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**FIELD DEPENDENT TENSORS IN**

**SOLID STATE PHYSICS**

**by**

**AZAM POURGHAZI, M.Sc.**

**Graduate Society**

**A thesis submitted to the University of Durham**

**in candidature for the degree of**

**Doctor of Philosophy**

**August 1977**

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*To my parents*

## ABSTRACT

The concept of field-dependent tensors (tensors the components of which depend on the direction of an applied field) is generalized to define quantities which have different tensorial character in different subspaces (field subspace and geometrical or physical subspace) of the whole space. The transformation laws for these field-dependent tensors are worked out and the weighted and relative field dependent tensors are defined.

The calculus of field dependent tensors is established through which the operations of addition, subtraction, inner and outer multiplication, contraction and differentiation of field dependent tensors are defined and the conditions under which each operation can be performed are discussed, and the quotient law for field dependent tensors is also worked out.

The effect of magnetic crystal symmetry on the forms of field-dependent tensors is considered and a generalized Neumann's principle is defined. Furthermore, it is proved that in working out the magnetic point group of symmetry operations, identification of the magnetic moment inversion operator with the time-inversion operator is not correct.

The effect of the symmetry operations of the magnetic point groups on the field dependent tensors representing the transport properties of a magnetic crystal is considered. Different prescriptions (A, B and C) given by different workers for finding the magnetic symmetry restricted forms of the magnetoconductivity tensor  $\sigma_{ij}(\vec{B})$  are discussed, the objections to each prescription are pointed out and then a new prescription (D) is given. Following prescription D, the restriction on

the forms of the magnetoconductivity tensor  $\sigma_{ij}(\vec{H})$ , the magnetoresistivity tensor  $\rho_{ij}(\vec{H})$ , the magnetothermoelectric power  $\alpha_{ij}(\vec{H})$ , the magnetothermal conductivity  $K_{ij}(\vec{H})$  and the magneto-Peltier effect  $\pi_{ij}(\vec{H})$ , imposed by the symmetry of crystals belonging to each magnetic point group are found.

Finally the way in which the permittivity of a crystal belonging to a magnetic point group can be represented by a field dependent tensor is discussed.

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CHAPTER 1

GENERAL INTRODUCTION

1.1 Tensors

Most physical properties of crystals, which are defined by relations between two or more measurable quantities associated with the crystals, can be represented by mathematical entities called tensors. Tensors are defined by their transformation laws from one set of coordinate axis to another, and are classified by their rank. Scalars and vectors are tensors of zero and first rank respectively. A physical property which inter-relates two vectors is a second rank tensor. As an example of this, the conductivity,  $\sigma_{ij}$ , of a crystal may be considered where

$$\begin{aligned} J_1 &= \sigma_{11} E_1 + \sigma_{12} E_2 + \sigma_{13} E_3 \\ J_2 &= \sigma_{21} E_1 + \sigma_{22} E_2 + \sigma_{23} E_3 \\ J_3 &= \sigma_{31} E_1 + \sigma_{32} E_2 + \sigma_{33} E_3 \end{aligned} \tag{1.1}$$

There are tensors of higher rank also. A tensor of rank  $h$  has  $(n)^h$  components in an  $n$  dimensional space. Crystal symmetry dictates some relations between the components of a tensor representing a property of the crystal and therefore reduces the number of its independent components. The detailed simplification which can be made in the forms of tensor properties are considered, for example, in the book by Nye (1972), for tensors of various ranks and for all the 32 crystallographic point groups.

There are a number of physical properties of crystals which are best described by tensors, the components of which are themselves functions of an applied field. The magnetoconductivity tensor  $\sigma_{ij}(\vec{H})$ , the magnetothermoelectric power  $\alpha_{ij}(\vec{H})$  and the magnetothermal conductivity  $K_{ij}(\vec{H})$



of a magnetic crystal are examples of this kind of tensor. The components of all these tensors depend on the magnetic field. Grabner and Swanson (1962) have called these tensors "field-dependent tensors" and have worked out their transformation law under a spatial transformation operation. They have stated that a symmetry operation acts on both the (field-dependent) tensor and its arguments. Failure to recognise this has led some earlier workers (Birss 1963, 1966 and Cracknell 1973) to incorrect simplification of certain tensors. Akgöz and Saunders (1975 a,b) have shown how to use the transformation law of field dependent tensors in conjunction with Onsager's relations (intrinsic symmetry) to establish the form of the magnetoconductivity tensor  $\sigma_{ij}(\vec{H})$  and the magnetothermoelectric power  $\alpha_{ij}(\vec{H})$  for each of the 32 classical point groups G. Although Akgöz and Saunders have recognised the need to use the transformation law of field dependent tensors, a detailed mathematical substructure to their work has up until now been missing. One major objective of this thesis has been to develop the mathematics of field dependent tensors on a formal basis. Thus in part the work is devoted to giving a general definition of field dependent tensors and to establish their transformation laws under any transformation operation either in the geometrical subspace or in the field subspace (Chapter 3). Furthermore, the calculus of field dependent tensors is worked out (Chapter 4). This investigation has put the studies of Akgöz and Saunders on a firmer foundation.

## 1.2 Generalized symmetry and field dependent tensors

By introducing the concept of antisymmetry, Shubnikov (see for example Shubnikov and Belov 1964) added a new dimension to the study of symmetry of the geometrical objects. He employed an antisymmetry operation in addition to the spatial symmetry operations to develop what are now

known as the type I, II and III Heesch-Shubnikov groups. By identification of the magnetic moment inversion operation with this antisymmetry operation it has proved possible to put the structure and properties of magnetic materials on a group theoretical basis (see Mackay 1957, Donnay et al 1958 and Cracknell 1969). Furthermore, since the operation of time inversion has the effect of reversing the direction of the magnetic moment, it has become a common practice to identify the time inversion operator with the magnetic moment inversion operator (see, for example, Opechowski and Guccione 1965, Tavger and Zaitsev 1956, Birss 1966, Kleiner 1966, 1967 and 1969, and Cracknell 1973). In this thesis it is shown that this identification is not always correct. Furthermore there are a number of magnetic structures that cannot adequately be described by using the magnetic moment inversion operation (or time inversion operation). To describe these structures it is necessary to adopt other operations (rotations) on the magnetic moment (or spin) of the atoms as well (see Brinkman and Elliott 1966 a,b and Litvin 1973). This leads to what is called the generalized symmetry (see Cracknell 1975).

Some workers (Birss 1966, Kleiner 1966, 1967, 1969 and Cracknell 1973) have tried to find the restrictions imposed on the form of magnetic field-dependent transport tensors by the simple magnetic symmetry where only the operation of inversion on the magnetic moment is involved. But due to lack of a transformation law for field-dependent tensors under the transformation operations of the field subspace and also because of the incorrect identification of the magnetic moment inversion operation with time inversion operation, the results are neither correct nor consistent with each other. Akgöz and Saunders (1975 a,b) have found the restrictions on the forms of magnetoconductivity and other transport properties imposed by spatial symmetry operations. Now this has been extended here

to find the restrictions imposed by the magnetic symmetry operations (without identifying the magnetic moment inversion operator with the time-inversion operator) using the transformation law for field-dependent tensors (see Section 6.3.4).

### 1.3 Some remarks on the nomenclature

The terms field-dependent tensor, field-independent tensor, constant tensor and tensor field are used frequently in the text. Thus a thorough definition of them may be found useful. A constant tensor is a tensor, the components of which have the same value at every point in the space. That is the components of a constant tensor, measured at a point in the space, do not depend on the coordinates of the point. While a tensor field is a tensor the components of which have values which vary from one point in space to another. A field-dependent tensor is a tensor the components of which not only may depend on the coordinates of a point, but also on the direction of an applied field. This definition is generalized in Chapter 3 to describe a field-dependent tensor as a tensor the components of which have one type of tensorial dependence on the coordinates in the geometrical subspace and another type of tensorial dependence on the coordinates in the field subspace. A field-independent tensor is a tensor the components of which do not depend on the coordinates in the field subspace. A further extension of the nomenclature would correspond to a property which is a field dependent tensor which has values which can vary from one point in space to another - such a system would comprise a field dependent tensor field.

CHAPTER 2

FIELD INDEPENDENT TENSORS

This chapter constitutes the necessary background for the study of field dependent tensors and their analysis, and it is not intended to cover the whole subject of field independent tensors (tensors which have components independent of any field) and their applications. For the sake of brevity, throughout this chapter the word tensor has been used to denote field independent tensors.

2.1 Tensors

Tensors are abstract objects (such as physical quantities) whose properties are independent of the reference frame used to describe them. As an example the position of a point in geometrical space can be considered. A point in this three dimensional space can be denoted by an ordered set of three numbers in a special cartesian coordinate system. In another cartesian coordinate system the same point will be represented by a different set of numbers. The position vector of the point is a tensor, which is independent of the choice of the reference frame, and each set of three numbers forms its components with respect to the corresponding coordinate system.

Scalars are a special kind of tensor (tensors of rank zero). In an  $n$  dimensional space a scalar has one component ( $n^0 = 1$ ) which is the same in all the different coordinate systems. Vectors are another kind of tensor (being tensors of the first rank) which in an  $n$  dimensional space have  $n$  components ( $n^1 = n$ ) with respect to each coordinate system (three in a three dimensional space). These  $n$  components transform into a new set of  $n$  components in a new coordinate system. Then there are

tensors of higher rank ( $h$ ) which have  $n^h$  components with respect to each coordinate system ( $n$  is the dimension of the space and  $h$  is the rank of the tensor). Tensors can be more precisely defined by the transformation laws of their components from one reference frame to another.

2.2 Linear orthogonal transformation of coordinate axes and the summation convention

First we consider the simple case of transformation of one rectangular cartesian system of coordinates  $X(X_1, X_2, X_3)$  into another rectangular cartesian system of coordinates  $X'(X'_1, X'_2, X'_3)$  which describe the three dimensional geometrical space. In addition we assume that there is no translation of axes, that is, the origin  $O$  remains the same after the transformation. The relation between the axes in the old system  $X$  and the new system  $X'$  may be specified by the following table:

		old			
		$X_1$	$X_2$	$X_3$	
	$X'_1$	$a_{11}$	$a_{12}$	$a_{13}$	
new	$X'_2$	$a_{21}$	$a_{22}$	$a_{23}$	(2.1)
	$X'_3$	$a_{31}$	$a_{32}$	$a_{33}$	

where  $a_{ij}$  is the direction cosine of  $X'_i$  with respect to  $X_j$  and is a constant for a given cartesian coordinate transformation. A point  $B$  in the space can be described either by its coordinates  $(x^1, x^2, x^3)$  with respect to the  $X$ -system or equally well by  $(x'^1, x'^2, x'^3)$  with respect to the  $X'$ -system. The following relations hold between these two sets of coordinates:

$$\begin{aligned}x'^1 &= a_{11} x^1 + a_{12} x^2 + a_{13} x^3 \\x'^2 &= a_{21} x^1 + a_{22} x^2 + a_{23} x^3 \\x'^3 &= a_{31} x^1 + a_{32} x^2 + a_{33} x^3\end{aligned}\tag{2.2}$$

Equations (2.2) may also be written in matrix notations ,

$$\begin{bmatrix} x'^1 \\ x'^2 \\ x'^3 \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} x^1 \\ x^2 \\ x^3 \end{bmatrix}\tag{2.3}$$

where the array  $a_{ij}$  is called the transformation matrix and is the operator which transforms one set of axes  $X$  into another set  $X'$ . The equations (2.2) may also be concisely written as

$$x'^i = \sum_{j=1}^3 a_{ij} x^j \quad (i, j = 1, 2, 3)\tag{2.4}$$

We will now introduce the Einstein summation convention; namely, if a suffix is repeated in a term, then it is understood that a summation with respect to that suffix over the range  $1, 2, \dots, N$  is implied. An unrepeated suffix is called a free suffix, while, the repeated one is called a dummy or umbral suffix, as it can be replaced by any other symbol except the ones already used to express free suffixes. The summation convention will be employed throughout the rest of this thesis.

Therefore equation (2.4) may be written as

$$x'^i = a_{ij} x^j \quad (i, j = 1, 2, 3)\tag{2.5}$$



In this chapter the range of values of all suffixes is 1, 2, 3 unless otherwise stated.

In the special case of rectangular cartesian coordinates the reverse transformation will have ~~the same~~ <sup>a similar</sup> transformation operator, that is

$$x^i = a_{ji} x'^j \quad (2.6)$$

The nine  $a_{ij}$  are not independent of one another, and in fact (Nye 1972)

$$a_{ik} a_{pk} = \delta_{ip} \quad (2.7)$$

where  $\delta_{ip}$  is the Kronecker delta ,

$$\delta_{ip} \begin{cases} = 1 & \text{when } i = p \\ = 0 & \text{when } i \neq p. \end{cases} \quad (2.8)$$

The relations (2.7) are called the orthogonality relations. Transformations in which the coefficients satisfy the orthogonality relations are called linear orthogonal transformations. The transformation matrix for such a transformation has an inverse equal to its transpose and is called an orthogonal matrix.

When two linear orthogonal transformations of coordinate axes are applied successively, the resulting transformation from the initial coordinate system to the final one, which is called the product transformation, is also linear orthogonal. To show this, let the transformations be

$$x'^k = a_{kj} x^j \quad (2.9)$$

and

$$x''^i = b_{ik} x'^k \quad (2.10)$$

And let the product transformation be

$$x''^i = C_{ij} x^j. \quad (2.11)$$

Substituting for  $x'^j$  from (2.9) into (2.10), we get

$$x''^i = b_{ik} a_{kj} x^j. \quad (2.12)$$

Comparing (2.12) and (2.11), we obtain

$$C_{ij} = b_{ik} a_{kj}. \quad (2.13)$$

Equation (2.13) shows that  $C_{ij}$  is an orthogonal matrix, as the product of two orthogonal matrices is orthogonal. Therefore the product transformation is also a linear orthogonal transformation. This result may be extended to the product of any number of transformations.

Another characteristic property of linear orthogonal transformations is that the determinant of the transformation matrix  $(a_{ij})$ , which we write as  $|a_{ij}|$ , is equal to  $-1$  or  $+1$  according to whether the hand of the axes is changed or unchanged by the transformation (Jeffreys 1931).

### 2.3 Linear transformation of axes

The linear orthogonal transformation of coordinate axes is a special case of linear transformation of axes. When a linear transformation of axes is applied in an  $n$  dimensional space, there exists a set of  $n$  linear relations between the new coordinates and the old ones, that is

$$x'^i = a_{ij} x^j, \quad (a_{ij} \text{ is constant } i, j=1, \dots, n). \quad (2.14)$$

We shall suppose that the transformation is non-singular,  $|a_{ij}| \neq 0$ , so that the set of  $n$  linear equations (2.14) can be solved for the  $x^i$

in terms of  $x'^i$ . The solution of equations (2.14) for the  $x$ 's yields

$$x^i = \frac{A_{ji}}{a} x'^j \quad (2.15)$$

where  $A_{ij}$  is the co-factor of the element  $a_{ij}$  in  $|a_{ij}| \equiv a$ .  $(A_{ji}/a)$  forms the transformation matrix for the reverse transformation.

If we have two successive linear transformations

$$x'^j = a_{ij} x^j \quad (2.16)$$

and

$$x''^k = b_{ki} x'^i, \quad (i, j, k = 1, \dots, n) \quad (2.17)$$

then the direct transformation from  $x^i$  coordinate system to  $x''^i$  coordinate is

$$x''^k = b_{ki} a_{ij} x^j, \quad (i, j, k = 1, \dots, n), \quad (2.18)$$

this is called the product transformation. Writing this transformation in matrix notation yields

$$x'' = B A X \quad (2.19)$$

Since the product  $BA$ , in general, is not equal to  $AB$ , we see that the order in which the transformations are performed is not immaterial.

