

TABULATION OF THE NUMBER OF INDEPENDENT COMPONENTS OF PHYSICAL TENSORS FOR THE MAGNETIC CLASSES*

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ABSTRACT

Following the method of Bhagavantam and Pantulu⁸ the number of independent components of tensors up to 4th rank is derived for the magnetic classes. This method is extended by Lyubarskii¹ to cases of tensors having intrinsic symmetry. The results cover all cases of tensors lacking intrinsic symmetry as well as of tensors having the symmetries of Table II, and are in agreement with previous results.^{5, 8}

1. INTRODUCTION

MANY physical properties of materials are represented by tensors. Because of the symmetries of the material and of the tensor, the number of independent components of the tensor is reduced from the maximum possible. If, in particular, the number of independent components of a tensor reduces to zero, the material does not possess the property represented by this tensor.

The symmetry of a crystal is given by its space group. But since macroscopic properties depend only on the directional symmetry of the crystal,¹ they are determined by the point group of the crystal. For magnetic properties there are 90 classes of directional symmetry represented by the 90 magnetic point groups.²⁻⁴

The problem of tensors in the magnetic classes has already been considered in previous works.⁵⁻⁸ Bhagavantam⁷ investigated several physical properties in the ordinary 32 crystal classes and Bhagavantam and Pantulu⁸

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considered the number of independent components of several physical tensors in the magnetic classes.

In this paper we derive the number of independent components of tensors up to the 4th rank in the various magnetic classes. We follow the method of Bhagavantam and Pantulu⁸ and extended by Lyubarskii¹ to cases of tensors having intrinsic symmetry. By intrinsic symmetry is meant the symmetry resulting from the definition of the tensor, *e.g.*, the symmetry of its indices.

2. DESCRIPTION OF METHOD

The number of independent components of a tensor in a given symmetry group is equal to the number of times the identity representation of the group is contained in the reducible representation according to which the tensor transforms.^{1,8} If n_i denotes how many times an irreducible representation of a group with character χ_i occurs in a representation with character χ then

$$n_i = \frac{1}{N} \sum_{\mathbf{R}} \chi(\mathbf{R}) \chi_i(\mathbf{R}) \quad (1)$$

where N is the order of the group, $\chi(\mathbf{R})$ the character of an element \mathbf{R} in the given representation, $\chi_i(\mathbf{R})$ the character of \mathbf{R} in the irreducible representation and the summation is over all elements of the group. For the identity representation $\chi_i(\mathbf{R}) = 1$ for all \mathbf{R} . Therefore the number of independent components, n , of a tensor in a symmetry group is given by

$$n = \frac{1}{N} \sum_{\mathbf{R}} \chi(\mathbf{R}) \quad (2)$$

where $\chi(\mathbf{R})$ is the character of the element \mathbf{R} in the (reducible) representation according to which the tensor transforms.

Thus, in order to find the number of independent components of a tensor in a given point group it is enough to know the characters of all elements of the group discussed in the reducible representation according to which the tensor transforms.

To find these characters we proceed as follows. We express the representation of the tensor as a combination of representations of the rotation group augmented by time and space reversal which we denote by U . If D_j (integral j) is a representation of weight j and dimensionality $2j + 1$ of the proper rotation group then a (proper) tensor of rank m trans-

forms like D_1^m . D_1 is the so-called vector representation. The augmented rotation group U has four single-valued representations for every integral weight j according to their behaviour with respect to time and space reversal. Let us denote them as follows: D_{jg} —invariant with respect to both time and space reversal. D_{ju} —invariant under time reversal but changes sign under space inversion. \bar{D}_{jg} —invariant under space inversion but changes sign under time reversal. \bar{D}_{ju} —changes sign under both time and space reversal. D_1^m can be calculated according to the multiplication rule

$$D_j \times D_{j'} = \sum_{i=|j-j'|}^{j+j'} D_i \quad (3)$$

The generalised formulae for the representations of U are:

