Pramāṇa – J. Phys., Vol. 26, No. 4, April 1986, pp. 355–360. © Printed in India.

Magnetic symmetry and transport properties in crystals

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MS received 3 June 1985; revised 13 December 1985

Abstract. The number of non-vanishing independent tensor components in respect of the known transport properties for the magnetic variants of the crystallographic point groups are obtained by adopting a different procedure. This method fulfils the orthogonality conditions of group theory.

Keywords. Transport property; magnetic variant; alternating representation.

PACS No. 61·50; 02·20

1. Introduction

The effects of magnetic field on the electrical and thermoelectric properties in the absence of a temperature gradient are known as galvanomagnetic effects. Examples are the Hall effect, the magneto-resistance effect, the Ettingshausen effect and their related higher order effects. The effects of magnetic field on the thermoelectric and thermal properties in the absence of an electric current are called thermomagnetic effects. Examples are Nernst effect, the magnetothermoelectric power, the Leduc-Righi effect and the magnetothermal conductivity and their related higher order effects. Studies on these effects have gained importance in semiconductor physics and are therefore of interest.

Bhagavantam and Pantulu (1964) used the character method (Bhagavantam and Suryanarayana 1949) to obtain the number of non-vanishing independent constants needed by each one of the 32 crystal classes for the known galvanomagnetic, thermomagnetic and piezo-galvanomagnetic effects. Identical results in respect of the various physical properties have been obtained by Krishnamurty and Gopalakrishnamurti (1968) employing the method of Jahn (1949) for reduction of a representation.

In recent years some debate is going on regarding the symmetry restricted forms of the transport property tensors for magnetic crystals. Birss (1963, 1964—prescription A) assumed the validity of Onsager reciprocity relations regarding the transport properties in crystals, which possess time inversion as a symmetry operation. Kleiner (1966, 1967, 1969—prescription B) generalized the classical Onsager relations, which hold good in the presence of or in the absence of an external magnetic field for the magnetic as well as non-magnetic crystal classes. These generalized Onsager relations have been employed by Pantulu and Radhakrishna (1969) for deriving the non-vanishing independent constants required for the description of the galvanomagnetic and thermomagnetic effects in the 122 crystal classes. Cracknell (1973—prescription C) discussed the symmetry-restricted transport coefficients of magnetic crystals both from the macroscopic and the microscopic points of view. While prescription A ignores the antiunitary symmetry operations, the use of these operations is included in both prescriptions B and C. However prescriptions A, B and C often lead to different results. Pourghazi *et al* (1976), while accepting Cracknell's objections to the arguments of both Birss and Kleiner, modified and gave a new prescription (D) which did not consider any specific transport property but gave three general outlines to enumerate the transport coefficients.

Krishnamurty and Gopalakrishnamurti (1969) showed that the method of computing the number of independent constants required to describe a magnetic property for a magnetic variant G' of a point group G is the same as determining that number against that alternating representation (AR) of G, which induces the magnetic variant G'. Krishnamurty and Appalanarasimham (1970) established that the above method can be used to find the number of independent constants required to describe a physical property in respect of the 58 magnetic groups which are induced by the distinct ARs of the 32-point groups.

2. Hall effect tensor

In the present paper, the method of Krishnamurty and Appalanarasimham (1970) is applied to transport properties. Our prescription E relates to the method of computing the number of non-vanishing independent constants and the symmetry restricted tensor describing a transport property in respect of a magnetic point group G'. This number is the same as that number in respect of the transport property determined against that AR (of the point group G) which induces the magnetic variant G'. As an illustration the symmetry restricted Hall effect tensor for $62'2'$ is obtained in the following manner.

The symmetry-restricted Hall effect tensor whose character is $4c^2 \pm 4c + 1$ (where $c = \cos\phi$ and the upper and lower signs refer respectively to proper rotation and improper rotation (table VII(b) of Bhagavantam 1966)) for the single colour group 622 whose generators are

$$C_6 = \begin{bmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad C_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

is calculated using equation (6) of Pantulu and Radhakrishna (1969) and is found to be

$$\begin{bmatrix} \rho_{xx} & 0 & 0 \\ 0 & \rho_{yy} & 0 \\ 0 & 0 & \rho_{zz} \end{bmatrix}.$$

The AR A_2 (Herzberg 1945) of 622 induces the magnetic group $62'2'$ (Krishnamurty and Gopalakrishnamurti 1969). According to our prescription E the symmetry-restricted Hall effect tensor for the magnetic group $62'2'$ is the same as the one determined against the AR A_2 (of 622) which induces the magnetic group $62'2'$. The symmetry restricted

Hall effect tensor for 62′2′, calculated by this new method, is found to be

$$\begin{bmatrix} 0 & \rho_{xy} & 0 \\ -\rho_{xy} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

Thus, the symmetry-restricted Hall effect tensor has one independent component for 62′2′ and this is in agreement with table 3 which is constructed using the character method. Further this agrees with the extraordinary Hall effect in ferromagnetic metals like Co whose Laue group is 62′2′ (Kleiner 1969). It may also be noted that the tensor components representing the Hall effect for the single colour group 622 and the double colour group 62′2′ are orthogonal. Following this new approach (prescription E), the number of independent constants required to describe the 10 transport properties for the 58 magnetic groups are calculated in the present paper.