#### 2.4 General transformation of coordinate axes

Let us consider the coordinate system  $x^i$  ( $i = 1, \dots, n$ ) in an  $n$ -dimensional space. A general transformation of coordinates to a new reference frame can be defined by  $n$  independent equations

$$x'^i = \psi^i(x^1, x^2, \dots, x^n), \quad (i = 1, \dots, n) \quad (2.20)$$

where the  $\psi^i$  are single-valued continuous differentiable functions of

the coordinates. A necessary and sufficient condition for  $n$  equations (2.20) to be independent is that the Jacobian determinant formed from the partial derivatives  $\partial x'^i / \partial x^j$  does not vanish (Sokolnikoff 1956). Under this condition we can solve equations (2.20) for the  $x'^i$  as functions of the  $x'^i$  and obtain

$$x'^i = \psi^i(x'^1, x'^2, \dots, x'^n) \quad (i = 1, 2, \dots, n). \quad (2.21)$$

Now differentiation of (2.20) yields

$$dx'^i = \frac{\partial x'^i}{\partial x^r} dx^r. \quad (2.22)$$

Here matrix formed from the partial derivatives  $\partial x'^i / \partial x^r = a_{ir}$  is the transformation matrix. Generally, the elements of this matrix are not constant with respect to the corresponding coordinate axes. But in the case of linear transformation the  $a_{ir} = \partial x'^i / \partial x^r$  are a set of  $n^2$  constants and the transformation, as it has been shown before (2.14), can be rewritten as

$$x'^i = a_{ir} x^r \quad \text{or} \quad x'^i = \frac{\partial x'^i}{\partial x^r} x^r. \quad (2.23)$$

And, in the case of orthogonal linear transformation we have the condition ,

$$\frac{\partial x'^i}{\partial x^r} = \frac{\partial x^r}{\partial x'^i}. \quad (2.24)$$

### 2.5 Transformation by invariance

Let  $f(P) = f(x^1, \dots, x^n)$  be a function of the  $n$  components  $x^i$  of the point  $P$  with respect to  $X$ -coordinate system in an  $n$ -dimensional space. This function is called an "invariant" or a "scalar function" or, simply, a "scalar" with respect to a transformation of coordinates

from X-system into X'-system, if  $f(P) = f'(P)$ , where  $f(P)$  and  $f'(P)$  are the values of this function in X and X'-coordinate systems. The functional form of  $f(P)$  in the X'-coordinate system will be  $f'(x'^1, \dots, x'^n)$ .

Therefore

$$f \left[ x^1(x'^1, \dots, x'^n), \dots, x^n(x'^1, \dots, x'^n) \right] = f'(x'^1, \dots, x'^n), \quad (2.25)$$

since the value of  $f(x^1, \dots, x^n)$  at  $P(x^1, \dots, x^n)$  is the same (invariant) as that of  $f'(x'^1, \dots, x'^n)$  at  $P(x'^1, \dots, x'^n)$ . We can regard equation (2.25) as being the definition of a scalar function; that is, the functions having the transformation laws typified by formula (2.25) are scalar functions. A transformation of the kind (2.25) is called "transformation by invariance".

## 2.6 Transformation by contravariance and covariance

A set of  $n$  functions  $A^i(x)$  of the  $n$  coordinates  $x^i$  are said to be the components of a contravariant vector, associated with the X-coordinate system, if they transform according to the equation

$$A'^i(x') = \frac{\partial x'^i}{\partial x^\alpha} A^\alpha(x) \quad (2.26)$$

on the change of the coordinates  $x^i$  to  $x'^i$ . Equations (2.26) define the  $n$  components of the vector in the new coordinate system X'. When we examine equation (2.22)

$$dx'^i = \frac{\partial x'^i}{\partial x^r} dx^r \quad (2.22)$$

we see that the differentials,  $dx'^i$ , which determine the displacement vector from a point  $P_1(x^1, \dots, x^n)$  to another point  $P_2(x^1 + dx^1, \dots, x^n + dx^n)$ , form the components of a contravariant vector, whose components in any other system of coordinates are the set of differentials,

$dx'^i$ , in that system. The coordinates  $x^i$  will only behave like the components of a contravariant vector with respect to linear transformations. A transformation of the kind (2.26) is called a "transformation by contravariance".

There exists another law of transformation of vectors, which is quite different from the law typified by formula (2.26), and is called the "transformation by covariance". It can be defined in the following way:

A set of  $n$  functions  $A_i(x)$  of the  $n$  coordinates  $x^i$ , associated with the  $X$ -coordinate system, are the  $n$  components of a covariant vector in an  $n$ -dimensional space, if they transform according to the equation

$$A'_i(x') = \frac{\partial x^\alpha}{\partial x'^i} A_\alpha(x) \quad (2.27)$$

on the change of the coordinates  $x^i$  to  $x'^i$ . Equations (2.27) define the  $n$  components of the vector in the new coordinate system  $X'$ . As an example of a covariant vector consider the set of  $n$  partial derivatives of a scalar function  $f$ . Since  $\partial f / \partial x'^i = (\partial f / \partial x^\alpha) (\partial x^\alpha / \partial x'^i)$ , it follows immediately from (2.27) that the quantities  $\partial f / \partial x^i$  are the components of a covariant vector, whose components are the corresponding partial derivatives  $\partial f / \partial x'^i$ . Such a covariant vector is called "the gradient of  $f$ ".

A covariant vector will always be denoted by a single subscript, while a single superscript will denote a contravariant vector, unless otherwise stated. The coordinates  $x^i$  are an exception to this, since with respect to general transformations of coordinates, the  $x^i$  do not form the components of a contravariant vector.

There is no distinction between contravariant and covariant vectors when we restrict ourselves to linear orthogonal transformations, since

according to (2.24)

$$\partial x^\alpha / \partial x'^i = \partial x'^i / \partial x^\alpha .$$

## 2.7 Definition of tensors by their transformation laws

We can define a tensor as "a system of numbers or functions (components of the tensor) representing a quantity in an n-dimensional space, which obeys a certain law of transformation when the coordinates undergo a transformation." We have already defined the transformation law for scalars or tensors of rank zero (equation (2.25)), and also the two different transformation laws for contravariant and covariant vectors or tensors of rank one (equations (2.26) and (2.27)).

The next requirement is to state the transformation law for tensors of ranks higher than one. To do this, we start with second rank tensors. Consider the set of  $n^2$  functions  $A^{ij}(x)$  whose transformation law is

$$A'^{ij}(x') = \frac{\partial x'^i}{\partial x^k} \frac{\partial x'^j}{\partial x^l} A^{kl}(x) , \quad (2.28)$$

then we call  $A^{ij}(x)$  the components of a contravariant tensor of second rank. Similarly, if we have a set of  $n^2$  functions whose transformation law is

$$A'_{ij}(x') = \frac{\partial x^k}{\partial x'^i} \frac{\partial x^l}{\partial x'^j} A_{kl}(x) , \quad (2.29)$$

we call  $A_{ij}(x)$  the components of a covariant tensor of second rank.

Further, if we have a set of  $n^2$  functions  $A_j^i(x)$  whose transformation law is

$$A_j'^i(x') = \frac{\partial x'^i}{\partial x^k} \frac{\partial x^l}{\partial x'^j} A_l^k(x) , \quad (2.30)$$

we call  $A_j^i(x)$  the components of a mixed tensor of second rank. Super-  
scripts and subscripts always correspond to respectively contravariance  
and covariance properties.

From what has been said above, we can generalize the definition  
of a tensor in the following way:

A set of  $n^{s+p}$  functions  $A_{q_1 q_2 \dots q_p}^{t_1 t_2 \dots t_s}(x)$  of the  $n$  coordinate system  $x^i$ ,  
associated with  $X$ -coordinate system are said to be the components of a  
mixed tensor of rank  $(s+p)$ , contravariant of the  $s$ -th rank and covariant  
of the  $p$ -th rank, if they transform according to the equation

$$A_{r_1 r_2 \dots r_p}^{u_1 u_2 \dots u_s}(x') = \frac{\partial x'^{u_1}}{\partial x^{t_1}} \dots \frac{\partial x'^{u_s}}{\partial x^{t_s}} \frac{\partial x^{q_1}}{\partial x'^{r_1}} \dots \frac{\partial x^{q_p}}{\partial x'^{r_p}} A_{q_1 q_2 \dots q_p}^{t_1 t_2 \dots t_s}(x), \quad (2.31)$$

on the change of coordinates  $x^i$  to  $x'^i$ . Equations (2.31) define the  
 $n^{s+p}$  components in the new coordinate system  $X'$ .

Now we establish a useful property of the law of the transformation  
of tensors. If we are given the components  $A^j(x)$  of a contravariant  
vector in  $X$ -coordinate system, by using the transformation law of a  
contravariant vector, (equation (2.26)),  $A'^i(x') = \partial x'^i / \partial x^j A^j(x)$ , the  
components of the same vector in  $X'$ -system,  $A'^i(x')$  can be found. On  
multiplying equation (2.26) by  $\partial x^k / \partial x'^i$  and summing over the index  
 $i$  from 1 to  $n$ , we obtain

$$\frac{\partial x^k}{\partial x'^i} A'^i(x') = \frac{\partial x^k}{\partial x'^i} \frac{\partial x'^i}{\partial x^j} A^j(x) = \frac{\partial x^k}{\partial x^j} A^j(x) = \delta_j^k A^j(x) = A^k(x). \quad (2.32)$$

That is

$$A^k(x) = \frac{\partial x^k}{\partial x'^i} A'^i(x'). \quad (2.33)$$



Generalising, we can state that:

"Let the components of a mixed tensor in the X-coordinate system

be denoted by  $A_{\alpha_1 \dots \alpha_r}^{\beta_1 \dots \beta_s}(x)$  and its components in the X'-coordinate system by  $A'_{i_1 \dots i_r}{}^{j_1 \dots j_s}(x')$ . Then, from the law of transformation of mixed tensors we can write

$$A'_{i_1 \dots i_r}{}^{j_1 \dots j_s}(x') = \frac{\partial x^{\alpha_1}}{\partial x'^{i_1}} \dots \frac{\partial x^{\alpha_r}}{\partial x'^{i_r}} \cdot \frac{\partial x'^{j_1}}{\partial x^{\beta_1}} \dots \frac{\partial x'^{j_s}}{\partial x^{\beta_s}} A_{\alpha_1 \dots \alpha_r}^{\beta_1 \dots \beta_s}(x). \quad (2.34)$$

On the other hand, if we are given the components  $A'_{i_1 \dots i_r}{}^{j_1 \dots j_s}(x')$ , the

components  $A_{\alpha_1 \dots \alpha_r}^{\beta_1 \dots \beta_s}(x)$  of the same tensor in the X-coordinate system

are determined by

$$A_{\alpha_1 \dots \alpha_r}^{\beta_1 \dots \beta_s}(x) = \frac{\partial x'^{i_1}}{\partial x^{\alpha_1}} \dots \frac{\partial x'^{i_r}}{\partial x^{\alpha_r}} \cdot \frac{\partial x^{\beta_1}}{\partial x'^{j_1}} \dots \frac{\partial x^{\beta_s}}{\partial x'^{j_s}} A'_{i_1 \dots i_r}{}^{j_1 \dots j_s}(x'). \quad (2.35)$$

From the two equations (2.34) and (2.35) we can deduce an important theorem, namely

"If all components of a tensor vanish in a particular coordinate system, then they necessarily vanish in every other coordinate system."

The significance of this theorem in finding the null properties of crystals has been discussed by Birss (1966, p.71).

## 2.8 Symmetrical and antisymmetrical tensors

When two covariant (or contravariant) indices in the components

$A_{j_1 \dots j_r}{}^{i_1 \dots i_s}(x)$  of a tensor can be interchanged without altering the value of those components, the tensor is said to be symmetric with respect to

those indices. It can be shown that the symmetry of the components of a symmetric tensor is preserved under the coordinate transformations (Sokolnikoff, 1956).

A tensor is said to be antisymmetric with respect to two certain indices (both covariant or both contravariant), if an interchange of those two indices in the components changes the sign and not the magnitude of the components. The antisymmetry is also an invariant property (Sokolnikoff, 1956). A second order symmetric tensor has got  $\frac{1}{2} n (n + 1)$  different non-zero components.

## 2.9 Constant tensors and tensor field

The words "constant tensor" and "tensor field" will be used frequently throughout this thesis, therefore it is beneficial to give a short definition of them here.

### (a) Constant tensors

Constant tensors are those tensors whose components have the same value at every point in the space (or the subspace) over which they have been defined. These are the type of tensors which are usually encountered in solid state physics and have been described in detail in standard texts such as that by Nye (1972). The transformation law for these tensors is

$$A_{i_1 \dots i_r}^{j_1 \dots j_s} = \frac{\partial x^{\alpha_1}}{\partial x'^{i_1}} \dots \frac{\partial x^{\alpha_r}}{\partial x'^{i_r}} \cdot \frac{\partial x'^{j_1}}{\partial x^{\beta_1}} \dots \frac{\partial x'^{j_s}}{\partial x^{\beta_s}} A_{\alpha_1 \dots \alpha_r}^{\beta_1 \dots \beta_s} \quad (2.36)$$

### (b) Tensor-field

A tensor field is a tensor which has different values for its components at different points in the space over which the tensor has been defined, in other words the components of a tensor-field depend on the position of the point, at which the tensor has been defined, in the

space. Equation (2.34) is the transformation law for these tensors. Constant tensors are a special kind of tensor field. In this thesis, the word tensor has been used to mean tensor-field unless otherwise stated.

### 2.10 Relative or weighted tensors (polar and axial tensors)

We shall now extend the definition of a tensor to include relative or weighted tensors. By a relative tensor-field of weight  $\omega$  ( $\omega$  is a constant), we shall mean an object with components whose transformation law differs from the transformation law of a tensor-field by the appearance of the determinant of the transformation matrix to the  $\omega^{\text{th}}$  power in the transformation law. That is

$$A_{i_1 \dots i_r}^{j_1 \dots j_s}(x') = \left| \frac{\partial x^\beta}{\partial x'^j} \right|^\omega \frac{\partial x'^{j_1}}{\partial x^{\alpha_1}} \dots \frac{\partial x'^{j_s}}{\partial x^{\alpha_s}} \cdot \frac{\partial x^{\beta_1}}{\partial x'^{i_1}} \dots \frac{\partial x^{\beta_r}}{\partial x'^{i_r}} A_{\beta_1 \dots \beta_r}^{\alpha_1 \dots \alpha_s}(x) \quad (2.37)$$

where  $\left| \frac{\partial x^\beta}{\partial x'^j} \right|$  denotes the Jacobian of the transformation; in other words, the determinant of the transformation matrix.

In the special case of linear orthogonal transformation,

$$\left| \frac{\partial x^\beta}{\partial x'^j} \right| = \pm 1 \quad (+ \text{ sign for transformation which keep the hands of axes unchanged and } - \text{ sign for those which change the hands of axes}).$$

Therefore, considering the fact that for linear orthogonal transformation of coordinate axes, there is no difference between the covariance and contravariance properties (see Section 2.6), the transformation law of tensors, for such transformation of axes, will be

$$B_{i_1 \dots i_s}^{j_1 \dots j_s}(x') = (\pm 1)^\omega a_{i_1 j_1} \dots a_{i_s j_s} B_{j_1 \dots j_s}^{j_1 \dots j_s}(x) \quad (2.38)$$

where  $a_{i_m j_m}$  constants are the elements of the corresponding transformation

matrix. Therefore, we will have two kinds of tensors:

(i) tensors which transform according to the following law

$$B'_{i_1 \dots i_s}(x') = a_{i_1 j_1} \dots a_{i_s j_s} B_{j_1 \dots j_s}(x) \quad (2.39)$$

these are tensors of even weight and are referred to as "polar tensors".

(ii) tensors which transform according to

$$B'_{i_1 \dots i_s}(x') = \pm a_{i_1 j_1} \dots a_{i_s j_s} B_{j_1 \dots j_s}(x) \quad (2.40)$$

or,

$$B'_{i_1 \dots i_s}(x') = |a_{ij}| a_{i_1 j_1} \dots a_{i_s j_s} B_{j_1 \dots j_s}(x) \quad (2.41)$$

these are tensors of odd weight and are referred to as "axial tensors".

## 2.11 Algebra of tensors

(i) Addition and subtraction

Consider two unweighted tensors  $A(x)$  and  $B(x)$  of the same type and rank defined at the same point  $P$ , and the corresponding laws of transformation

$$B'_{i_1 \dots i_r}(x') = \frac{\partial x^{\alpha_1}}{\partial x'^{i_1}} \dots \frac{\partial x^{\alpha_r}}{\partial x'^{i_r}} \cdot \frac{\partial x^{j_1}}{\partial x^{\beta_1}} \dots \frac{\partial x^{j_s}}{\partial x^{\beta_s}} B_{\alpha_1 \dots \alpha_r \beta_1 \dots \beta_s}(x) \quad (2.42)$$

$$A'_{i_1 \dots i_r}(x') = \frac{\partial x^{\alpha_1}}{\partial x'^{i_1}} \dots \frac{\partial x^{\alpha_r}}{\partial x'^{i_r}} \cdot \frac{\partial x^{j_1}}{\partial x^{\beta_1}} \dots \frac{\partial x^{j_s}}{\partial x^{\beta_s}} A_{\alpha_1 \dots \alpha_r \beta_1 \dots \beta_s}(x) \quad (2.43)$$

Now we prove that the sum of (or the difference between) these two

tensors is again a tensor of the same type and rank as the two tensors. Performing the summation we get,

$$B_{i_1 \dots i_r}^{j_1 \dots j_s}(x') \pm A_{i_1 \dots i_r}^{j_1 \dots j_s}(x') = \left( \frac{\partial x^{\alpha_1}}{\partial x'^{i_1}} \dots \frac{\partial x^{\alpha_r}}{\partial x'^{i_r}} \right) \cdot \left( \frac{\partial x'^{j_1}}{\partial x^{\beta_1}} \dots \frac{\partial x'^{j_s}}{\partial x^{\beta_s}} \right) \cdot \left[ B_{\alpha_1 \dots \alpha_r}^{\beta_1 \dots \beta_s}(x) \pm A_{\alpha_1 \dots \alpha_r}^{\beta_1 \dots \beta_s}(x) \right], \quad (2.44)$$

and it immediately follows that  $A(x) + B(x)$  is a tensor which has the same number of covariant and the same number of contravariant indices as the original tensors, and each of its components is the sum of the corresponding components of the summand tensors. The summation operation can be extended to three or more tensors. It can also be easily shown that, if each component of a tensor is multiplied by a constant, the resulting set of functions is a tensor of the same type and rank. Therefore, any linear combination of tensors of the same rank and the same type is a tensor of the same type and the same rank.

