matrices $\tilde{\Gamma}_{\mathbf{k}}$. The only change here, which mainly affects the vocabulary, is that these matrices do not form a representation, because the equality

$$\Gamma(\tilde{g}\tilde{g}') = \Gamma(\tilde{g})\Gamma(\tilde{g}') \tag{19}$$

holds only if $\tilde{g}$ is linear (i.e. it belongs to set (i)). In contrast, if $\tilde{g}$ is antilinear (i.e. it belongs to set (ii)), then

$$\Gamma(\tilde{g}\tilde{g}') = \Gamma(\tilde{g})\Gamma^*(\tilde{g}'). \tag{20}$$

This property is characteristic of a 'corepresentation' [9,10]. The matrices $\tilde{\Gamma}_{\mathbf{k}}$ form the 'natural' corepresentation of $G^{(2)}_{\mathbf{k}}$. Corepresentations can be reduced as representations. Indeed the matrices $\tilde{\Gamma}_{\mathbf{k}}(\tilde{g})$ are ordinary matrices, i.e. linear operators. The task is to find basis vectors which are such that those matrices take the form

$$\tilde{\Gamma}_{\mathbf{k}}(\tilde{g}) = \begin{bmatrix} \tilde{\Gamma}^{(1)}_{\mathbf{k}}(\tilde{g}) & 0 & 0 & \ldots \\ 0 & \tilde{\Gamma}^{(2)}_{\mathbf{k}}(\tilde{g}) & 0 & \ldots \\ 0 & 0 & \tilde{\Gamma}^{(3)}_{\mathbf{k}}(\tilde{g}) & \ldots \\ \ldots & \ldots & \ldots & \ldots \end{bmatrix} \tag{21}$$

Table 4. Irreducible corepresentations of $G^{(2)}_0(\mathbf{k})$.

	h_1	h_{13}	Ch_{25}	Ch_{37}
τ_1	1	1	1	1
τ_2	1	−1	1	−1
τ_3	1	1	−1	−1
τ_4	1	−1	−1	1

where the blocks $\tilde{\Gamma}^{(1)}_{\mathbf{k}}(\tilde{g})$, $\tilde{\Gamma}^{(2)}_{\mathbf{k}}(\tilde{g})$, ... are smaller matrices and constitute irreducible corepresentations of $G^{(2)}_{\mathbf{k}}$. The matrix elements of $\tilde{\chi}(\mathbf{k})$ between basis vectors belonging to different irreducible corepresentations vanish, so that any eigenvector of $\tilde{\chi}(\mathbf{k})$ should combine basis vectors belonging to a single irreducible corepresentation.

The calculation will be explicitly done for $CeAl_2$. In this case, the group $G_{\mathbf{k}}$ is symmorphic. This implies that

$$\Gamma(\{\tilde{h}|\mathbf{T}\}) = \Gamma(\tilde{h})\exp(-i\mathbf{k}.\mathbf{T}) \tag{22}$$

where the 12×12 matrices $\Gamma(\tilde{h}) = \Gamma(\{\tilde{h}|0\})$ form a corepresentation (the 'natural' one) of the abelian group $G^{(2)}_{0,\mathbf{k}}$ formed by the 4 elements $\tilde{h} = h_1,\ h_{13},\ CI = Ch_{25}$ (to use Kovalev's notation) and $Ch_{37} = Ch_{25}h_{13}$. The matrices $\Gamma(\tilde{g})$ are easily obtained from Table 3. The irreducible corepresentations of this group are of dimension 1 and displayed by Table 4. It is of interest to note that if choice A were made (refraining to introduce the conjugation operator C), the situation would be more complicated, because the irreducible representations of the group formed by $(\{h_1|\mathbf{T}\})$, $(\{h_{13}|\mathbf{T}\})$, $(\{h_{25}|\mathbf{T}\})$, $(\{h_{37}|\mathbf{T}\})$ are two-dimensional as seen from textbooks [8,9,13].

In $CeAl_2$, the group $G^{(2)}_{0,\mathbf{k}}$ is abelian. It follows that the 4 matrices $\tilde{\Gamma}(\tilde{h})$ have the same eigenvectors. These eigenvectors can be taken as basis vectors. Since the four operators $\tilde{h}$ of $G^{(2)}_{0,\mathbf{k}}$ have their square $\tilde{h}^2$ equal to the unit matrix, the eigenvalues are equal to 1 or −1. The eigenvectors of h_{13} are given by (5) and (6) but should be rewritten as column matrices of 12 instead of 6 elements. Let the vector $\mathbf{e}_{i\alpha}$ be defined as having all its components equal to 0 except $m_{i\alpha} = 1$. Let $\bar{\mathbf{e}}_{i\alpha}$ be defined as having all its components equal to 0 except $m^*_{i\alpha} = 1$. Then the eigenvectors of h_{13} are the vectors $\mathbf{u}^{\pm}_i$ defined by (5) and (6), and the vectors $\bar{\mathbf{u}}^{\pm}_i$ defined in an obvious, analogous way. It is seen from (5), (6) and Table 3 that Ch_{25} transforms $\mathbf{u}^{\pm}_1$ into $\mp\bar{\mathbf{u}}^{\pm}_2$, $\mathbf{u}^{\pm}_2$ into $\mp\bar{\mathbf{u}}^{\pm}_1$, and $\mathbf{u}^{\pm}_3$ into $\mp\bar{\mathbf{u}}^{\pm}_3$. Common eigenvectors of h_{13} and Ch_{25} are easily deduced and can