$$\left. \begin{aligned} D_{jg} \times D_{j'g} &= D_{ju} \times D_{j'u} = \bar{D}_{jg} \times \bar{D}_{j'g} = \bar{D}_{ju} \times \bar{D}_{j'u} = \sum_i D_{ig} \\ D_{jg} \times D_{j'u} &= D_{ju} \times D_{j'g} = \bar{D}_{jg} \times \bar{D}_{j'u} = \bar{D}_{ju} \times \bar{D}_{j'g} = \sum_i D_{iu} \\ \bar{D}_{jg} \times D_{j'g} &= D_{jg} \times \bar{D}_{j'g} = \bar{D}_{ju} \times D_{j'u} = D_{ju} \times \bar{D}_{j'u} = \sum_i \bar{D}_{ig} \\ \bar{D}_{jg} \times D_{j'u} &= D_{jg} \times \bar{D}_{j'u} = \bar{D}_{ju} \times D_{j'g} = D_{ju} \times \bar{D}_{j'g} = \sum_i \bar{D}_{iu} \end{aligned} \right\} \quad (4)$$

For tensors up to the 4th rank we find:

$$\left. \begin{aligned} \text{1st rank} & D_1 \\ \text{2nd rank} & D_1^2 = D_2 + D_1 + D_0 \\ \text{3rd rank} & D_1^3 = D_3 + 2D_2 + 3D_1 + D_0 \\ \text{4th rank} & D_1^4 = D_4 + 3D_3 + 6D_2 + 6D_1 + 3D_0 \end{aligned} \right\} \quad (5)$$

On the right side we have to choose the appropriate representations of U according to the nature of the tensor discussed, e.g., $\bar{D}_{1g}^2 = \bar{D}_{2g} + \bar{D}_{1g} + \bar{D}_{0g}$. (5) is valid for tensors with no intrinsic symmetry.

With the help of Eq. (2) we calculated the number of independent components of the four kinds of representations of U (also called spinors) up to the 4th weight in all magnetic point groups. We used the expression

$$\chi_j(C_\psi) = 1 + 2 \cos \psi + \dots + 2 \cos j\psi = \frac{\sin [(2j+1)\psi/2]}{\sin \psi/2} \quad (6)$$

for the character of D_j for a proper rotation C_ψ through an angle ψ and the corresponding expressions for the representations of U . The results are summarised in Table I.

TABLE I

System	Magnetic point group	D_{00}	D_{10}	D_{20}	D_{30}	D_{40}	D_{0u}	D_{1u}	D_{2u}	D_{3u}	D_{4u}	\bar{D}_{00}	\bar{D}_{10}	\bar{D}_{20}	\bar{D}_{30}	\bar{D}_{40}	\bar{D}_{0u}	\bar{D}_{1u}	\bar{D}_{2u}	\bar{D}_{3u}	\bar{D}_{4u}	
Triclinic	1	1	3	5	7	9	1	3	5	7	9	1	3	5	7	9	1	3	5	7	9	
	$\bar{1}$	1	3	5	7	9	0	0	0	0	0	1	3	5	7	9	0	0	0	0	0	
	$\bar{1}$	1	3	5	7	9	0	0	0	0	0	0	0	0	0	0	1	3	5	7	9	
Monoclinic	2	1	1	3	3	5	1	1	3	3	5	1	1	3	3	5	1	1	3	3	5	
	$\underline{2}$	1	1	3	3	5	1	1	3	3	5	0	2	2	4	4	0	2	2	4	4	
	m	1	1	3	3	5	0	2	2	4	4	1	1	3	3	5	0	2	2	4	4	
	\underline{m}	1	1	3	3	5	0	2	2	4	4	0	2	2	4	4	1	1	3	3	5	
	2/m	1	1	3	3	5	0	0	0	0	0	1	1	3	3	5	0	0	0	0	0	
	$\underline{2/m}$	1	1	3	3	5	0	0	0	0	0	0	2	2	4	4	0	0	0	0	0	
	$\underline{2/m}$	1	1	3	3	5	0	0	0	0	0	0	0	0	0	0	1	1	3	3	5	
	$\underline{2/m}$	1	1	3	3	5	0	0	0	0	0	0	0	0	0	0	0	2	2	4	4	
Orthorhombic	222	1	0	2	1	3	1	0	2	1	3	1	0	2	1	3	1	0	2	1	3	
	$\underline{222}$	1	0	2	1	3	1	0	2	1	3	0	1	1	2	2	0	1	1	2	2	
	mm2	1	0	2	1	3	0	1	1	2	2	1	0	2	1	3	0	1	1	2	2	
	$\underline{mm2}$	1	0	2	1	3	0	1	1	2	2	0	1	1	2	2	1	0	2	1	3	
	$\underline{mm2}$	1	0	2	1	3	0	1	1	2	2	0	1	1	2	2	0	1	1	2	2	
	mmm	1	0	2	1	3	0	0	0	0	0	1	0	2	1	3	0	0	0	0	0	
	\underline{mmm}	1	0	2	1	3	0	0	0	0	0	0	1	1	2	2	0	0	0	0		
	\underline{mmm}	1	0	2	1	3	0	0	0	0	0	0	0	0	0	0	0	1	0	2	1	3
	\underline{mmm}	1	0	2	1	3	0	0	0	0	0	0	0	0	0	0	0	0	1	1	2	2
Tetragonal	4	1	1	1	1	3	1	1	1	1	3	1	1	1	1	3	1	1	1	1	3	
	$\underline{4}$	1	1	1	1	3	1	1	1	1	3	0	0	2	2	2	0	0	2	2	2	
	$\bar{4}$	1	1	1	1	3	0	0	2	2	2	1	1	1	1	3	0	0	2	2	2	
	$\bar{4}$	1	1	1	1	3	0	0	2	2	2	0	0	2	2	2	1	1	1	1	3	
	4/m	1	1	1	1	3	0	0	0	0	0	1	1	1	1	3	0	0	0	0	0	
	$\underline{4/m}$	1	1	1	1	3	0	0	0	0	0	0	0	2	2	2	0	0	0	0	0	
	$\underline{4/m}$	1	1	1	1	3	0	0	0	0	0	0	0	0	0	0	1	1	1	1	3	
	$\underline{4/m}$	1	1	1	1	3	0	0	0	0	0	0	0	0	0	0	0	0	0	2	2	2
	422	1	0	1	0	2	1	0	1	0	2	1	0	1	0	2	1	0	1	0	2	
	$\underline{422}$	1	0	1	0	2	1	0	1	0	2	0	0	1	1	1	0	0	1	1	1	