We can generalize the addition of tensors to include relative tensors as well. It can be easily shown that relative tensors of the same weight and rank and the same type (having equal number of covariance and equal number of contravariance indices) can be added together, and the sum will be a relative tensor of the same weight, rank and type. For the case of a linear orthogonal transformation, the addition of a polar and an axial tensor is not defined. That is, if two tensors are to be added together, they should be of the same rank and the same polarity.

(ii) Multiplication: Outer product

Consider two tensors (not necessarily of the same rank or type

or weight)  $A^{i_1 \dots i_q}_{j_1 \dots j_p}(x)$  of weight  $\omega_1$ , and  $B^{\ell_1 \dots \ell_s}_{k_1 \dots k_r}(x)$  of weight  $\omega_2$ .

The set of quantities consisting of the product of each component of

the tensor  $B^{\ell_1 \dots \ell_s}_{k_1 \dots k_r}(x)$  by each component of the tensor  $A^{i_1 \dots i_q}_{j_1 \dots j_p}(x)$

forms a tensor  $C(x)$ , called the "outer product" of tensors  $B(x)$  and  $A(x)$ . By using the transformation law for relative tensors  $A(x)$  and  $B(x)$  (equation (2.37)) it can be easily shown that this tensor,  $C(x)$ , is contravariant of rank  $q + s$  and covariant of rank  $p + r$ , and its weight is  $\omega_1 + \omega_2$ . In  $X$ -coordinate system the components of tensor  $C(x)$  are given by the following formula:

$$C^{i_1 \dots i_q \ell_1 \dots \ell_s}_{k_1 \dots k_r j_1 \dots j_p}(x) = B^{\ell_1 \dots \ell_s}_{k_1 \dots k_r}(x) A^{i_1 \dots i_q}_{j_1 \dots j_p}(x) \quad (2.45)$$

(iii) Tensor contraction

Consider a mixed tensor,  $A^{i_1 \dots i_s}_{j_1 \dots j_r}(x)$ , and equate a covariant and a contravariant index and sum with respect to that index. The resulting set of  $n^{r+s-2}$  sums is a mixed tensor, covariant of rank  $r-1$  and contravariant of rank  $s-1$ . To show this, consider a mixed tensor like  $A^{ijk}_{lm}(x)$ , from the transformation law of tensors (equation (2.31)) we have

$$A'^{rst}_{pq}(x') = \frac{\partial x'^r}{\partial x^i} \frac{\partial x'^s}{\partial x^j} \frac{\partial x'^t}{\partial x^k} \frac{\partial x^\ell}{\partial x'^p} \frac{\partial x^m}{\partial x'^q} A^{\ell m}_{ijk}(x) \quad (2.46)$$

Now if we equate  $t$  and  $q$  we will get

$$\begin{aligned}
 A'^{rst}_{pt}(x') &= \frac{\partial x'^r}{\partial x^i} \frac{\partial x'^s}{\partial x^j} \frac{\partial x'^t}{\partial x^k} \frac{\partial x^\ell}{\partial x'^p} \frac{\partial x^m}{\partial x'^t} A_{\ell m}^{ijk}(x) \\
 &= \frac{\partial x'^r}{\partial x^i} \frac{\partial x'^s}{\partial x^j} \frac{\partial x^\ell}{\partial x'^p} \delta_j^m A_{\ell m}^{ijk}(x) .
 \end{aligned}$$

$$A'^{rst}_{pt}(x') = \frac{\partial x'^r}{\partial x^i} \frac{\partial x'^s}{\partial x^j} \frac{\partial x^\ell}{\partial x'^p} A_{\ell k}^{ijk}(x) . \tag{2.47}$$

Therefore  $A_{\ell k}^{ijk}$  is a mixed tensor, contravariant of the second rank and covariant of the first rank. This process of reducing the rank of a tensor in contravariant and covariant indices is called the operation of contraction and it can be applied to all the indices of a tensor, one after another, as far as there are indices of both types present. The operation of contraction on a relative tensor yields a relative tensor of the same weight as the original tensor.

(iv) Inner product

Inner multiplication is performed by combining the two operations of outer multiplication and contraction, and the resulting tensor is called the inner product of the original tensors upon which the operations are applied. To find the inner product of two tensors, first we find the outer product of them, and then we apply the operation of contraction (if it is possible).

2.12 Quotient law

The direct method of establishing the tensor character of sets of functions is to find out how they transform from one coordinate system to another. The quotient law provides a means of doing this

without having to study transformation properties in detail, which in practice is troublesome. It states that  $n^k$  functions of  $x^i$  coordinates form the components of a tensor of rank  $h$ , (with certain contravariant and covariant character), provided that an inner product of these functions with an arbitrary tensor is itself a tensor, (the term "inner product" has been used here for sums of the form  $A(\alpha, i_2, \dots, i_h) A_\alpha$ , or  $A(\alpha, i_2, \dots, i_h) A^\alpha$ , whether the set of functions  $A(i_1, i_2, \dots, i_h)$  represents a tensor or not). It will suffice to establish the proof for the particular case of the set of  $n^3$  functions  $A(i, j, k)$ , which has all features of the more involved cases. Now let us suppose that the inner product  $A(i, j, k) B_j^{ip}(x)$  for an arbitrary tensor  $B_j^{ip}(x)$  yields a tensor of the type  $C^{pk}(x)$ :

$$A(i, j, k) B_j^{ip}(x) = C^{pk}(x) \quad (2.48)$$

The transformed quantities, referred to a new system of coordinates  $x'^i$ , satisfy the equations

$$A'(i, j, k) B_j'^{ip}(x') = C'^{pk}(x') \quad (2.49)$$

Substituting for  $B_j'^{ip}(x')$  and  $C'^{pk}(x')$  from their transformation laws (equation (2.31)), we have

$$A'(i, j, k) \frac{\partial x'^i}{\partial x^\ell} \frac{\partial x'^p}{\partial x^m} \frac{\partial x^n}{\partial x'^j} B_n^{\ell m}(x) = \frac{\partial x'^p}{\partial x^q} \frac{\partial x'^k}{\partial x^r} C^{qr}(x) \quad (2.50)$$

Substituting for  $C^{qr}(x)$  from equation (2.48) into equation (2.50) and changing the dummy indices, we get

$$\frac{\partial x'^p}{\partial x^m} \left[ A'(i, j, k) \frac{\partial x'^i}{\partial x^\ell} \frac{\partial x^u}{\partial x'^j} - A(\ell, u, r) \frac{\partial x'^k}{\partial x^r} \right] B_u^{\ell m}(x) = 0 \quad (2.51)$$



On inner multiplication by  $\partial x^s / \partial x'^p$  we obtain

$$\left[ A'(i, j, k) \frac{\partial x'^i}{\partial x^\ell} \frac{\partial x^u}{\partial x'^j} - A(\ell, u, r) \frac{\partial x'^k}{\partial x^r} \right] B_u^{\ell s}(x) = 0. \quad (2.52)$$

Since  $B_u^{\ell s}(x)$  is an arbitrary tensor, the expression in brackets is identically zero, that is

$$A'(i, j, k) \frac{\partial x'^i}{\partial x^\ell} \frac{\partial x^u}{\partial x'^j} = A(\ell, u, r) \frac{\partial x'^k}{\partial x^r}. \quad (2.53)$$

Inner multiplication of this equation by  $\frac{\partial x^\ell}{\partial x'^s} \frac{\partial x'^t}{\partial x^u}$  yields

$$A'(s, t, k) = \frac{\partial x^\ell}{\partial x'^s} \frac{\partial x'^t}{\partial x^u} \frac{\partial x'^k}{\partial x^r} A(m, u, r), \quad (2.54)$$

which shows that  $A(m, u, r)$  is a tensor of third rank and contravariant in  $m$  and  $n$ , and covariant in  $r$ ,  $A_r^{mu}$ .

### 2.13 Differentiation of tensors

We have seen in Section(2.6) that the set of partial derivatives (gradient) of a scalar function,  $f(x)$ , forms a covariant tensor of rank one. If we form the set of partial derivatives of this covariant vector  $\frac{\partial f}{\partial x^i}$  we get

$$\frac{\partial^2 f}{\partial x'^i \partial x'^i} = \frac{\partial}{\partial x'^i} \left( \frac{\partial f}{\partial x^\alpha} \frac{\partial x^\alpha}{\partial x'^i} \right) = \frac{\partial^2 f}{\partial x^\alpha \partial x^\beta} \frac{\partial x^\beta}{\partial x'^i} \frac{\partial x^\alpha}{\partial x'^i} + \frac{\partial f}{\partial x^\alpha} \frac{\partial^2 x^\alpha}{\partial x'^i \partial x'^i}. \quad (2.55)$$

Therefore for general transformation of coordinate axes, where

$\frac{\partial^2 x^\alpha}{\partial x'^i \partial x'^i} \neq 0$ , this set of partial derivatives of the covariant tensor  $\frac{\partial f}{\partial x^\alpha}$  does not represent a tensor. This can be generalized to any kind of vector, to show that the set of partial derivatives of a

contravariant or a covariant vector do not form a tensor for general transformation of coordinates.

Consider a covariant vector  $A_\alpha(x)$ , then

$$A'_i(x') = \frac{\partial x^\alpha}{\partial x'^i} A_\alpha(x) \quad (2.56)$$

Differentiating this with respect to coordinates  $x'^i$ , we get

$$\frac{\partial A'_i(x')}{\partial x'^i} = \frac{\partial x^\alpha}{\partial x'^i} \frac{\partial x^\beta}{\partial x'^j} \frac{\partial A_\alpha(x)}{\partial x^\beta} + \frac{\partial^2 x^\alpha}{\partial x'^i \partial x'^j} A_\alpha(x) \quad (2.57)$$

which is not the transformation rule for a tensor, that is,  $\frac{\partial A_\alpha(x)}{\partial x^\beta}$  is not a tensor.

Similarly, for a contravariant vector  $A^\alpha(x)$ , we get

$$\frac{\partial A'^i(x')}{\partial x'^i} = \frac{\partial A^\alpha(x)}{\partial x^\beta} \frac{\partial x^\beta}{\partial x'^j} \frac{\partial x'^i}{\partial x^\alpha} + A^\alpha(x) \frac{\partial^2 x'^i}{\partial x^\alpha \partial x^\beta} \frac{\partial x^\beta}{\partial x'^j} \quad (2.58)$$

which shows that  $\frac{\partial A^\alpha(x)}{\partial x^\beta}$  is not a tensor.

This can be extended to mixed tensors of any rank to show that the set of partial derivatives of a tensor does not form a tensor. But for linear transformation where  $\partial x^\alpha / \partial x'^i$  is a constant the partial derivative operator acts like a covariant vector, and adds one covariant index to the indices of the original tensor. That is, the tensor formed by the set of partial derivatives of the tensor  $A_{j_1 \dots j_r}^{i_1 \dots i_s}(x)$  will have  $s$  contravariant and  $r + 1$  covariant indices. The transformation law for such a tensor will be ,

$$\frac{\partial A'_{j_1 \dots j_r}^{i_1 \dots i_s}(x')}{\partial x'^k} = \frac{\partial x^\ell}{\partial x'^k} \frac{\partial x'^{i_1}}{\partial x^{\alpha_1}} \dots \frac{\partial x'^{i_s}}{\partial x^{\alpha_s}} \cdot \frac{\partial x^{\beta_1}}{\partial x'^{j_1}} \dots \frac{\partial x^{\beta_r}}{\partial x'^{j_r}} \frac{A_{\beta_1 \dots \beta_r}^{\alpha_1 \dots \alpha_s}(x)}{\partial x^\ell} \quad (2.59)$$

In the preparation of this chapter, text books by the following authors have been consulted: Sokolnikoff (1956), Brand (1948), Spain (1956), Brillouin (1964), McConnell (1957), Nye (1972) and Birss (1966).

CHAPTER 3

FIELD DEPENDENT TENSORS (I):

DEFINITION AND TRANSFORMATION LAWS

3.1 Introduction

In the study of tensor properties of materials in the presence of an external field, such as a magnetic field or strain, one encounters properties, for instance the conductivity, with components which depend on the applied field. These tensors have been named "field dependent" tensors (Grabner and Swanson 1962).

In Sections 3.2, 3.3 and 3.4, the way field dependent tensor properties have been dealt with in the past has been discussed and the need for a more general approach has been recognized. The rest of this chapter is devoted to giving a general definition of field dependent tensors and to finding their transformation laws from one system of coordinates to another.

3.2 Expansion of the field dependent tensor components in terms of field components

In dealing with field dependent tensor properties, previous practice has been to expand the tensor components as a power series in the applied field and to restrict the calculations and measurements to the low field coefficients (which are constant with respect to the field components). The formulation of this procedure for some special properties, in orthogonal coordinate system, can be found in many articles (for example see Akgöz and Saunders 1974, Birss 1966, Juretschke 1955, Mason et al 1953). We generalize this to state that:

In a general coordinate system a field dependent tensor,

$A_{j_1 \dots j_r}^{i_1 \dots i_s}(\vec{F})$  can be expanded according to the following formulas:

(a) in the presence of a field  $\vec{F}$ , which behaves like a covariant vector,

$$A_{j_1 \dots j_r}^{i_1 \dots i_s}(\vec{F}) = A_{j_1 \dots j_r}^{i_1 \dots i_s(0)} + A_{j_1 \dots j_r}^{i_1 \dots i_s k_1(1)} F_{k_1} + A_{j_1 \dots j_r}^{i_1 \dots i_s k_1 k_2(2)} F_{k_1} F_{k_2} + \dots \quad (3.1)$$

(b) in the presence of a field  $\vec{F}$ , which behaves like a contravariant vector,

$$A_{j_1 \dots j_r}^{i_1 \dots i_s}(\vec{F}) = A_{j_1 \dots j_r}^{i_1 \dots i_s(0)} + A_{j_1 \dots j_r k_1}^{i_1 \dots i_s(1)} F^{k_1} + A_{j_1 \dots j_r k_1 k_2}^{i_1 \dots i_s(2)} F^{k_1} F^{k_2} + \dots \quad (3.2)$$

The coefficients  $A_{j_1 \dots j_r k_1 \dots k_N}^{i_1 \dots i_s(N)}$  or  $A_{j_1 \dots j_r}^{i_1 \dots i_s k_1 \dots k_N(N)}$  are now field

independent tensors and are given by

$$A_{j_1 \dots j_r k_1 \dots k_N}^{i_1 \dots i_s(N)} = \left( \frac{1}{N!} \right) \left( \frac{\partial^N A_{j_1 \dots j_r}^{i_1 \dots i_s}(\vec{F})}{\partial F^{k_1} \dots \partial F^{k_N}} \right) \Big|_{\vec{F}=0} \quad (3.3)$$

and

$$A_{j_1 \dots j_r}^{i_1 \dots i_s k_1 \dots k_N(N)} = \left( \frac{1}{N!} \right) \left( \frac{\partial^N A_{j_1 \dots j_r}^{i_1 \dots i_s}(\vec{F})}{\partial F^{k_1} \dots \partial F^{k_N}} \right) \Big|_{\vec{F}=0} \quad (3.4)$$

The new set of components of each of the coefficient tensors, in a new reference frame, can be found by employing the transformation law for

field independent tensors (equation 2.31). By substituting these transformed coefficients into equation (3.1) and (3.2), the transformed set of components of the tensor  $A_{j_1 \dots j_r}^{i_1 \dots i_s}(\vec{F})$  is then obtained. Experimental measurements and theoretical interpretation of the low field (field independent) coefficients for some field dependent properties have been done in the past. As an example the magnetoconductivity can be considered:

For the magnetoconductivity tensor  $\sigma_{ij}(\vec{B})$  (in an orthogonal reference frame) this procedure gives (see Drabble et al 1956, Akgöz and Saunders 1974):

$$\sigma_{ij}(\vec{B}) = \sigma_{ij}^{(0)} + \sigma_{ij k_1}^{(1)} B_{k_1} + \sigma_{ij k_1 k_2}^{(2)} B_{k_1} B_{k_2} + \dots \quad (3.5)$$

where

$$\sigma_{ij k_1 k_2 \dots k_N}^{(N)} = \left( \frac{1}{N!} \right) \left( \frac{\partial^N \sigma_{ij}(\vec{B})}{\partial B_{k_1} \dots \partial B_{k_N}} \right) \Bigg|_{\vec{B} = 0} \quad (3.6)$$

Experimental measurements of these low field coefficients have then usually been interpreted in terms of carrier densities and mobilities, and Fermi surface parameters. (For more detail see Zitter 1962, Öktü and Saunders 1967, Jeavons and Saunders 1969, Michenaud and Issi 1972, Akgöz and Saunders 1974, Turetken et al 1974).