3. Prescription E: illustration

The transport properties and their characters are taken from table VII(b) of Bhagavantam (1966). The number of constants appearing against the distinct ARs of the 32-point groups in respect of these transport properties is obtained using the well-known formula:

$$n_i = \frac{1}{N} \sum h_{\hat{\rho}} \chi'_{\rho}(R) \chi_i(R), \tag{1}$$

where $h_{\hat{\rho}}$ is the number of elements in the ρth conjugate class, $\chi'_{\rho}(R)$ is the character of the symmetry operation R, belonging to the ρth conjugate class, in respect of the transport property and $\chi_i(R)$ is the character of the operation R in the ith irreducible representation (IR) of G. That these distinct ARs of the 32-point groups induce the 58 magnetic groups is already known (Krishnamurty and Gopalakrishnamurti 1969). Now let us consider, for example, the magnetic variant m' of the point group m and the transport property 1 (table VII(b) of Bhagavantam 1966), *viz* electrical resistivity and thermal conductivity whose character is $4c^2 \pm 2c$. The character table of m is given in table 1. It is seen that $\chi'(R) = 4c^2 \pm 2c$ is the character of the element R for the electrical resistivity and thermal conductivity, $\chi'_1(E) = 6$, $\chi'_2(\sigma_h) = 2$. Using this $\chi'(R)$ in (1) we get n_i against A' and A'' as shown in table 1. The number of constants required to describe the property 1 appearing against the AR A'' of m is 2. We know from Krishnamurty and Gopalakrishnamurti (1969) that the AR A'' of the point group m

Table 1. Character table of m.

m	E	σ_h	n_i
A'	1	1	4
A''	1	−1	2
$\chi'(R) = 4c^2 \pm 2c$	6	2	

Table 2. Character table of the point group $2/m$.

$2/m$	E	C_2	i	σ_h	n_i
A_g	1	1	1	1	4
A_u	1	1	−1	−1	—
B_g	1	−1	1	−1	2
B_u	1	−1	−1	1	—
$\chi'(R) = 4c^2 \pm 2c$	6	2	6	2	

induces the magnetic variant m' of m. Thus, the number of constants required to describe property 1 of table VII(b) of Bhagavantam (1966) for the magnetic variant m' is 2.

The AR of the point group 2 induces the magnetic variant $2'$ and the property 1 requires 2 constants for the magnetic variant $2'$ which can be easily seen from the character table of the point group 2.

Now let us consider another point group $2/m$ whose character table is given in table 2. The AR B_g of $2/m$ induces the magnetic variant $2'/m'$ and hence property 1 of table VII(b) of Bhagavantam (1966) requires 2 constants for the magnetic variant $2'/m'$. The AR'S A_u and B_u induce the magnetic variants $2/m'$ and $2'/m$ respectively and it is seen from the above table that the property 1 requires no constants for these magnetic variants. The reason for this is that the character of i in these two AR'S is -1 and $\chi'(E) = \chi'(i)$.

Thus each of these three magnetic groups m', $2'$ and $2'/m'$ require 2 constants for this property 1. Similarly proceeding with the other nine properties of table VII(b) of Bhagavantam (1966), we find that these three magnetic groups require 4 constants to describe the transport property 2 of table VII(b) of Bhagavantam (1966). Following this procedure (prescription E), the numbers of independent constants required to describe these studied transport properties for the 58 magnetic groups are obtained (table 3).

4. Results and discussion

It may be observed that, using the character formulae given in table VII(b) of Bhagavantam (1966),

$$\chi'(E) = \chi'(i), \qquad \chi'(C_2) = \chi'(\sigma),$$
$$\chi'(C_3) = \chi'(S_6) = 0, \quad \chi'(C_4) = \chi'(S_4), \quad \chi'(C_6) = \chi'(S_3)$$

hold good for each of the 10 transport properties (table VII(b) of Bhagavantam 1966) as they are centro-symmetric. As a consequence of the fact $\chi'(E) = \chi'(i)$, the 21 ARs of the 32-point groups, in each of which the centre of inversion is represented by character -1, do not require any constants to describe these 10 transport properties. This, in turn, implies that the 10 transport properties do not require any constants for the 21 magnetic variants induced by these 21 ARs. The remaining 37 magnetic variants can be

Table 3. Number of transport coefficients in the double-coloured crystal classes.