TABLE I (Contd.)

System	Magnetic point group	D_{0g}	D_{1g}	D_{2g}	D_{3g}	D_{4g}	D_{0u}	D_{1u}	D_{2u}	D_{3u}	D_{4u}	\bar{D}_{0g}	\bar{D}_{1g}	\bar{D}_{2g}	\bar{D}_{3g}	\bar{D}_{4g}	\bar{D}_{0u}	\bar{D}_{1u}	\bar{D}_{2u}	\bar{D}_{3u}	\bar{D}_{4u}	
Tetragonal	$\underline{422}$	1	0	1	0	2	1	0	1	0	2	0	1	0	1	1	0	1	0	1	1	
	$\underline{4mm}$	1	0	1	0	2	0	1	0	1	1	1	0	1	0	2	0	1	0	1	1	
	$\underline{4mm}$	1	0	1	0	2	0	1	0	1	1	0	0	1	1	1	0	0	1	1		
	$\underline{4mm}$	1	0	1	0	2	0	1	0	1	1	0	1	0	1	1	1	0	1	0	1	
	$\underline{42m}$	1	0	1	0	2	0	0	1	1	1	1	0	1	0	2	0	0	1	1	2	
	$\underline{42m}$	1	0	1	0	2	0	0	1	1	1	0	0	1	1	1	1	0	1	0	2	
	$\underline{42m}$	1	0	1	0	2	0	0	1	1	1	0	0	1	1	1	0	1	0	1	1	
	$\underline{42m}$	1	0	1	0	2	0	0	1	1	1	0	1	0	1	1	0	0	1	1	1	
	$\underline{4/mmm}$	1	0	1	0	2	0	0	0	0	0	0	1	0	1	0	2	0	0	0	0	
	$\underline{4/mmm}$	1	0	1	0	2	0	0	0	0	0	0	0	1	1	1	0	0	0	0	0	
	$\underline{4/mmm}$	1	0	1	0	2	0	0	0	0	0	0	1	0	1	1	0	0	0	0	0	
	$\underline{4/mmm}$	1	0	1	0	2	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	2
	$\underline{4/mmm}$	1	0	1	0	2	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	1
	Trigonal	$\underline{3}$	1	1	1	3	3	1	1	1	3	3	1	1	1	3	3	1	1	1	3	3
$\bar{3}$		1	1	1	3	3	0	0	0	0	0	1	1	1	3	3	0	0	0	0	0	
$\bar{3}$		1	1	1	3	3	0	0	0	0	0	0	0	0	0	0	1	1	1	3	3	
$\underline{32}$		1	0	1	1	2	1	0	1	1	2	1	0	1	1	2	1	0	1	1	2	
$\underline{32}$		1	0	1	1	2	1	0	1	1	2	0	1	0	2	1	0	1	0	2	1	
$\underline{3m}$		1	0	1	1	2	0	1	0	2	1	1	0	1	1	2	0	1	0	2	1	
$\underline{3m}$		1	0	1	1	2	0	1	0	2	1	0	1	0	2	1	1	0	1	1	2	
$\bar{3}m$		1	0	1	1	2	0	0	0	0	0	1	0	1	1	2	0	0	0	0	0	
$\bar{3}m$		1	0	1	1	2	0	0	0	0	0	0	1	0	2	1	0	0	0	0	0	
$\bar{3}m$		1	0	1	1	2	0	0	0	0	0	0	0	0	0	0	0	1	0	1	1	2
$\bar{3}m$		1	0	1	1	2	0	0	0	0	0	0	0	0	0	0	0	0	1	0	2	1
Hexagonal		$\underline{6}$	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	$\underline{6}$	1	1	1	1	1	1	1	1	1	1	0	0	2	2	0	0	0	2	2		
	$\bar{6}$	1	1	1	1	1	0	0	0	2	2	1	1	1	1	1	0	0	0	2	2	
	$\bar{6}$	1	1	1	1	1	0	0	0	2	2	0	0	0	2	2	1	1	1	1	1	
	$\underline{6/m}$	1	1	1	1	1	0	0	0	0	0	1	1	1	1	1	0	0	0	0	0	