### 3.3 Grabner and Swanson transformation law for field dependent tensors

A transformation law for a field dependent tensor  $d_{ijk}(\vec{F}_{np\dots})$ , with respect to a linear orthogonal transformation of coordinates was first suggested by Grabner and Swanson (1962) which can be written as

$$d'_{ijk\dots}(\vec{F}'_{np\dots}) = a_{ir} a_{js} a_{kt} \dots d_{rst\dots}(\vec{F}_{mo\dots}) \quad (3.7)$$

where  $[a_{ij}]$  is the transformation matrix. That is, the transformation law for a field dependent tensor requires that both the matter components and their arguments be transformed. Using transformation law (3.7) enables one to work with field dependent tensor components rather than the low field coefficients, and important practical advantages accrue from this.

(i) they are easier to measure because the applied field can take any value - there is no longer any necessity to ensure that the low field limit is achieved - and so it can be assured that the induced effects are larger,

(ii) since the measurements can be made over a wide range of field, much more comprehensive data can be obtained,

(iii) in many cases the number of samples needed to obtain the required information is less than that demanded by the low field method,

(iv) direct studies of non-linear effects in the physical properties of solids - an area of much interest at present - can be made.

Solution of the Boltzmann transport equation has enabled expression of field dependent transport tensors in terms of band model parameters for materials with simple many-valleyed Fermi surfaces. (For more detail see Fuchser et al 1970, Aubrey 1971, and Sümengen et al 1972). As a result the microscopic formulation is no longer restricted to the low field condition ( $\mu B \ll 1$ ) but now includes the intermediate field region for which galvanomagnetic data could not previously be interpreted quantitatively. Analysis of experimental data of the field and orientation dependence of  $\rho_{ij}(\vec{B})$  (the magnetoresistivity tensor) and  $\alpha_{ij}(\vec{B})$  (the magnetothermoelectric power tensor) for bismuth (see Sümengen et al 1972,

Saunders et al 1972, and Türetken et al 1974) and arsenic-antimony alloy (see Akgöz et al 1974) has established that the band model parameters found by the field dependent tensor components are the same within experimental error as those obtained from the low field coefficients. Thus using the transformation law (3.7) has great advantages.

### 3.4 Inadequacy of Grabner and Swanson transformation law

As long as the spatial transformation operators are being considered, there is no difficulty in obtaining the transformed tensor components of a field dependent tensor. But there are cases where more complicated transformation operators are considered, that is transformation operators composed of spatial transformation operators and operators which operate only on the field components. As an example of this kind of transformation, a transformation operator in "spin space" (see Litvin 1973, Brinkman et al 1966 a,b, and Cracknell 1975) can be considered. This operator can be denoted by  $\{ R_p | R_i | v_{ip} \}$ , where  $\{ v_{ip} \}$  is a translation,  $\{ R_i \}$  a rotation or rotation-inversion operator acting on the spatial coordinates of the spin arrangement, and  $\{ R_p \}$  a rotation or rotation-inversion operator acting on the spin directions of that spin arrangement (through the rest of this thesis operators have been notified with barred letters like  $\bar{A}$  or  $\bar{R}$  to avoid confusion). Now for a tensor defined in the geometrical space with components depending on the spin directions, the effect of the  $\{ R_i | v_{ip} \}$  part of the transformation operator can be obtained using the transformation law (3.7), but the  $\{ R_p \}$  part needs further consideration. Before this can be done it is necessary to define the space of the physical problem under consideration.



### 3.5 N-dimensional space

An N-dimensional space, denoted by  $V_N$ , can be defined as any set of objects that can be placed in a one-to-one correspondence with the totality of ordered sets of N numbers  $x_1, x_2, \dots, x_N$ . These numbers are called coordinates of the objects (points) (see Sokolnikoff 1956, page 9). As an example consider physical space - a three dimensional space with the objects being the geometrical points and with the coordinates of a point being  $x_1, x_2, x_3$  with respect to three coordinate axes. In general by "objects" a broader meaning than just geometrical points is understood: in different cases "objects" may imply different sets of physical properties such as electric field, magnetic field, spin of a particle, position vector, temperature gradient, pressure, time, etc. These physical properties can be the coordinate axes of a space. It must be remembered that in a definition of an N-dimensional space, there is no suggestion of the concept of distance between pairs of points (objects). If a rule for the measurement of the distance in a space is defined, that space is called a "metric space."

In addition to the points in an N-dimensional space, we need a second kind of mathematical entity, that is the vector, which is related to the points through the following postulates:

(i) every pair of points in the N-dimensional space determines an entity which is called a vector,

(ii) any two vectors  $\vec{A}$  and  $\vec{B}$  have a sum  $\vec{A} + \vec{B}$  which obeys the following laws:

(a) commutative law  $\vec{A} + \vec{B} = \vec{B} + \vec{A}$  ,

(b) associative law  $(\vec{A} + \vec{B}) + \vec{C} = \vec{A} + (\vec{B} + \vec{C})$  ,

(c) if  $\vec{A}$  and  $\vec{B}$  are vectors, there exists a unique vector  $\vec{X}$  such that  $\vec{A} = \vec{B} + \vec{X}$ , thus it follows that the operation of subtraction of vectors is unique and there exists a vector  $\vec{0}$  (zero) such that  $\vec{A} + \vec{0} = \vec{A}$ ,

(iii) for every real number  $\alpha$  and a vector  $\vec{A}$  there exists a vector  $\alpha\vec{A} = \vec{A}\alpha$  such that

$$(\alpha_1 + \alpha_2)\vec{A} = \alpha_1\vec{A} + \alpha_2\vec{A},$$

and

$$\alpha(\vec{A} + \vec{B}) = \alpha\vec{A} + \alpha\vec{B},$$

and

$$\alpha_1(\alpha_2\vec{A}) = (\alpha_1\alpha_2)\vec{A}.$$

The totality of vectors defined in this way in the N-dimensional space constitutes a linear vector space of N dimensions. A linear vector space is called a metric vector space when to every pair of vectors  $\vec{A}$  and  $\vec{B}$  of the space a number  $\vec{A} \cdot \vec{B}$  is assigned, called the "inner" or "scalar" product of these vectors, such that

$$\vec{A} \cdot \vec{A} > 0, \quad \text{unless } \vec{A} = \vec{0},$$

$$\vec{A} \cdot \vec{B} = \vec{B} \cdot \vec{A},$$

$$\vec{A} \cdot (\vec{B} + \vec{C}) = \vec{A} \cdot \vec{B} + \vec{A} \cdot \vec{C},$$

and

$$\alpha(\vec{A} \cdot \vec{B}) = \alpha\vec{A} \cdot \vec{B}.$$

In an N-dimensional space there exist N independent vectors, called basis vectors, and every set of N + 1 vectors is linearly dependent. When a basis  $\vec{X}_k$ ,  $k = 1, \dots, N$ , is defined in an N-dimensional vector space, then each vector  $\vec{A}$  of the space is uniquely determined by

a set of  $N$  numbers  $a^k$ ,  $k = 1, \dots, N$ , such that

$$\vec{A} = \sum_k \vec{X}_k a^k .$$

The numbers  $a^k$  are called the components of the vector  $A$  with respect to the given basis. These basis vectors form the coordinate axes and the transformation matrix introduced in equation (2.22) represents a change of basis vectors.

### 3.6 Subspace

A subspace can be defined as any subset of a vector space which satisfies the following condition (see Gerretsen 1962):

If  $\vec{A}$  and  $\vec{B}$  are vectors belonging to the subset, then all the vectors  $\alpha\vec{A} + \beta\vec{B}$ , where  $\alpha$  and  $\beta$  are arbitrary real numbers, also belong to the subset.

The whole space is a subspace of itself, called the "improper subspace". A "proper subspace" is a subspace which does not contain all the elements of the whole space. The set of basis vectors of a proper subspace is a subset of the set of basis vectors of the whole space, and therefore the dimension of the subspace, that is the number of vectors in its basis, is less than the dimension of the whole space.

A transformation operator corresponding to a change of basis vectors in an  $N$ -dimensional space can then be decomposed into an operator acting on the basis vectors of a subspace and an operator which acts on the other basis vectors of the whole space.

This approach will be relevant when we consider later (Section 3.7), magnetic materials (which can have complicated magnetic ordering), in which case we will be dealing with a six-dimensional space,  $V_M$  (six

degrees of freedom) composed of the three-dimensional geometrical subspace  $V$ , and the three-dimensional magnetic subspace  $M$ . In this six-dimensional space the transformation operator corresponding to a change of basic vectors can be written as  $\{R_p | R_i | W_{ip}\}$  (see Section 3.4), (Brinkman et al 1966 a,b and Litvin 1973) where  $\{R_i\}$  acts on the coordinates in the geometrical subspace and  $\{R_p\}$  acts on the coordinates in the magnetic subspace, and  $\{W_{ip}\}$  is a translation operator.

### 3.7 Formal Definition of a field dependent tensor

In a variety of circumstances one encounters situations where a physical property, which can be identified as a tensor in one subspace of the whole space, has components depending on the variables defined in the other subspaces. We generalize the idea one step further to say that the dependence of the tensor components defined in one subspace, on the basis vectors of another subspace might be more complicated than being just a scalar function.

For example in the six-dimensional space of the last section, a physical property can be considered which in the absence of magnetic field behaves like a tensor of rank  $n$ , that is, it is a tensor of rank  $n$  in the geometrical subspace  $V$ . After introducing the magnetic field the transformation operator will become more complicated and will involve  $\{R_p\}$ . Therefore the transformation law for this physical property (tensor of rank  $n$  in  $V$ ) has to be generalized to take operations  $\{R_p\}$  into account. To do this we have to seek the transformation law of the property corresponding to a change of basis vectors in magnetic subspace  $M$ , and find out what sort of tensorial dependence this property has on the magnetic subspace coordinates. That is, what is its rank,  $\ell$ , in this space; this rank  $\ell$  does not have to be the same as  $n$ , the rank of the property in  $V$ .  $\ell$  depends

entirely on each special property and the physical laws concerning that property. The process of finding  $\ell$  is similar to the ordinary case of field independent tensors (namely quotient law, see Section 4.6).

The transformation law for a tensor property A with rank n in V and rank  $\ell$  in M, which to maintain the generality is considered to be a tensor field in both subspaces can be written

$$\begin{aligned} \{R_p | R_i\} A_{i_1 \dots i_\ell j_1 \dots j_n}^{(m, r)} = \\ \underbrace{\quad}_{\ell} \underbrace{\quad}_{n} \\ = A'_{\alpha_1 \dots \alpha_\ell \beta_1 \dots \beta_n} (\{R_p\}^m, \{R_i\}^r), \end{aligned} \tag{3.8}$$

where  $m^1, \dots, m^\ell, m^{\alpha_1}, \dots, m^{\alpha_\ell}$  indices refer to the coordinate axes in M subspace and  $r^{j_1}, \dots, r^{j_n}, r^{\beta_1}, \dots, r^{\beta_n}$  indices refer to the coordinate axes in V subspace, and they all range from one to three (number of coordinate axes in a three-dimensional space). The transformation operator  $\{R_p\}$  has the matrix representation with components  $(R_p)^i_{m e} \alpha'_f$ , and the components of the representation matrix for operation  $\{R_i\}$  are  $(R_i)^j_e \beta_f$ . Therefore the operator  $\{R_p | R_i\}$  on the left hand side of equation (3.8) can be represented by

$$\begin{aligned} \{R_p | R_i\} = \underbrace{(R_p)^{i_1 \alpha_1}_{m_1 m_1} \dots (R_p)^{i_\ell \alpha_\ell}_{m_\ell m_\ell}}_{\ell} \\ \cdot \underbrace{(R_i)^{j_1 \beta_1}_{r_1 r_1} \dots (R_i)^{j_n \beta_n}_{r_n r_n}}_{n} \end{aligned} \tag{3.9}$$

The combined operation  $\{R_p | R_i\}$  acts in the following way: first operation  $\{R_i\}$  transforms the  $3^n$  components of the tensor A, in the subspace V, into their new values in the new reference frame in V, then each of these components which has  $3^\ell$  components in M is operated upon by  $\{R_p\}$  and is transformed into a set of  $3^\ell$  new values in the new set of  $m_1$  (which for instance could be magnetic coordinates). The number 3 is the dimension of the subspace in each case. Therefore our tensor property has indeed  $(3)^n \times (3)^\ell = 3^{\ell+n}$  components. In general, in a space composed of two subspaces V( $h_1$  - dimensional) and M( $h_2$  - dimensional), a tensor of rank n in V and rank  $\ell$  in M will have  $(h_1)^n + (h_2)^\ell$  components. Supposing that this tensor has t contravariant and s covariant indices in V ( $T + s = n$ ) and v contravariant and u covariant indices in M ( $v + u = \ell$ ), the transformation law for its components will be

$$\begin{aligned}
 & \underbrace{g_1 \dots g_v}_{m^1 \dots m^v} \quad \underbrace{j_1 \dots j_t}_{r^1 \dots r^t} \\
 A' & (m^1, r^1) = \frac{\partial m^{\alpha_1} g_1}{\partial m^1} \dots \frac{\partial m^{\alpha_v} g_v}{\partial m^v} \cdot \frac{\partial \beta_1}{\partial m^1} \dots \frac{\partial \beta_u}{\partial m^u} \cdot \frac{\partial r^{j_1}}{\partial r^1} \\
 & \underbrace{i_1 \dots i_u}_{m^1 \dots m^u} \quad \underbrace{k_1 \dots k_s}_{r^1 \dots r^s} \\
 & \dots \frac{\partial r^{j_t}}{\partial r^t} \frac{\partial \delta_1}{\partial r^1} \dots \frac{\partial \delta_s}{\partial r^s} A \begin{matrix} \alpha_1 & \dots & \alpha_v & \gamma_1 & \dots & \gamma_t \\ m^1 & \dots & m^v & r^1 & \dots & r^t \\ \beta_1 & \dots & \beta_u & \delta_1 & \dots & \delta_s \\ m^1 & \dots & m^u & r^1 & \dots & r^s \end{matrix} (m, r) \quad (3.10)
 \end{aligned}$$

For a relative, field dependent tensor, B, of weight  $\omega_1$  in V, and of weight  $\omega_2$  in M, and of the same rank and covariance and contravariance property as the tensor A in equations (3.10), the transformation law will be

$$\begin{aligned}
 B'_{m_1 \dots m_u r_1 \dots r_s}^{g_1 \dots g_v j_1 \dots j_t} (m', r') &= \left| \frac{\partial m^\alpha}{\partial m'^g} \right|^{\omega_1} \frac{\partial m'^{g_1}}{\partial m^{\alpha_1}} \dots \frac{\partial m'^{g_v}}{\partial m^{\alpha_v}} \\
 &\cdot \frac{\partial m^{\beta_1}}{\partial m'^{i_1}} \dots \frac{\partial m^{\beta_u}}{\partial m'^{i_u}} \cdot \left| \frac{\partial r^\gamma}{\partial r'^j} \right|^{\omega_2} \frac{\partial r'^{j_1}}{\partial r^{\gamma_1}} \dots \frac{\partial r'^{j_t}}{\partial r^{\gamma_t}} \cdot \frac{\partial r^{\delta_1}}{\partial r'^{k_1}} \dots \\
 &\cdot \frac{\partial r^{\delta_s}}{\partial r'^{k_s}} B_{m_1 \dots m_u r_1 \dots r_s}^{\alpha_1 \dots \alpha_v \gamma_1 \dots \gamma_t} (m, r) , \quad (3.11)
 \end{aligned}$$

where  $\left| \frac{\partial m^\alpha}{\partial m'^g} \right|$  and  $\left| \frac{\partial r^\gamma}{\partial r'^j} \right|$  are the determinants of the transformation matrices in M and V subspace. Equation (3.11) is the general transformation law for field dependent tensors. For a transformation operator, which is composed of orthogonal transformation of coordinate axes in all the subspaces of the whole space, there is no difference between covariant and contravariant indices and the transformation law (3.11) can be written as

$$\begin{aligned}
 A'_{m_{i_1} \dots m_{i_\ell} r_{j_1} \dots r_{j_m}} (m', r') &= \left| \frac{\partial m^\alpha}{\partial m'^i} \right|^{q_1} \cdot \left| \frac{\partial r^\beta}{\partial r'^j} \right|^{q_2} \frac{\partial m^{\alpha_1}}{\partial m'^{i_1}} \dots \\
 &\cdot \frac{\partial m^{\alpha_\ell}}{\partial m'^{i_\ell}} \cdot \frac{\partial r^{\beta_1}}{\partial r'^{j_1}} \dots \frac{\partial r^{\beta_n}}{\partial r'^{j_n}} A_{m_{\alpha_1} \dots m_{\alpha_\ell} r_{\beta_1} \dots r_{\beta_n}} (m, r) , \quad (3.12)
 \end{aligned}$$

where  $q_1 = \begin{cases} 0 & \text{for even } \omega_1 \text{ (polar in M) ,} \\ 1 & \text{for odd } \omega_1 \text{ axial in M) ,} \end{cases}$

and

$q_2 = \begin{cases} 0 & \text{for even } \omega_2 \text{ (polar in V) ,} \\ 1 & \text{for odd } \omega_2 \text{ (axial in V) .} \end{cases}$