be written

$$\mathbf{e}_{1x}(\mathbf{k}) - \epsilon\mathbf{e}_{2y}(\mathbf{k}) + \epsilon'\bar{\mathbf{e}}_{2x}(\mathbf{k}) - \epsilon\epsilon'\bar{\mathbf{e}}_{1y}(\mathbf{k}) \quad (23)$$

$$\mathbf{e}_{1y}(\mathbf{k}) - \epsilon\mathbf{e}_{2x}(\mathbf{k}) + \epsilon'\bar{\mathbf{e}}_{2y}(\mathbf{k}) - \epsilon\epsilon'\bar{\mathbf{e}}_{1x}(\mathbf{k}) \quad (24)$$

$$\mathbf{e}_{1z}(\mathbf{k}) - \epsilon\mathbf{e}_{2z}(\mathbf{k}) + \epsilon'\bar{\mathbf{e}}_{2z}(\mathbf{k}) - \epsilon\epsilon'\bar{\mathbf{e}}_{1z}(\mathbf{k}). \quad (25)$$

These vectors can be taken as basis vectors. It follows that the eigenvectors of the susceptibility matrix have the form

$$\begin{aligned}\mathbf{w} = {} & \lambda[\mathbf{e}_{1x}(\mathbf{k}) - \epsilon\mathbf{e}_{2y}(\mathbf{k}) + \epsilon'\bar{\mathbf{e}}_{2x}(\mathbf{k}) - \epsilon\epsilon'\bar{\mathbf{e}}_{1y}(\mathbf{k})] \\ & + \mu[\mathbf{e}_{1y}(\mathbf{k}) - \epsilon\mathbf{e}_{2x}(\mathbf{k}) + \epsilon'\bar{\mathbf{e}}_{2y}(\mathbf{k}) - \epsilon\epsilon'\bar{\mathbf{e}}_{1x}(\mathbf{k})] \\ & + \nu[\mathbf{e}_{1z}(\mathbf{k}) - \epsilon\mathbf{e}_{2z}(\mathbf{k}) + \epsilon'\bar{\mathbf{e}}_{2z}(\mathbf{k}) - \epsilon\epsilon'\bar{\mathbf{e}}_{1z}(\mathbf{k})]. \quad (26)\end{aligned}$$

This leads to formulae (11) and (12) for the eigenvectors of the susceptibility matrix. The calculation proceeds as in Section 3

5 Conclusion

Since Bertaut's earlier works [4] it has been known that the number of parameters of a magnetic structure can be reduced by using group representations. However, it is often claimed that symmetry operations of the space group which can be exploited are only those which conserve $\mathbf{k}$. Various counter-examples of this statement are known, in which invariance under inversion brings additional information. An example is ferroelectric NiVO [15] Another example is $CeAl_2$, as shown by one of us [11] using antilinear operators and corepresentations. In the present work, it has been shown that the same results may be obtained from usual representation theory with linear operators only.

One can wonder whether it might not be appropriate to introduce operations which rotate $\mathbf{k}$ instead of reversing it. It is not so, and the reason is the following. As long as one does not worry about the reality of the magnetization, one can use the irreducible representations of the group of the $\mathbf{k}$ vector, or the irreducible representations of the group of $\mathbf{k}$ and $-\mathbf{k}$, or the irreducible representations of the full space group. In all cases the number of parameters is the same. This follows from the standard way [13] to construct the irreducible representations of a space group. In the example studied in the present article there are 3 complex parameters in (7) and (8). In (11) and (12), when inversion has been taken into account, the number of parameters is the same! However, when the complex solutions are combined with their complex conjugates to build a real magnetization density, the number of parameters is reduced when using (11) and (12), and *not* reduced when using (7) and (8). This simplification can *not* occur when combining two vectors $\mathbf{k}$ and $\mathbf{k}$' which are not opposite or equal.

The exploitation of inversion implies certain slight difficulties. One of them is the loss of translational invariance in (11) and (12), which results from the necessity to choose the relative position of the symmetry centre and the origin of the coordinates. Another difficulty is the appearance of a discrete degeneracy which replaces the continuous degeneracy corresponding to translation. In view of the tricks which have to be used, it may be appropriate to confirm the group theoretical treatment by a pedestrian diagonalization of the susceptibility matrix, taking all symmetries into account. The case of $CeAl_2$ is sufficiently simple to allow such an approach. We have done this and obtained the same results as by the various group theoretical methods developed in the present paper. Each of these methods has a its advantage.

Coming back to the magnetic structure of $CeAl_2$, described by (15), it turns out to be more complex than up to now believed. Besides the two possible couplings, positive or negative, between the two Ce atoms of the unit cell, a phase difference may exist between the propagation of the x component and the propagation of the z component, and the same phase but with an opposite sign between the y and the z components. The value of this phase is not given by symmetry arguments but is fixed by the exchange integrals and has to be determined experimentally. It was shown by Givord et al. [3] that, when the temperature is lowered below T_N, there is an experimental evidence of an evolution of the magnetic structure, and this evolution was attributed to a variation of the parameter u in (15). This evolution could also be attributed to the apparition and the increase of the phase shift. For the moment the question is not settled and needs more experimental data to disentangle the respective roles of the parameter u and the phase α.

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