Class symbol	Laue group	Transport properties* 1	2	3	4	5	6	7	8	9	10
$m', 2', 2'/m'$	$2'$	2	4	14	16	26	14	42	46	66	104
$2m'm', 2'mm', 2'2'2, m'm'm$	$2'2'2$	1	2	7	8	13	7	21	23	33	52
$4', \bar{4}', 4'/m$	$4'$	2	2	6	10	14	8	24	22	34	56
$4m'm', \bar{4}2'm', 42'2', 4/mm'm'$	$42'2'$	—	1	4	3	6	3	9	12	16	24
$4'mm', \bar{4}'2'm, \bar{4}'2m', 4'22', 4'/mmm'$	$4'22'$	1	1	3	5	7	4	12	11	17	28
$3m', 32', \bar{3}m'$	$32'$	—	1	5	4	8	4	12	16	21	32
$\bar{6}', 6', 6'/m'$	$6'$	—	—	2	4	6	4	14	14	22	32
$\bar{6}2'm', 6m'm', 62'2', 6/mm'm'$	$62'2'$	—	1	4	2	5	2	5	9	10	16
$\bar{6}'2m', \bar{6}'2'm, 6'm'm, 6'22', 6'/m'mm'$	$6'22'$	—	—	1	2	3	2	7	7	11	16
$\bar{4}'3m', 4'32', m3m'$	$4'32'$	—	—	1	1	2	1	3	4	5	8

*1 stands for physical properties such as electrical resistivity, thermal conductivity, 2 stands for Hall effect, Leduc–Righi effect and so on (see table VII(b) of Bhagavantam 1966).

Table 4. Number of independent constants required to describe the electrical conductivity or first order Hall effect for various magnetic point groups.

Magnetic point groups	Prescription A	Prescription B	Prescription C	Prescription E
$2', m', 2'/m'$	$2(2'), 4(m'), 0(2'/m')$	6	5	4
$2m'm', 2'mm', 2'2'2, m'm'm$	$3(2m'm'), 1(2'mm'), 1(2'2'2), 0(m'm'm)$	4	3	2
$4', \bar{4}', 4'/m$	$2(4'), 3(\bar{4}'), 0(4'/m)$	2	2	2
$4m'm', \bar{4}2'm', 42'2', 4/mm'm'$	$2(4m'm'), 1(\bar{4}2'm'), 1(42'2'), 0(4/mm'm')$	3	2	1
$4'mm', \bar{4}'2'm, \bar{4}'2m', 4'22', 4'/mmm'$	$1(4'mm'), 1(\bar{4}'2'm), 2(\bar{4}'2m'), 0(4'22'), 0(4'/mmm')$	2	2	1
$3m', 32', \bar{3}m'$	$2(3m'), 1(32'), 0(\bar{3}m')$	3	2	1
$6', 6'/m', \bar{6}'$	$0(6'), 0(6'/m'), 3(\bar{6}')$	2	2	0
$\bar{6}2'm', 6m'm', 62'2', 6/mm'm'$	$0(\bar{6}2'm'), 2(6m'm'), 1(62'2'), 0(6/mm'm')$	3	2	1
$\bar{6}'2m', \bar{6}'2'm, 6'm'm, 6'22', 6'/m'mm'$	$2(\bar{6}'2m'), 1(\bar{6}'2'm), 0(6'm'm), 0(6'22'), 0(6'/m'mm')$	2	2	0
$\bar{4}'3m', 4'32', m3m'$	$1(\bar{4}'3m'), 0(4'32'), 0(m3m')$	1	1	0

grouped into 10 sets as far as the number of constants required to describe these transport properties is concerned and these are tabulated in table 3. Incidentally these 10 classes coincide with the ten sets of the magnetic point groups associated with the 10 Laue groups under category C of Kleiner (1966).

We find from table 6 of Birss (1963), table VI of Kleiner (1966) and table 1 of Cracknell (1973) that symmetry-restricted matrices representing electrical conductivity or first order Hall effect have different forms in certain magnetic point groups. To have a comparative view about these four prescriptions, some of the results from table 6 of Birss (1963), table VI of Kleiner (1966), table 1 of Cracknell (1973) and table 3 of our prescription *E* are given in table 4 of this paper. A perusal of this table shows that these prescriptions yield different results in most cases. But for a majority of the magnetic point groups, prescriptions A and E agree with each other. In enumerating the number of independent constants for any transport property, the earlier prescriptions consider one or more of the following: (1) Onsager relations (2) modified Onsager relations and (3) antiunitary symmetry operations. Our prescription E solely depends upon the representation theory of groups and the well-known formula (1) of §3. In this prescription E, the number of constants required to describe a transport property in respect of a magnetic point group G' is the same as that number in respect of the transport property determined against that AR (of the point group G) which induces the magnetic variant G'. Perhaps this may be the reason why our results disagree with those of the earlier prescriptions. As suggested by Cracknell (1973), perhaps, it should be possible to distinguish experimentally between these various prescriptions, for example, by taking up studies of the extraordinary Hall effect.

Acknowledgements

The author thanks Prof. T S G Krishnamurty and Prof. L S R K Prasad for their interest and suggestions.

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