As an example the conductivity tensor in the space composed of the three-dimensional geometrical subspace and the three-dimensional momentum subspace, can be considered. In this space a transformation of coordinates may be represented by the operator  $\{R_p | R_i | v_{ip}\}$  with  $R_p$  a rotation operation in the momentum subspace,  $R_i$  a rotation operation in the geometrical subspace, and  $v_{ip}$  a translation operation. The form of the Ohm's law in the three-dimensional geometrical subspace is

$$J_i = \sigma_{ij} E_j, \quad (3.13)$$

with  $J$  and  $E$  acting as vectors, or first rank tensors and  $\sigma_{ij}$  as a second rank tensor. Therefore the effect of  $R_i$  on  $\sigma_{ij}$  can be easily found. But for  $R_p$ , the behaviour of  $J$ ,  $E$  and  $\sigma$  in the momentum subspace has to be found first. Since electric field  $E$  at a point depends only on the distance between the point and the charged body, which is creating the field, every rotation of coordinate axes in the momentum subspace leaves  $E$  unchanged. Therefore electric field  $E$  behaves like a scalar in the momentum subspace. The current density  $J$  can be written as the product of electric charge density times electric charge velocity;  $J = \rho \cdot v$ . Electric charge density  $\rho$  is a scalar in momentum subspace and  $v$  the charge velocity is a vector. Therefore using the quotient law (see Section 4.6),  $J$ , the current density, is a tensor of first rank, or a vector, in the momentum subspace, and can be written as  $(J_i)_{m_k}$ , with nine components ( $m_k$  refers to coordinate axes in the momentum subspace). Now by using the quotient law it can be shown that conductivity is also a vector in the momentum subspace, and can be written as  $(\sigma_{ij})_{m_k}$  with twenty seven components. Thus we can conclude the generalized Ohm's law in the space composed of the geometrical subspace and the momentum subspace :

$$(J_i)_{m_k} = (\sigma_{ij})_{m_k} E_j \quad (3.14)$$



Spin-tensor quantities can be considered as another example of quantities with such multi-tensorial character. Spinors have been defined in the following way (Corson 1953):

Spinors are geometrical objects  $\psi_A$  which are defined over a two dimensional space (the spin-space) and obey the following transformation law ,

$$\psi'_A = S_A^B \psi_B \quad (A, B = 1, 2) \quad (3.15)$$

with  $S_A^B$  the transformation matrix in s-space (the spin-space).  $\psi_A$  defined in this way is a covariant spinor of first rank in the spin-space. In our terminology this will be a covariant tensor of first rank in the spin subspace. There are also higher rank spinors and weighted spinors. In addition spin-tensors are defined as those quantities which have both tensor and spinor indices and obey the transformation laws

$$\phi'_{\mu AB} = a_{\mu}^{\nu} \phi_{\nu AB} \quad (3.16)$$

under coordinate transformation  $a_{\mu}^{\nu}$  in the geometrical subspace ( $a_{\mu\nu}$  in notations used in this thesis), and

$$\phi'_{\mu AB} = S_A^C S_B^D \phi_{\mu CD} \quad (3.17)$$

under spin transformation in the spin-subspace. All these quantities might be defined in terms of field dependent tensor terminology. It is apparent that there will be many other quantities which arise in different field of physics that can be brought under a blanket definition of field dependent tensors.

### 3.8 The nature of coordinates in the field subspace

So far in the definition of field dependent tensors and their transformation laws we have just considered the dependence of the field dependent tensor components on extra coordinates (coordinates in the field subspace), without any special reference to the nature of the field. By the nature of field components, we mean the relation between the coordinates in the field subspace and the geometrical subspace. This relation will be investigated in this section.

First we consider the simple case where the field coordinates are scalar quantities in the geometrical subspace (quantities which are independent of the choice of coordinates in the geometrical subspace), such as temperature, colour or shape of the individual object (different colours or different shapes can be characterized by different numbers). In this case transformation operators of the geometrical subspace do not have any effect on the coordinates in the field subspace, and equations (3.8), (3.9), (3.10), (3.11) and (3.12) can be used to find the transformed set of field dependent tensor components.

There are other cases where the coordinates in the field subspace depend on the direction of coordinate axes in the geometrical subspace. Examples of this are the space composed of momentum and geometrical subspaces, described in the last section, where momentum is itself a vector in the geometrical subspace, or the space of a magnetic crystal where the magnetic moments (coordinates of the field subspace) are vectors in the geometrical subspace. In constructing the set of symmetry operations of such spaces the effect of each symmetry operation on every coordinate axis should be specified. In this sense there are different possibilities for symmetry operations;

- (i) the symmetry operations of the geometrical subspace are sufficient to satisfy the symmetry requirements of the field subspace,
- (ii) extra operations in the field subspace must be added to each transformation operation of the geometrical subspace to satisfy the symmetry requirements of the field subspace,
- (iii) the operations which satisfy the symmetry requirements of the field subspace are quite different from those in the geometrical subspace, which are supposed to leave the coordinates in the field subspace unchanged. Here, to find the set of transformed components of a field dependent tensor, the transformation law (one of the equations (3.8), (3.9), (3.10), (3.11) or (3.12) according to the kind of tensor under consideration) of the last section can be employed.

For spaces of the kind (i) and (ii) where one transformation operator may act on both of the subspaces the situation is slightly different. To explain this let us consider tensor properties which act like scalar functions in the field subspace. Under a transformation of coordinates in the geometrical subspace, denoted by operator  $\{R\}$ , the transformation law for such a tensor property will have one of the following forms:

- (a) when the coordinates in the field subspace are vectors in the geometrical subspace;

$$\begin{aligned}
 & B, r_1^{j_1} \dots r_t^{j_t} \left( \frac{\partial r^\alpha}{\partial r'^i} m_\alpha, \frac{\partial r'^\beta}{\partial r^\beta} r^\beta \right) = \frac{\partial r'^{j_1}}{\partial r^{Y_1}} \dots \frac{\partial r'^{j_t}}{\partial r^{Y_t}} \cdot \frac{\partial r^{\delta_1}}{\partial r^{k_1}} \dots \\
 & \cdot \frac{\partial r^{\delta_s}}{\partial r'^s} \cdot B, r_1^{Y_1} \dots r_t^{Y_t} \left( m_\alpha, r^\beta \right), \quad (3.18)
 \end{aligned}$$

where  $\frac{\partial r^i}{\partial r'^j}$  is the  $|R|_{ij}$  element of the transformation matrix. (R) ,

(b) when the coordinates in the field subspace are second rank tensors in the geometrical subspace:

$$\begin{aligned}
 & B, r_1^{j_1} \dots r_t^{j_t} \left( \frac{\partial r^{\alpha_1}}{\partial r'^{i_1}} \cdot \frac{\partial r^{\alpha_2}}{\partial r'^{i_2}} m_{\alpha_1 \alpha_2}, \frac{\partial r'^g}{\partial r^\beta} r^\beta \right) = \frac{\partial r'^{j_1}}{\partial r^{Y_1}} \dots \frac{\partial r'^{j_t}}{\partial r^{Y_t}} \\
 & \cdot \frac{\partial r^{\delta_1}}{\partial r'^{k_1}} \dots \frac{\partial r^{\delta_s}}{\partial r'^{k_s}} B, r_1^{Y_1} \dots r_t^{Y_t} \left( m_{\alpha_1 \alpha_2}, r^\beta \right), \quad (3.19)
 \end{aligned}$$

where  $m_{i_1 i_2}$  are the components of the field tensor along the coordinate axes in the geometrical subspace, (the field tensor could have contra-variant indices as well),

(c) when the coordinates in the field subspace are tensors of ranks higher than two:

$$\begin{aligned}
 & B^{r_1 \dots r_t} \left( \frac{\partial x^{\alpha_1}}{\partial x'^{i_1}} \dots \frac{\partial x^{\alpha_a}}{\partial x'^i} m_{\alpha_1 \dots \alpha_a}, \frac{\partial x'^g}{\partial x'^\beta} r^\beta \right) = \frac{\partial x'^{j_1}}{\partial x'^{Y_1}} \dots \frac{\partial x'^{j_t}}{\partial x'^{Y_t}} \frac{\partial x^{\delta_1}}{\partial x'^{k_1}} \\
 & \dots \frac{\partial x^{\delta_s}}{\partial x'^{k_s}} B^{r_1 \dots r_t} \left( m_{\alpha_1 \dots \alpha_a}, r^\beta \right), \quad (3.20)
 \end{aligned}$$

the field tensor could also have contravariant indices.

We may extend what has been said also to the case of field dependent tensor properties which have ranks higher than zero in the field subspace, where the field components are themselves tensors in the geometrical subspace. Then for spaces of kind (i) and (ii), a transformation operator  $\{R\}$  in the geometrical subspace which can satisfy a part of or all the symmetry requirements of the field subspace will transform the components of the field tensor in the geometrical subspace in the following way:

$$m'_{\alpha_1 \dots \alpha_u} = \frac{\partial x^{i_1}}{\partial x'^1} \dots \frac{\partial x^{i_u}}{\partial x'^{\alpha_u}} m_{i_1 \dots i_u}, \quad (3.21)$$

where  $m'_{\alpha_1 \dots \alpha_u}$  are the field components along the coordinate axes in the geometrical subspace. Now we can construct the transformation operator  $\{R_p\}$  in the field subspace, corresponding to the transformation operator  $\{R\}$  in the geometrical subspace. We can write,

$$m'_a = \{R_p\}_{ab} m_b, \quad (3.22)$$

where  $m'_a = m'_{\alpha_1 \dots \alpha_u}$ , and  $m_b = m_{i_1 \dots i_u}$ , and

$$\{R_p\} = \frac{\partial x^{i_1}}{\partial x'^{\alpha_1}} \dots \frac{\partial x^{i_u}}{\partial x'^{\alpha_u}} \quad (3.23)$$

Then equation (3.8) can be used as the transformation law for field dependent tensors with operation  $\{R_p\}$  as defined in equation (3.23).

CHAPTER 4

FIELD DEPENDENT TENSORS (II):

CALCULUS

4.1 Introduction

The basic concepts and theorems of the algebra of field independent tensors (Sections 2.11, 2.12 and 2.13) such as addition and subtraction operations can be generalized to establish the algebra of field dependent tensors. This is done here for the first time. In this chapter the way the operations of addition, subtraction, inner and outer multiplication, contraction and differentiation of field dependent tensors act are worked out, and the conditions under which these operations can be performed are discussed. Furthermore, the quotient law is generalized to include field dependent tensors.

4.2 Addition and subtraction

Theorem 1:

In the space composed of two subspaces R and M, it will be shown that the sum (or difference) of two field dependent tensors  $A(r,m)$  and  $B(r,m)$  ( $r$  and  $m$  refer to the coordinate axes in R and M subspaces) which have the same rank  $h$  (with the same number of covariant  $f$  and the same number of contravariant  $e$  indices ( $f + e = h$ )) in R and the same rank  $n$  (with the same number of covariant  $p$  and the same number of contravariant  $q$  indices ( $p + q = n$ )) in M, defined at the same point is again a field dependent tensor  $C(r,m)$  of the same rank and type in R and the same rank and type in M.

Proof: The corresponding transformation laws (equation 3.10) for  $A(r,m)$  and  $B(r,m)$  are

$$\begin{aligned}
 & \underbrace{g_1 \dots g_q}_{q} \quad \underbrace{j_1 \dots j_e}_{e} \\
 A'_{m'1} \dots m'q & \quad r_1 \dots r_e \\
 & \underbrace{i_1 \dots i_p}_{p} \quad \underbrace{k_1 \dots k_f}_{f} \\
 & m_1 \dots m_p \quad r_1 \dots r_f \\
 (r', m') & = \frac{\partial m'_1}{\alpha_1} \dots \frac{\partial m'_q}{\alpha_q} \cdot \frac{\partial m_1}{\beta_1} \dots \frac{\partial m_p}{\beta_p} \\
 & \cdot \frac{\partial r'_1}{\gamma_1} \dots \frac{\partial r'_e}{\gamma_e} \cdot \frac{\partial r_1}{\delta_1} \dots \frac{\partial r_f}{\delta_f} \quad A \quad \begin{matrix} \alpha_1 \dots \alpha_q & \gamma_1 \dots \gamma_e \\ \beta_1 \dots \beta_p & \delta_1 \dots \delta_f \end{matrix} \quad (r, m) , \\
 & \hspace{15em} (4.1)
 \end{aligned}$$

$$\begin{aligned}
 & \underbrace{g_1 \dots g_q}_{q} \quad \underbrace{j_1 \dots j_e}_{e} \\
 B'_{m'1} \dots m'q & \quad r_1 \dots r_e \\
 & \underbrace{i_1 \dots i_p}_{p} \quad \underbrace{k_1 \dots k_f}_{f} \\
 & m_1 \dots m_p \quad r_1 \dots r_f \\
 (r', m') & = \frac{\partial m'_1}{\alpha_1} \dots \frac{\partial m'_q}{\alpha_q} \cdot \frac{\partial m_1}{\beta_1} \dots \frac{\partial m_p}{\beta_p} \\
 & \cdot \frac{\partial r'_1}{\gamma_1} \dots \frac{\partial r'_e}{\gamma_e} \cdot \frac{\partial r_1}{\delta_1} \dots \frac{\partial r_f}{\delta_f} \quad B \quad \begin{matrix} \alpha_1 \dots \alpha_q & \gamma_1 \dots \gamma_e \\ \beta_1 \dots \beta_p & \delta_1 \dots \delta_f \end{matrix} \quad (r, m) . \\
 & \hspace{15em} (4.2)
 \end{aligned}$$

Then adding each component of A' from equation (4.1) to the corresponding component of B' from equation (4.2), we arrive at a set with the same number of components which obeys the following transformation law



$$\begin{aligned}
 & A' \begin{matrix} g_1 & \dots & g_q & j_1 & \dots & j_e \\ m_1 & \dots & m_q & r_1 & \dots & r_e \end{matrix} (r', m') \pm B' \begin{matrix} g_1 & \dots & g_q & j_1 & \dots & j_e \\ m_1 & \dots & m_q & r_1 & \dots & r_e \end{matrix} (r', m') = \\
 & \begin{matrix} i_1 & \dots & i_p & k_1 & \dots & k_f \\ m_1 & \dots & m_p & r_1 & \dots & r_f \end{matrix} \\
 & = \frac{\partial m_1^{g_1}}{\partial m^{\alpha_1}} \dots \frac{\partial m_q^{g_q}}{\partial m^{\alpha_q}} \cdot \frac{\partial m_1^{\beta_1}}{\partial m^{i_1}} \dots \frac{\partial m_p^{\beta_p}}{\partial m^{i_p}} \cdot \frac{\partial r_1^{j_1}}{\partial r^{\gamma_1}} \dots \frac{\partial r_e^{j_e}}{\partial r^{\gamma_e}} \cdot \frac{\partial r_1^{\delta_1}}{\partial r^{k_1}} \dots \frac{\partial r_f^{\delta_f}}{\partial r^{k_f}} \\
 & \cdot \left( \begin{matrix} \alpha_1 & \dots & \alpha_q & \gamma_1 & \dots & \gamma_e \\ m_1 & \dots & m_q & r_1 & \dots & r_e \end{matrix} (r, m) \pm \begin{matrix} \alpha_1 & \dots & \alpha_q & \gamma_1 & \dots & \gamma_e \\ m_1 & \dots & m_q & r_1 & \dots & r_e \end{matrix} (r, m) \right). \tag{4.3}
 \end{aligned}$$

Therefore the set of components ,

$$\begin{aligned}
 & C \begin{matrix} \overbrace{\alpha_1 \dots \alpha_q}^q & \overbrace{\gamma_1 \dots \gamma_e}^e \\ m_1 \dots m_q & r_1 \dots r_e \end{matrix} (r, m) = \\
 & \begin{matrix} \overbrace{\beta_1 \dots \beta_p}^p & \overbrace{\delta_1 \dots \delta_f}^f \\ m_1 \dots m_p & r_1 \dots r_f \end{matrix} \\
 & A \begin{matrix} \alpha_1 & \dots & \alpha_q & \gamma_1 & \dots & \gamma_e \\ m_1 & \dots & m_q & r_1 & \dots & r_e \end{matrix} (r, m) \pm B \begin{matrix} \alpha_1 & \dots & \alpha_q & \gamma_1 & \dots & \gamma_e \\ m_1 & \dots & m_q & r_1 & \dots & r_e \end{matrix} (r, m), \tag{4.4} \\
 & \begin{matrix} \beta_1 & \dots & \beta_p & \delta_1 & \dots & \delta_f \\ m_1 & \dots & m_p & r_1 & \dots & r_f \end{matrix}
 \end{aligned}$$

forms a field dependent tensor of the same rank and type as the two original tensors A and B, in each subspace.