Using (5) it is possible to find the number of independent components of tensors with no intrinsic symmetry. Whether or not the tensor discussed is invariant under inversion or time reversal, that is which kind of representations of U we have to consider, is found from direct inspection of the tensor.

In cases of tensors with intrinsic symmetry we use the formula for the character given by Lyubarskii,¹ namely:

$$\chi^\circ(g) = \frac{1}{N_P} \sum_{p \in P} \chi(g^{l_1}) \cdots \chi(g^{l_f}) \quad (7)$$

In this formula P is the permutation group of the tensor indices, N_P its order; f the number of cycles in the permutation p ; $l_1 \cdots l_f$ the lengths of the cycles and $\chi(g)$ is the character of the symmetry element g in the vector representation of the symmetry group of the crystal (*i.e.*, transforms like D_1). Summation is over all permutations. Once $\chi^\circ(g)$ is known for all elements g of the point group of the crystal it is possible to find the number of independent components of the tensor according to a formula similar to (2) namely:

$$n = \frac{1}{N} \sum_g \chi^\circ(g) \quad (8)$$

Instead, we express $\chi^\circ(g)$ in (7) for a proper rotation C_ψ as a combination of the $\chi_j(C_\psi)$'s in (6). In other words, we express the representation with character $\chi^\circ(g)$ according to which the tensor with intrinsic symmetry transforms as a combination of the D_j 's. So, again we may use Table 1 to get the number of independent components. The appropriate combinations of the D_j 's thus found for several cases of intrinsic symmetry are summarised in Table II.

3. RESULTS AND USE OF TABLES

As already stated, Table I gives the number of independent components of the four kinds of representations of the augmented (by time and space reversal) rotation group U , up to weight 4 in the magnetic classes. It contains only the 90 classes with magnetic structure. For the 32 non-magnetic classes, in which time reversal is a symmetry element of the magnetic point group, one of the following two cases may occur. For tensors invariant with respect to time reversal the results are the same as for the corresponding crystallographic point group. For tensors which change sign under time reversal all the components are identically zero.