General extension of the theorem: the operation of addition can be immediately extended to find the (algebraic) sum of any number of field dependent tensors, provided they all have the same rank and are all of the same type (equal number of covariant indices and equal number of contravariant indices) in every subspace of the whole space. But the operation of addition does not apply to field dependent tensors which have different ranks or are of different types in a subspace.

Theorem II:

The set of functions formed by multiplying each component of a field dependent tensor by a constant  $\psi$  is itself a field dependent tensor with the same tensorial character (the same rank and type in every subspace). This is readily proved by multiplying both sides of equation (4.1) by a constant  $\psi$ . From this fact together with the definition of the addition operation, it can be stated that:

Any linear combination of field dependent tensors of the same tensorial character is a field dependent tensor of the same character.

#### 4.3 Outer multiplication of two field dependent tensors

Definition:

In a space composed of two subspaces M (with  $m_i$  as coordinate axes) and R (with  $r_i$  as coordinate axes), consider two field dependent tensors:  $A(r,m)$  of rank  $k$  (with  $s$  contravariant and  $p$  covariant indices  $s + p = k$ ) in M subspace and of rank  $\ell$  (with  $t$  contravariant and  $q$  covariant indices  $t + q = \ell$ ) in R subspace, and  $B(r,m)$  of rank  $n$  (with  $i$  contravariant and  $u$  covariant indices  $i + u = n$ ) in M subspace and of  $\sigma$  rank (with  $j$  contravariant and  $v$  covariant  $j + v = \sigma$ ) in R subspace. The outer product of these two field dependent tensors can be defined as the set of

elements  $C(r,m)$  formed by multiplying each component of  $A(r,m)$  by each component of the tensor  $B(r,m)$ . That is

$$\begin{array}{c}
 \overbrace{a_1 \dots a_s}^s \quad \overbrace{b_1 \dots b_t}^t \\
 m_1 \dots m_s \quad r_1 \dots r_t \\
 A \quad \overbrace{c_1 \dots c_p}^p \quad \overbrace{d_1 \dots d_q}^q \quad (r,m) \cdot B \quad \overbrace{e_1 \dots e_i}^i \quad \overbrace{f_1 \dots f_j}^j \\
 m_1 \dots m_p \quad r_1 \dots r_q \quad \overbrace{g_1 \dots g_u}^u \quad \overbrace{h_1 \dots h_v}^v \quad (r,m) \equiv \\
 \\
 \equiv C \quad \overbrace{a_1 \dots a_s \quad e_1 \dots e_i}^{s+i} \quad \overbrace{b_1 \dots b_t \quad f_1 \dots f_j}^{t+j} \\
 m_1 \dots m_s \quad m_1 \dots m_i \quad r_1 \dots r_t \quad r_1 \dots r_j \\
 \overbrace{c_1 \dots c_p \quad g_1 \dots g_u}^{p+u} \quad \overbrace{d_1 \dots d_q \quad h_1 \dots h_v}^{q+v} \\
 m_1 \dots m_p \quad m_1 \dots m_u \quad r_1 \dots r_q \quad r_1 \dots r_v \\
 (r,m) \cdot \quad (4.5)
 \end{array}$$

After the transformation of coordinate axes  $(r,m)$  into new axes  $(r',m')$  the outer product can be written as

$$\begin{array}{c}
 \alpha_1 \dots \alpha_s \quad \epsilon_1 \dots \epsilon_i \quad \beta_1 \dots \beta_t \quad \eta_1 \dots \eta_j \\
 m_1 \dots m_s \quad m_1 \dots m_i \quad r_1 \dots r_t \quad r_1 \dots r_j \\
 C' \quad \gamma_1 \dots \gamma_p \quad \lambda_1 \dots \lambda_u \quad \delta_1 \dots \delta_q \quad \mu_1 \dots \mu_v \\
 m_1 \dots m_p \quad m_1 \dots m_u \quad r_1 \dots r_q \quad r_1 \dots r_v \\
 (r',m') \equiv \\
 \\
 \equiv A' \quad \alpha_1 \dots \alpha_s \quad \beta_1 \dots \beta_t \quad \epsilon_1 \dots \epsilon_i \quad \eta_1 \dots \eta_j \\
 m_1 \dots m_s \quad r_1 \dots r_t \quad m_1 \dots m_i \quad r_1 \dots r_j \\
 (r',m') \cdot B' \quad \gamma_1 \dots \gamma_p \quad \delta_1 \dots \delta_q \quad \lambda_1 \dots \lambda_u \quad \mu_1 \dots \mu_v \\
 m_1 \dots m_p \quad r_1 \dots r_q \quad m_1 \dots m_u \quad r_1 \dots r_v \\
 (r',m') \cdot \\
 \\
 (4.6)
 \end{array}$$

Changing the dummy suffixes in equations (4.1) and (4.2), and substituting for  $A'(r,m)$  and  $B'(r,m)$  from these equations into equation (4.6) shows that the set of elements of the outer product  $C(r,m)$  forms a field dependent

tensor of rank  $k + n$  (with  $s + i$  contravariant and  $p + u$  covariant indices  $s + i + p + u = k + n$ ) in  $M$  and of rank  $\ell + 0$  (with  $t + j$  contravariant and  $q + v$  covariant indices  $t + j + q + v = \ell + 0$ ) in  $R$  subspace.

#### 4.4 Contraction of field dependent tensors

In a space composed of two subspaces  $R$  ( $n$ -dimensional) and  $M$  ( $\ell$ -dimensional) consider a field dependent tensor

$$A \begin{matrix} a_1 & \dots & a_s & b_1 & \dots & b_t \\ m_1 & \dots & m_s & r_1 & \dots & r_t \\ c_1 & \dots & c_p & d_1 & \dots & d_q \\ m_1 & \dots & m_p & r_1 & \dots & r_q \end{matrix} (r, m) \text{ of rank } s + p \text{ in } M \text{ and rank } t + q \text{ in } R \text{ (}$$

and  $t$  contravariant,  $p$  and  $q$  covariant). Equating a covariant index  $m_{c_j}$  and a contravariant index  $m_{a_i}$  in the same subspace  $M$  and summing with respect to this index will result in a set of  $(\ell)^{s+p-2} (m)^{t+q}$  functions. This is the operation of contraction. It will be shown that this set of functions forms a field dependent tensor of rank  $s + p - 2$  in  $M$  subspace and  $t + q$  in  $R$  subspace. In order to avoid writing out long formulae with many covariant and contravariant indices in each subspace we illustrate the proof by considering a field dependent tensor

$$A \begin{matrix} a_1 & a_2 & b_1 & b_2 \\ m_1 & m_2 & r_1 & r_2 \\ c_1 & c_2 & c_3 & d_1 \\ m_1 & m_2 & m_3 & r_1 \end{matrix} (r, m). \text{ The transformation law for this tensor is (see}$$

equation 4.1)

$$A' \begin{matrix} a_1 & a_2 & b_1 & b_2 \\ m_1 & m_2 & r_1 & r_2 \\ c_1 & c_2 & c_3 & d_1 \\ m_1 & m_2 & m_3 & r_1 \end{matrix} (r', m') = \left( \frac{\partial m'^{a_1}}{\partial m^{a_1}} \cdot \frac{\partial m'^{a_2}}{\partial m^{a_2}} \cdot \frac{\partial m^{\gamma_1}}{\partial m'^{c_1}} \cdot \frac{\partial m^{\gamma_2}}{\partial m'^{c_2}} \cdot \frac{\partial m^{\gamma_3}}{\partial m'^{c_2}} \right)$$

$$\cdot \left( \frac{\partial r'^{b_1}}{\partial r^{\beta_1}} \cdot \frac{\partial r'^{b_2}}{\partial r^{\beta_2}} \cdot \frac{\partial r^{\delta_1}}{\partial r'^{d_1}} \right) \begin{matrix} a_1 & a_2 & \beta_1 & \beta_2 \\ m_1 & m_2 & r_1 & r_2 \\ \gamma_1 & \gamma_2 & \gamma_3 & \delta_1 \\ m_1 & m_2 & m_3 & r_1 \end{matrix} (r, m) \quad (4.7)$$

Now if we equate  $m^{a_2}$  and  $m^{c_3}$  in equation (4.7) we obtain

$$A' \begin{matrix} a_1 & a_2 & b_1 & b_2 \\ m_1 & m_2 & r_1 & r_2 \\ c_1 & c_2 & c_3 & d_1 \end{matrix} (r', m') = \frac{\partial m^{a_1}}{\partial m^{\alpha_1}} \cdot \frac{\partial m^{a_2}}{\partial m^{\alpha_2}} \cdot \frac{\partial m^{\gamma_1}}{\partial m^{c_1}} \cdot \frac{\partial m^{\gamma_2}}{\partial m^{c_2}} \cdot \frac{\partial m^{\gamma_3}}{\partial m^{a_2}}$$

$$\cdot \frac{\partial r^{b_1}}{\partial r^{\beta_1}} \cdot \frac{\partial r^{b_2}}{\partial r^{\beta_2}} \cdot \frac{\partial r^{\delta_1}}{\partial r^{d_1}} \begin{matrix} \alpha_1 & \alpha_2 & \beta_1 & \beta_2 \\ m_1 & m_2 & r_1 & r_2 \\ \gamma_1 & \gamma_2 & \gamma_3 & \delta_1 \end{matrix} (r, m)$$

Therefore ,

$$A' \begin{matrix} a_1 & a_2 & b_1 & b_2 \\ m_1 & m_2 & r_1 & r_2 \\ c_1 & c_2 & c_3 & d_1 \end{matrix} (r', m') = \frac{\partial m^{a_1}}{\partial m^{\alpha_1}} \cdot \frac{\partial m^{\gamma_1}}{\partial m^{c_1}} \cdot \frac{\partial m^{\gamma_2}}{\partial m^{c_2}} \cdot \frac{\partial r^{b_1}}{\partial r^{\beta_1}} \cdot \frac{\partial r^{b_2}}{\partial r^{\beta_2}}$$

$$\cdot \frac{\partial r^{\delta_1}}{\partial r^{d_1}} \begin{matrix} \alpha_2 & \alpha_1 & \alpha_2 & \beta_1 & \beta_2 \\ m_2 & m_1 & m_2 & r_1 & r_2 \\ \gamma_3 & \gamma_1 & \gamma_2 & \gamma_3 & \delta_1 \end{matrix} (r, m)$$

That is:

$$A' \begin{matrix} a_1 & a_2 & b_1 & b_2 \\ m_1 & m_2 & r_1 & r_2 \\ c_1 & c_2 & a_2 & d_1 \end{matrix} (r', m') = \frac{\partial m^{a_1}}{\partial m^{\alpha_1}} \cdot \frac{\partial m^{\gamma_1}}{\partial m^{c_1}} \cdot \frac{\partial m^{\gamma_2}}{\partial m^{c_2}} \cdot \frac{\partial r^{b_1}}{\partial r^{\beta_1}} \cdot \frac{\partial r^{b_2}}{\partial r^{\beta_2}}$$

$$\cdot \frac{\partial r^{\delta_1}}{\partial r^{d_1}} \begin{matrix} \alpha_1 & \alpha_2 & \beta_1 & \beta_2 \\ m_1 & m_2 & r_1 & r_2 \\ \gamma_1 & \gamma_2 & \alpha_2 & \delta_1 \end{matrix} (r, m) \tag{4.8}$$

Equation (4.8) shows that  $A \begin{matrix} a_1 & a_2 & b_1 & b_2 \\ m_1 & m_2 & r_1 & r_2 \\ c_1 & c_2 & a_2 & d_1 \\ m_1 & m_2 & m_2 & r_1 \end{matrix} (r,m)$  is a field dependent

tensor of the same rank as  $A \begin{matrix} a_1 & a_2 & b_1 & b_2 \\ m_1 & m_2 & r_1 & r_2 \\ c_1 & c_2 & c_3 & d_1 \\ m_1 & m_2 & m_2 & r_1 \end{matrix} (r,m)$  in R subspace but of

rank less than  $A \begin{matrix} a_1 & a_2 & b_1 & b_2 \\ m_1 & m_2 & r_1 & r_2 \\ c_1 & c_2 & c_3 & d_1 \\ m_1 & m_2 & m_2 & r_1 \end{matrix} (r,m)$  by two (one contravariant, one

covariant), in M subspace. It should be borne in mind that the operation of contraction (lowering the number of covariant and contravariant indices by one) can only be applied to two indices which are of different types and refer to the axes defined in one subspace. Moreover the operation of contraction can be carried out for all the indices of a field dependent tensor one after another, as far as there are indices of both types present in the same subspace.

#### 4.5 Inner multiplication of field dependent tensors

The operation of inner multiplication of two field dependent tensors is a combination of the operations of outer multiplication and tensor contraction. That is, to find the inner product of two field dependent tensors, first we find their outer product and then we apply the operation of contraction. As an example, consider two field dependent tensors

$$A \begin{matrix} a_1 & b_1 \\ m_1 & r_1 \\ c_1 & c_2 & d_1 \\ m_1 & m_2 & r_1 \end{matrix} (r,m) \quad \text{and} \quad B \begin{matrix} e_1 & e_2 \\ m_1 & m_2 \\ g_1 & h_1 \\ m_1 & m_1 \end{matrix} (r,m); \quad \text{then forming their outer product,}$$

we obtain

$$\begin{matrix} a_1 & e_1 & e_2 & b_1 \\ m_1 & m_1 & m_2 & r_1 \end{matrix} \begin{matrix} c_1 & c_2 & g_1 & d_1 & h_1 \\ m_1 & m_2 & m_1 & r_1 & r_1 \end{matrix} (r,m) = \begin{matrix} a_1 & b_1 \\ m_1 & r_1 \end{matrix} (r,m) \begin{matrix} e_1 & e_2 \\ m_1 & m_2 \end{matrix} \begin{matrix} g_1 & h_1 \\ m_1 & m_1 \end{matrix} (r,m) .$$

The field dependent tensor  $\begin{matrix} a_1 & e_1 & e_2 & b_1 \\ m_1 & m_1 & m_2 & r_1 \end{matrix} \begin{matrix} c_1 & c_2 & g_1 & d_1 & h_1 \\ m_1 & m_2 & m_1 & r_1 & r_1 \end{matrix} (r,m)$  can be contracted

three times in M subspace and once in R subspace (these contractions can be performed in several ways: two different ways in R and six different ways in M).

#### 4.6 The quotient law of field dependent tensors

The quotient law, defined in Section 2.12 for field independent tensors, can be generalized to include field dependent tensors in the following way. That is, it can be stated that in the space composed of two subspaces R (n-dimensional) and M (l-dimensional), the set of  $(n^h)(l^k)$  functions of coordinates r and m forms a field dependent tensor of rank h in R subspace and of rank k in M subspace (with a certain number of contravariant and covariant indices), provided that an inner product of this set of functions with an arbitrary field dependent tensor is itself a field dependent tensor, (the inner product of a tensor and a set of functions means the sum of the form

$$A(m^\alpha, m^{i_2}, \dots, m^{i_k}, r^{j_1}, \dots, r^{j_k}) A_\alpha, \text{ or } A(m^\alpha, m^{i_2}, \dots, m^{i_k}, r^{j_1}, \dots, r^{j_k}) A^m_\alpha .$$

Writing out the general proof for this statement involves long formulae with many contravariant and covariant indices. To avoid this the proof is given here for the following special case which has all the features of the general case. Consider the set of  $(m^3) \times (l^2)$  functions  $A(m^a, m^b, m^c, r^d, r^e)$ . Now let us suppose that the inner product ,

$$A(m^a, m^b, m^c, r^d, r^e) B_{m^c}^{m^a r^f} (r, m),$$

for an arbitrary field dependent tensor  $B_{m^c}^{m^a r^f} (r, m)$  yields a field dependent tensor  $C_{r^e r^d}^{m^b r^f} (r, m)$  of first rank (contravariant) in M and of third rank (two covariant and one contravariant) in R. That is

$$A(m^a, m^b, m^c, r^d, r^e) B_{m^c}^{m^a r^f} (r, m) = C_{r^e r^d}^{m^b r^f} (r, m) \quad (4.9)$$

The transformed quantities, referred to a new system of coordinates  $(r', m')$ , satisfy the following equation

$$A'(m'^a, m'^b, m'^c, r'^d, r'^e) B'_{m'^c}^{m'^a r'^f} (r', m') = C'_{r'^e r'^d}^{m'^b r'^f} (r', m') \quad (4.10)$$

Substituting for  $B'_{m'^c}^{m'^a r'^f} (r', m')$  and  $C'_{r'^e r'^d}^{m'^b r'^f} (r', m')$  from their trans-

formation laws (equation 4.1) into equation (4.10), we obtain

$$A'(m'^a, m'^b, m'^c, r'^d, r'^e) \frac{\partial m'^a}{\partial m^\alpha} \cdot \frac{\partial m^\gamma}{\partial m'^c} \cdot \frac{\partial r'^f}{\partial r^\mu} B_{m^\gamma}^{m^\alpha r^\mu} (r, m) =$$

$$= \frac{\partial m'^b}{\partial m^\beta} \cdot \frac{\partial r^e}{\partial r'^e} \cdot \frac{\partial r'^f}{\partial r^\mu} \cdot \frac{\partial r^\delta}{\partial r'^d} C_{r^e r^\delta}^{m^\beta r^\mu} (r, m) \quad (4.11)$$

Substituting for  $C_{r^e r^\delta}^{m^\beta r^\mu} (r, m)$  from equation (4.9) into equation (4.11) and changing the dummy indices, we get



$$\frac{\partial x'^f}{\partial x'^\mu} \left[ A'(m^a, m^b, m^c, r^d, r^e) \frac{\partial m'^a}{\partial m^\alpha} \cdot \frac{\partial m^\gamma}{\partial m'^c} - A(m^\alpha, m^\beta, m^\gamma, r^\delta, r^\epsilon) \cdot \frac{\partial m'^b}{\partial m^\beta} \cdot \frac{\partial r^\epsilon}{\partial m'^e} \cdot \frac{\partial r^\delta}{\partial r'^d} \right] B_{m^\gamma}^{m^\alpha r^\mu} (x, m) \equiv 0 \quad (4.12)$$

Equation (4.12) should hold for every  $B_{m^\gamma}^{m^\alpha r^\mu} (x, m)$ , the arbitrary tensor.

Therefore the expression in the bracket is identically zero, that is

$$A'(m^a, m^b, m^c, r^d, r^e) = \frac{\partial m^\alpha}{\partial m'^a} \cdot \frac{\partial m'^b}{\partial m^\beta} \cdot \frac{\partial m'^c}{\partial m^\gamma} \cdot \frac{\partial r^\epsilon}{\partial r'^e} \cdot \frac{\partial r^\delta}{\partial r'^d} \cdot A(m^\alpha, m^\beta, m^\gamma, r^\delta, r^\epsilon), \quad (4.13)$$

which shows that  $A(m^\alpha, m^\beta, m^\gamma, r^\delta, r^\epsilon)$  is a field dependent tensor of rank three in M subspace (contravariant in  $m^\beta$  and  $m^\gamma$ , and covariant in  $m^\alpha$ ) and of rank two in R subspace (covariant in both  $r^\delta$  and  $r^\epsilon$ ), that is

$$A(m^\alpha, m^\beta, m^\gamma, r^\delta, r^\epsilon) = A_{m^\alpha r^\delta r^\epsilon}^{m^\beta m^\gamma} (x, m). \quad (4.14)$$

The tensorial character of a set of functions can also be investigated in each subspace separately by means of the quotient law. The quotient law can then be stated in the following way:

A set of functions forms a field dependent tensor of certain rank (with certain covariant and contravariant indices) in a subspace if an inner product of this set of functions with an arbitrary field dependent tensor in that subspace is again a field dependent tensor in the same subspace.

#### 4.7 Differentiation of field dependent tensors

The way in which the differentiation operator has been dealt with for field independent tensors in Section 2.13 can be followed for the components of a field dependent tensor in one subspace. That is, it can be stated that, in a space composed of two subspaces R(n-dimensional) and M (l-dimensional), the set of partial derivatives  $\frac{\partial}{\partial m^a}$  (with respect to the coordinates in M) of a field dependent tensor which behaves like a scalar function in M, forms a field dependent tensor which acts like a covariant tensor of rank one in M. The tensorial character of this field dependent tensor in the subspace R does not change after differentiation. This field dependent tensor (scalar in the subspace M) can be denoted as  $A_{(r)}(r,m)$ , where the suffix (r) shows that the tensor  $A_{(r)}(r,m)$  has an undefined character in the subspace R. The set of partial derivatives can then be denoted as  $\frac{\partial A_{(r)}(r,m)}{\partial m^a}$ . Now if we form the set of partial derivatives with respect to the coordinates in the subspace M of the field dependent covariant vector  $\frac{\partial A_{(r)}(r,m)}{\partial m^a}$  (to avoid complication we drop the suffix (r) bearing in mind that  $A(r,m)$  is not a scalar function in R) we get

$$\begin{aligned} \frac{\partial^2 A(r,m)}{\partial m'^a \partial m'^a} &= \frac{\partial}{\partial m'^a} \left( \frac{\partial A(r,m)}{\partial m^\alpha} \frac{\partial m^\alpha}{\partial m'^a} \right) \\ &= \frac{\partial^2 A(r,m)}{\partial m^\alpha \partial m^\beta} \frac{\partial m^\beta}{\partial m'^a} \frac{\partial m^\alpha}{\partial m'^a} + \frac{\partial A(r,m)}{\partial m^\alpha} \frac{\partial^2 m^\alpha}{\partial m'^a \partial m'^a} . \end{aligned} \quad (4.15)$$

Therefore for a general transformation of coordinate axes in the subspace M, where  $\partial^2 m^\alpha / (\partial m'^a \partial m'^a) \neq 0$ , this set of partial derivatives of the covariant tensor in the subspace M does not represent a tensor. This can be generalized to any kind of field dependent tensor to show that the

partial derivatives of a field dependent tensor, with respect to the coordinate axes in one subspace, where a general transformation of coordinate axes in that subspace is considered, does not form the components of a tensor in that subspace. But for a linear transformation of coordinate axes in the subspace under consideration, where  $\partial_m^a / \partial m'^a$  is a constant the partial derivative operator in every subspace acts like a covariant vector in that subspace and adds one covariant index to the indices of the original field dependent tensor in that subspace. That is, the field dependent tensor formed by the set of partial derivatives, with respect to coordinate axes in the subspace M, of the field dependent

$$\text{tensor } A \begin{matrix} a_1 & \dots & a_g & b_1 & \dots & b_h \\ m^1 & \dots & m^g & r^1 & \dots & r^h \end{matrix} (r,m) \text{ with } g \text{ contravariant and } p \text{ covariant} \\ \begin{matrix} c_1 & \dots & c_p & d_1 & \dots & d_q \\ m^1 & \dots & m^p & r^1 & \dots & r^q \end{matrix}$$

indices in M, and h contravariant and q covariant indices in R, will have g contravariant and p + 1 covariant indices in M and h contravariant and q covariant indices in R. The transformation law for such a field dependent tensor will be

$$\frac{\partial}{\partial m'^e} A' \begin{matrix} a_1 & \dots & a_g & b_1 & \dots & b_h \\ m^1 & \dots & m^g & r^1 & \dots & r^h \end{matrix} (r',m') = \frac{\partial m^\epsilon}{\partial m'^e} \underbrace{\frac{\partial m^{\gamma_1}}{\partial m'^{c_1}} \dots \frac{\partial m^{\gamma_p}}{\partial m'^{c_p}}}_{p+1}$$

$$\underbrace{\frac{\partial m^{a_1}}{\partial m^{\alpha_1}} \dots \frac{\partial m^{a_g}}{\partial m^{\alpha_g}}}_g \cdot \underbrace{\frac{\partial r^{b_1}}{\partial r^{\beta_1}} \dots \frac{\partial r^{b_h}}{\partial r^{\beta_h}}}_h \cdot \underbrace{\frac{\partial r^{\delta_1}}{\partial r'^{d_1}} \dots \frac{\partial r^{\delta_q}}{\partial r'^{d_q}}}_q$$

$$\cdot \frac{\partial}{\partial m^\epsilon} A \begin{matrix} a_1 & \dots & a_g & b_1 & \dots & b_h \\ m^1 & \dots & m^g & r^1 & \dots & r^h \end{matrix} (r,m) \tag{4.16}$$

In the same way partial differentiation in the subspace  $R$  will also add one covariant index to the indices of a field dependent tensor in that subspace, only where a linear transformation of coordinate axes in that subspace is concerned.

CHAPTER 5

NEUMANN'S PRINCIPLE

EFFECT OF SYMMETRY ON TENSOR COMPONENTS

5.1 Introduction

The symmetry properties of the space, upon which a tensor is defined can restrict the form of that tensor in that space. These restrictions are dictated by a principle due to Neumann (see, for example, Nye 1957, p.20, or Birss, 1966, p.44). Through Neumann's principle every symmetry operation of the space under consideration defines relations between the components of the tensor defined on that space, and therefore reduces the number of its independent components.

Some authors have cast doubt on the validity of Neumann's principle when applied to some special kind of tensor (viz transport property tensors) defined over some special spaces (space composed of magnetic and geometric subspace, or in other words, space of a magnetic crystal). The aim of this chapter is to retain the validity of Neumann's principle and to show that the origin of the particular doubts expressed by these workers is unjustified and stems from use of symmetry operations, which are not exhibited by the space under consideration (i.e. the space of magnetic crystals). To facilitate the argument a short review of the nature of symmetry operations and the symmetry groups of ordinary crystals (ordinary geometrical space, where each point is identified only by its position vector) is given first and Neumann's principle is defined. Then the generalized symmetry, that is the symmetry of the space composed of coloured objects or the space composed of magnetic objects is discussed. Moreover it is shown that the identification of time inversion operator with the magnetic moment (or spin) inversion operator leads to incorrect results (the reason for doubt about the validity of Neumann's principle by previous workers).

## 5.2 Macroscopic symmetry operations and point groups

Symmetry operations are the displacements of an infinite rigid body which leave the body in a position undistinguishable from its original one. These operations can involve pure translation, pure rotation, pure reflection (or inversion), and, in general, combination of rotation, inversion and translation. A symmetry operation can be shown by  $\{R_i | v\}$ , where  $v$  denotes a translation and  $R_i$  denote rotation or rotation-inversion operations. Moreover the symmetry operations of a rigid body can be identified with the transformation of coordinate axes (section 2.4) and represented by transformation matrices.

The complete set of symmetry operations which restore a rigid body to itself forms a group and is referred to as a space group. That is:

- (i) the product of every two elements  $A$  and  $B$  of the set is itself a member of the set,
- (ii) combination (called multiplication) of the elements of the set is associative, that is, for any three elements  $A$ ,  $B$  and  $C$

$$(A B) C = A (B C) ,$$

- (iii) one of the elements of the set is the identity operator  $E$ , the symmetry operator which leaves the rigid body unmoved and for every element  $A$  of the set  $A E = E A = A$ ,
- (iv) for every element  $A$  of the set there exists an element  $B$  in the set such that  $A B = B A = E$ , the element  $B$  is called the inverse of  $A$  and is denoted by  $B = A^{-1}$ .

In dealing with macroscopic properties, however, we are concerned with the point group, which is a special sub-group of the space group, in which the translational part of symmetry operations are completely suppressed and only rotation and rotation-inversion symmetry operations are considered.

For identification of the group of symmetry elements of a rigid body only a few of the symmetry elements are necessary. These are called the generating elements of the group and the whole set of elements in the group can be generated by forming different combinations of these generating elements.

### 5.3 The symmetry of crystalline lattice and crystal classes

The symmetry of a crystalline lattice is described by considering it to be a three-dimensional array formed by repetition of physical objects, atoms or molecules or electric charges and current distributions. The crystal structure is then defined by specification of the pattern of repetition plus a complete description of the contents of the repetition unit (the unit cell). The existence of the spatial lattice (the three-dimensional array) restricts the number of possible rotation axes to five: one-, two-, three-, four- and six-fold axes of rotations. The space group of symmetry operations of an extended crystalline lattice is then described in terms of these rotation and inversion operations, together with the finite displacements of the lattice parallel to particular directions. There are 230 different space groups. Suppressing the translational components of the symmetry operations of the space group results in 32 possible point groups for a crystalline lattice. Detailed information about these point groups may be found in many books (see for example volume 1 of the "international tables for X-ray crystallography", Henry and Lonsdale 1965).

### 5.4 Neumann's principle and the effect of symmetry on physical properties

Neumann's principle states that (see for example, Nye, 1957, p.20 or Birss, 1966, p.44, or Bhagavantam, 1966, p.72) "the symmetry operations of any physical property of a crystal must include the symmetry operations

of the point group of the crystal". In other words when by symmetry considerations two different directions in a crystal are exactly the same, any physical property must have the same characteristics along these two directions. A physical property can have symmetry operations which do not exist in the point group of the crystal. These symmetry operations are called the intrinsic symmetry of a property. Many workers have studied the influence of macroscopic spatial symmetry on the tensor properties of crystals (see, for example, Voigt 1928, Love 1927, Wooster 1938, Mason 1947, Fumi 1952 a,b, Fieschi 1957, Nye 1972, Birss 1962, 1963, 1966).

The way a symmetry operation manifests itself in a physical tensor property can be shown in the following way: any symmetry operation,  $A$ , can be represented by a transformation of coordinate axes (with transformation matrix  $(a_{ij})$ ), which dictates the following relations between the components  $B_{i_1 \dots i_s} (x)$  of a tensor in the old and new coordinate system (equations 2.39 and 2.41).

$$B_{i_1 \dots i_s}^{(x'_k)} = a_{i_1 j_1} \dots a_{i_s j_s} B_{j_1 \dots j_s} (a_{kl} x_l) \quad (5.1)$$

for a polar tensor, and

$$B_{i_1 \dots i_s}^{(x'_k)} = |a_{ij}| a_{i_1 j_1} \dots a_{i_s j_s} B_{j_1 \dots j_s} (a_{kl} x_l) \quad (5.2)$$

for an axial tensor. Then through Neumann's principle,

$$B_{i_1 \dots i_s}^{(x'_k)} = B_{i_1 \dots i_s} (x_k) \quad (5.3)$$

Substituting for  $B_{i_1 \dots i_s}^{(x'_k)}$  from equations (5.1) and (5.2). for polar and axial tensors, into equation (5.3) we get

$$B_{i_1 \dots i_s} (x_k) = a_{i_1 j_1} \dots a_{i_s j_s} B_{j_1 \dots j_s} (a_{kl} x_l) \quad (5.4)$$

for a polar tensor and



$$B_{i_1 \dots i_s}^{(x^k)} = |a_{ij}| a_{i_1 j_1} \dots a_{i_s j_s} B_{j_1 \dots j_s}^{(a_{kl} x^l)} \quad (5.5)$$

for an axial tensor. Equations (5.4) or (5.5) are the analytical form of Neumann's principle, and define relations between the components of a polar or an axial tensor and thus reduce the number of independent components. The form of the Neumann's principle for a general (mixed and weighted) field independent tensor  $B_{i_1 \dots i_s}^{j_1 \dots j_r}(x^k)$  can be easily deduced as

$$B_{i_1 \dots i_s}^{j_1 \dots j_r}(x^k) = \left| \frac{\partial x^{i,j}}{\partial x^{i,j}} \right|^\omega \frac{\partial x^{j_1}}{\partial x^{\alpha_1}} \dots \frac{\partial x^{j_s}}{\partial x^{\alpha_s}} \cdot \frac{\partial x^{\beta_1}}{\partial x^{i_1}} \dots \frac{\partial x^{\beta_r}}{\partial x^{i_r}} B_{\beta_1 \dots \beta_r}^{\alpha_1 \dots \alpha_s} \left( \frac{\partial x^{i,k}}{\partial x^l} x^l \right).$$

(5.6)

and for a constant tensor (tensor with constant components with respect to the coordinate axes) in a cartesian frame of coordinates Neumann's principle can be written as

$$B_{i_1 \dots i_s} = a_{i_1 j_1} \dots a_{i_s j_s} B_{j_1 \dots j_s} \quad (5.7)$$

for a polar tensor and

$$B_{i_1 \dots i_s} = |a_{ij}| a_{i_1 j_1} \dots a_{i_s j_s} B_{j_1 \dots j_s} \quad (5.8)$$

for an axial tensor. To find the form of a physical tensor property for a crystal belonging to a special crystal system, the symmetry operations in the corresponding point group will be inserted one after another into the appropriate equation for Neumann's principle and all the restrictions found in this way are put together. To secure the maximum simplification in the form of a tensor, it is not always necessary to employ all the symmetry operators of a point group. The set of generating elements of the corresponding point group suffices to serve this purpose (see, for example, Birss, 1966, p.48). Different sets of generating

elements might be chosen for one crystal class. The following assemblage of generating elements used by Birss (Birss, 1966, p.48) has been employed in this thesis:

$$\sigma^{(0)} = [\bar{1}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \sigma^{(1)} = [\bar{1}] = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix},$$

$$\sigma^{(2)} = [2_y] = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \quad \sigma^{(3)} = [2_z] = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

$$\sigma^{(4)} = [\bar{2}_y] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \sigma^{(5)} = [\bar{2}_z] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix},$$

$$\sigma^{(6)} = [3_z] = \begin{bmatrix} -1/2 & \sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \sigma^{(7)} = [4_z] = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

$$\sigma^{(8)} = [\bar{4}_z] = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \quad \sigma^{(9)} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}.$$

Choosing this assemblage has the advantage that the number of generating matrices in any crystal point group is small and the relations between tensor components (obtained from one of the equations (5.4), (5.5),

(5.7) or (5.8) are simple. Sets of generating matrices (chosen from this assemblage) for the 32 crystal class are listed in Table 1.