TABLE II

No.	Rank of tensor	Type of intrinsic symmetry	Combination of D_j 's
1	2	No symmetry	$D_1^2 = D_2 + D_1 + D_0$
2		Symmetric $ij = ji$	$D_1^2 = D_2 + D_0$
3		Antisymmetric $ij = -ji$	$D_1^2 = D_1$
4	3	No symmetry	$D_1^3 = D_3 + 2D_2 + 3D_1 + D_0$
5		$ijk = ikj$ or $ijk = jik$	$D_1^3 = D_3 + D_2 + 2D_1$ $D_1^3 = D_3 + D_2 + 2D_1$
6		Full symmetry $ijk = ikj = jik$	$D_1^3 = D_3 + D_1$
7		$ijk = -jik$ or $ijk = -ikj$	$D_1^3 = D_2 + D_1 + D_0$
8		$\gamma_{ijk} = \gamma_{jik}$ $\Sigma \gamma_{ijk} = 0$ the antisymmetric tensor	$D_1^3 = D_2 + D_1$
9		$\gamma_{rj} = 0$ $j \neq r \neq 1$ $\gamma_{jrl} = \gamma_{ljr} = \gamma_{rlj} =$ $= -\gamma_{rjl} = -\gamma_{ljr} = -\gamma_{rlj}$	$D_1^3 = D_2 + D_1 + D_0$
10	4	No symmetry	$D_1^4 = D_4 + 3D_3 + 6D_2 + 6D_1 + 3D_0$
11		Full symmetry	$D_1^4 = D_4 + D_2 + D_0$
12		$ijkl = jikl = ijlk = klij$	$D_1^4 = D_4 + 2D_2 + 2D_0$
13		$ijkl = jikl = ijlk = jilk$	$D_1^4 = D_4 + D_3 + 3D_2 + D_1 + 2D_0$

In Table II are given the appropriate combination of the D_j 's for tensors with several types of intrinsic symmetry.

The tables are used as follows. According to the behaviour of the discussed tensor under time and space reversal, that is found by direct inspection, one may know which kind of D_j (e.g., D_{jg} , \bar{D}_{ju} , etc.) in Table I to use.

If the tensor has no intrinsic symmetry the number of independent components is found according to (5). If the tensor has one of the symmetries given in Table II, we find from this table how to add the D_j 's of Table I. If the tensor symmetry does not appear in Table II, the appropriate combination of the D_j 's may be found by the method described in the text.

As an example we consider the 3rd order tensor generated by the coefficients C_{ijk} of the third order terms in the expansion of the thermodynamic potential of a material in powers of a magnetic field. The general expansion is:

$$\phi = \text{const.} + \sigma_i H_i + \frac{1}{2} \chi_{ij} H_i H_j + \frac{1}{6} C_{ijk} H_i H_j H_k + \dots \quad (9)$$

where $i, j, k = x, y, z$ and summation is performed over repeated indices. σ_i and χ_{ij} are generally interpreted as the components of the spontaneous magnetic moment and the susceptibility tensor respectively. The tensor C_{ijk}^{9-11} causes a non-linear dependence of the magnetization on the magnetic field. The term $H_i H_j H_k$ is invariant under space inversion but changes sign under time reversal (a magnetic field is an axial vector and is reversed under time reversal). As each term in the expansion of the thermodynamic potential must be invariant under both space and time reversal the coefficients C_{ijk} are also invariant under space inversion but change sign under time reversal. We may conclude therefore that the third order tensor C_{ijk} is invariant under space inversion but changes sign under time reversal, and that in Table I we have to take the \bar{D}_{jg} 's. Further it is obvious that this tensor is symmetric in all three indices and according to Table II the desired combination is $\bar{D}_{3g} \diamond \bar{D}_{1g}$.

One may also derive the same information by considering the magnetization M_i in the i direction contributed by the third order terms, namely $M_i = \frac{1}{6} C_{ijk} H_j H_k$. As $H_j H_k$ is invariant under both space and time reversal C_{ijk} must behave under these operations like M_i .[†]

This example and other physical property tensors investigated similarly are summarised in Table III. This table gives the intrinsic symmetry of the tensor and its behavior under time and space reversal. + denotes invariance and - denotes changing of sign under the operation mentioned at the top of the column. The numbers cited in the column of intrinsic symmetry refer to Table II.

[†] For the validity of such arguments and Neuman's principle in case of dynamic properties see Refs. 6 and 12.

TABLE III

Property	Rank of tensor	Behavior under space inversion	Behavior under time inversion	Intrinsic symmetry
Ferromagnetism	.. 1	+	-	none
Ferroelectricity	.. 1	-	+	none
Pyromagnetism	.. 1	+	-	none
Pyroelectricity	1	-	+	none
Magnetic Susceptibility	.. 2	+	+	2
Electric Susceptibility	.. 2	+	+	2
Magnetoelectric Effect	.. 2	-	-	none
Piezomagnetism	.. 3	+	-	5
C_{ijk} (see Sec. 3)	.. 3	+	-	6
Elasticity Tensor	... 4	+	+	12

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