Using equations (5.7) and (5.8), the forms of constant tensor up to rank four in every crystal class have been worked out and their non-zero components have been listed by Birss (Birss, 1966, tables 4a, 4b, 4c, 4d, 4e and 4f).

However, these tables cannot be used to investigate the restrictions on tensor field and field dependent tensors such as transport properties of solids in the presence of an external field, and tensors in crystals with more complicated symmetry operations, such as magnetic moment inversion operation. The reason for this is that, to find the restrictions on the form of tensor fields, equations (5.4) and (5.5) should be employed instead of equations (5.7) and (5.8). That is the symmetry operation acts on the argument of the tensor components as well as on tensor components themselves. The non-zero components of such tensors have been worked out in Appendix I and listed in Tables A.3-A.14 in that appendix. As for field dependent tensors and tensors in the so-called generalized symmetric spaces, the analytical form of Neumann's principle will be derived in the subsequent sections of this chapter and their form will be given in the Tables A.1-A.14.

### 5.5 The symmetry of magnetic crystals (I):

#### Heesch-Shubnikov groups

In describing the spatial symmetry of a crystal the crystalline matter is conveniently regarded as a composition of similar groups of atoms or molecules located on definite points, without any reference to the movements of atoms around their equilibrium position or their magnetic moment direction or the spin direction of the electrons.

TABLE 1

System	Symbol of symmetry class				Number of symmetry operations	Generating matrices
	International		Schönflies	Shubnikov		
	Abbreviated	Full				
Triclinic	1	1	$C_1$	1	1	$\sigma^{(0)}$
	$\bar{1}$	$\bar{1}$	$C_1(S_2)$	$\bar{2}$	2	$\sigma^{(1)}$
Monoclinic	2	2	$C_2$	2	2	$\sigma^{(3)}$
	m	m	$C_s(C_{1h})$	m	2	$\sigma^{(5)}$
	2/m	$\frac{2}{m}$	$C_{2h}$	2:m	4	$\sigma^{(1)}, \sigma^{(3)}$
Orthorhombic	222	222	$D_2(V)$	2:2	4	$\sigma^{(2)}, \sigma^{(3)}$
	mm2	mm2	$C_{2v}$	2.m	4	$\sigma^{(3)}, \sigma^{(4)}$
	mmm	$\frac{222}{mmm}$	$D_{2h}(V_h)$	m.2:m	8	$\sigma^{(1)}, \sigma^{(2)}, \sigma^{(3)}$
Tetragonal	4	4	$C_4$	4	4	$\sigma^{(7)}$
	$\bar{4}$	$\bar{4}$	$S_4$	$\bar{4}$	4	$\sigma^{(8)}$
	4/m	$\frac{4}{m}$	$C_{4h}$	4:m	8	$\sigma^{(1)}, \sigma^{(7)}$
	422	422	$D_4$	4:2	8	$\sigma^{(2)}, \sigma^{(7)}$
	4mm	4mm	$C_{4v}$	4.m	8	$\sigma^{(4)}, \sigma^{(7)}$
	$\bar{4}2m$	$\bar{4}2m$	$D_{2d}(V_d)$	$\bar{4}.m$	8	$\sigma^{(2)}, \sigma^{(8)}$
	4/mmm	$\frac{422}{mmm}$	$D_{4h}$	m.4:m	16	$\sigma^{(1)}, \sigma^{(2)}, \sigma^{(7)}$

Table 1 continued overleaf

TABLE 1 (Continued)

System	Symbol of symmetry class				Number of symmetry operation	Generating matrices
	International		Schönflies	Shubnikov		
	Abbreviated	Full				
Trigonal	3	3	$C_3$	3	3	$\sigma^{(6)}$
	$\bar{3}$	$\bar{3}$	$C_{3i}(S_6)$	$\bar{6}$	6	$\sigma^{(1)}, \sigma^{(6)}$
	32	32	$D_3$	3:2	6	$\sigma^{(2)}, \sigma^{(6)}$
	3m	3m	$C_{3v}$	3.m	6	$\sigma^{(4)}, \sigma^{(6)}$
	$\bar{3}m$	$\bar{3} \frac{2}{m}$	$D_{3d}$	$\bar{6}.m$	12	$\sigma^{(1)}, \sigma^{(2)}, \sigma^{(6)}$
Hexagonal	6	6	$C_6$	6	6	$\sigma^{(3)}, \sigma^{(6)}$
	$\bar{6}$	$\bar{6}$	$C_{3h}$	3:m	6	$\sigma^{(5)}, \sigma^{(6)}$
	6/m	$\frac{6}{m}$	$C_{6h}$	6:m	12	$\sigma^{(1)}, \sigma^{(3)}, \sigma^{(6)}$
	622	622	$D_6$	6:2	12	$\sigma^{(2)}, \sigma^{(3)}, \sigma^{(6)}$
	6mm	6mm	$C_{6v}$	6.m	12	$\sigma^{(3)}, \sigma^{(4)}, \sigma^{(6)}$
	$\bar{6}m2$	$\bar{6}m2$	$D_{3h}$	m.3:m	12	$\sigma^{(2)}, \sigma^{(5)}, \sigma^{(6)}$
	6/mmm	$\frac{6}{m} \frac{2}{m} \frac{2}{m}$	$D_{6h}$	m.6:m	24	$\sigma^{(1)} \sigma^{(2)} \sigma^{(3)} \sigma^{(6)}$
	Cubic	23	23	T	3/2	12
m3		$\frac{2}{m} \bar{3}$	$T_h$	$\bar{6}/2$	24	$\sigma^{(1)}, \sigma^{(3)}, \sigma^{(9)}$
432		432	O	3/4	24	$\sigma^{(7)}, \sigma^{(9)}$
$\bar{4}3m$		$\bar{4}3m$	$T_d$	$3/\bar{4}$	24	$\sigma^{(8)}, \sigma^{(9)}$
m3m		$\frac{4}{m} \bar{3} \frac{2}{m}$	$O_h$	$\bar{6}/4$	48	$\sigma^{(1)}, \sigma^{(7)}, \sigma^{(9)}$

Such a description is statistical. Therefore in dealing with properties, such as transport properties of crystals, which depend on the dynamical characteristics of crystals, this aspect of crystal symmetry (spatial symmetry) fails to give correct predictions of the symmetry restrictions on these properties. In determination of the appropriate symmetry operations for these cases, the symmetry of the individual properties of groups of atoms (unit cells) as well as spatial symmetry must be taken into account. To do this new coordinate axes, representing the appropriate characteristics of the unit cell, such as the direction of its movements or the direction of its magnetic moment etc., may be introduced then the symmetry operators corresponding to the transformation of these coordinate axes can be combined together with the spatial transformation operators to give the appropriate symmetry operators. This has been done by Shubnikov in 1951 (see Shubnikov and Belov, 1964) for a simple case where one extra coordinate with two possible values has been introduced (atoms can be considered as black or white objects with the new coordinate being their colour, or in the case of simple magnetic structures, the new coordinate can be the direction of the magnetic moment of the atoms - parallel or antiparallel to a given axis). Then he defined the operation of antisymmetry as the operation which changes the value of this coordinate (black to white and white to black, for example). This concept of antisymmetry had been first introduced by Heesch (1929 a,b, 1930 a,b) but it was ignored because it did not have any immediate significance in physics at that time. The existence of black and white atoms (or atoms with two different directions of magnetic moment) will destroy the spatial symmetry of the crystal, unless they are distributed in a regular fashion;- in that case, part of classical symmetry (symmetry of crystal with similar atoms) will survive. That is, introducing the antisymmetry operation will result

in new sets of possible point groups and space groups, which are called Heesch-Shubnikov groups. There are three types of Heesch-Shubnikov point groups,  $G'$ , which are usually described as follows:

Type I the classical point groups (there are 32 of this type),

Type II: the grey point groups (there are 32 of this type),

Type III: the black and white point groups which are also called the magnetic point groups (there are 58 of this type),

the total number of these Heesch-Shubnikov point groups is therefore 122.

Type I point groups describe the symmetry of crystals composed of similar groups of atoms (all black or all white, or all with the magnetic moments in one direction), and they do not contain the operation of antisymmetry,  $A$ , that is they are the classical or ordinary point groups,  $G$ , i.e.  $G' = G$ .

Type II point groups, describe the symmetry of crystals with atoms of both kinds (black and white or with magnetic moments parallel and antiparallel to a given direction) present at each site simultaneously, so that any operation of a classical point group,  $G$ , leaves the fourth coordinate (the colour or the direction of the magnetic moment) unchanged, and the operation of antisymmetry,  $A$ , times any operation of  $G$  changes two different values of the fourth coordinate into each other, thereby leaving it unchanged. Thus  $G' = G + A G$ . That is, a grey point group contains twice the number of symmetry elements as the number of symmetry elements in the corresponding point group, with the antisymmetry operation,  $A$ , as an element on its own.

In the type III Heesch-Shubnikov, the antisymmetry operation,  $A$ , appears only in combination,  $A R$ , with the elements,  $R$ , of the corresponding classical point group,  $G$ , i.e.  $G' = H + A(G-H)$ , where  $H$  is a halving subgroup of the classical point group  $G$ .

The generating elements of the type I Heesch-Shubnikov point groups are exactly those given in Table 1. For the type II Heesch-Shubnikov point groups, the antisymmetry operation,  $A$ , must be added to the generating elements of the corresponding classical point group to form the set of their generating elements.

The identification of the elements in each of the 58 type III Heesch-Shubnikov point groups has been done by Tavger and Zaitsev (see Tavger and Zaitsev, 1956) and by other workers and the generating elements for these point groups are given in Table 2 (see Birss, 1966). Here the underlining of a symmetry operator indicates multiplication by the antisymmetry operator,  $A$ , i.e.  $\underline{S}_i = A S_i$

Heesch-Shubnikov (or coloured) space groups can be defined in the following way:

Type I the classical space groups (there are 230).

Type II the grey space groups (there are 230).

These two kinds of space groups can be formed by combining the corresponding point group together with the translational sub-group.

Type III black and white space groups, which are derived from the classical space groups (there are 674).

Type IV Heesch-Shubnikov space group,  $G'$ , which is another black and white space group and is based on a black and white Bravais lattice and consists of all the operations of a classical space group,  $G$ , together with an equal number of operations that involve the antisymmetry operation,  $A$ , i.e.  $G' = G + A \{ E | t \} G$  (there are 517 of these kind of space groups). The black and white Bravais lattices were derived by Belov et al (1955), and the black and white space groups were first derived by Zamorzaev in 1953 (see Belov et al., 1957; Shubnikov and Belov, 1964; Opechowski and Guccione, 1965; Bradley and Cracknell, 1972).



TABLE 2

System	Symbol of Symmetry class and magnetic point group G'		Symbol of classical sub-group H		Generating matrices of group G'	
	International	Shubnikov	International	Shubnikov	Generating matrices of sub-group H	Additional generating matrix
Triclinic	<u><math>\bar{1}</math></u>	<u><math>\bar{2}</math></u>	1	1	$\sigma^{(0)}$	<u><math>\sigma^{(1)}</math></u>
Monoclinic	<u>2</u>	<u>2</u>	1	1	$\sigma^{(0)}$	<u><math>\sigma^{(3)}</math></u>
	<u>m</u>	<u>m</u>	1	1	$\sigma^{(0)}$	<u><math>\sigma^{(5)}</math></u>
	<u>2/m</u>	<u>2:m</u>	$\bar{1}$	$\bar{2}$	$\sigma^{(1)}$	<u><math>\sigma^{(3)}</math></u>
	<u>2/m</u>	<u>2:m</u>	2	2	$\sigma^{(3)}$	<u><math>\sigma^{(1)}</math></u>
	<u>2/m</u>	<u>2:m</u>	m	m	$\sigma^{(5)}$	<u><math>\sigma^{(1)}</math></u>
	Orthorhombic	<u>222</u>	<u>2:2</u>	2	2	$\sigma^{(3)}$
<u>mm2</u>		<u>2:m</u>	2	2	$\sigma^{(3)}$	<u><math>\sigma^{(4)}</math></u>
<u>2mm</u>		<u>2:m</u>	m	m	$\sigma^{(5)}$	<u><math>\sigma^{(4)}</math></u>
<u>mmm</u>		<u>m.2:m</u>	2/m	2:m	$\sigma^{(1)}, \sigma^{(3)}$	<u><math>\sigma^{(2)}</math></u>
<u>mmm</u>		<u>m.2:m</u>	222	2:2	$\sigma^{(2)}, \sigma^{(3)}$	<u><math>\sigma^{(1)}</math></u>
<u>mmm</u>		<u>m.2:m</u>	mm2	2:m	$\sigma^{(3)}, \sigma^{(4)}$	<u><math>\sigma^{(1)}</math></u>
Tetragonal		<u>4</u>	<u>4</u>	2	2	$\sigma^{(3)}$
	<u><math>\bar{4}</math></u>	<u><math>\bar{4}</math></u>	2	2	$\sigma^{(3)}$	<u><math>\sigma^{(8)}</math></u>
	<u>4/m</u>	<u>4:m</u>	2/m	2:m	$\sigma^{(1)}, \sigma^{(3)}$	<u><math>\sigma^{(7)}</math></u>
	<u>4/m</u>	<u>4:m</u>	4	4	$\sigma^{(7)}$	<u><math>\sigma^{(1)}</math></u>
	<u>4/m</u>	<u>4:m</u>	$\bar{4}$	$\bar{4}$	$\sigma^{(8)}$	<u><math>\sigma^{(1)}</math></u>
	<u>422</u>	<u>4:2</u>	222	2:2	$\sigma^{(2)}, \sigma^{(3)}$	<u><math>\sigma^{(7)}</math></u>

Table 2 (Continued)

System	Symbol of Symmetry class and magnetic point group G'		Symbol of classical sub-group H		Generating matrices of group G'	
	International	Shubnikov	International	Shubnikov	Generating matrices of sub-group H	Additional generating matrix
Tetragonal	<u>422</u>	4: <u>2</u>	4	4	$\sigma^{(7)}$	$\underline{\sigma}^{(2)}$
	<u>4mm</u>	<u>4</u> .m	mm2	2.m	$\sigma^{(3)}, \sigma^{(4)}$	$\underline{\sigma}^{(7)}$
	<u>4mm</u>	4. <u>m</u>	4	4	$\sigma^{(7)}$	$\underline{\sigma}^{(4)}$
	<u>42m</u>	<u>4</u> .m	222	2:2	$\sigma^{(2)}, \sigma^{(3)}$	$\underline{\sigma}^{(8)}$
	<u>4m2</u>	<u>4</u> .m	mm2	2.m	$\sigma^{(3)}, \sigma^{(4)}$	$\underline{\sigma}^{(8)}$
	<u>42m</u>	<u>4</u> .m	<u>4</u>	<u>4</u>	$\sigma^{(8)}$	$\underline{\sigma}^{(2)}$
	<u>4/mmm</u>	m. <u>4</u> :m	mmm	m.2:m	$\sigma^{(1)}, \sigma^{(2)}, \sigma^{(3)}$	$\underline{\sigma}^{(7)}$
	<u>4/mmm</u>	<u>m</u> .4:m	4/m	4:m	$\sigma^{(1)}, \sigma^{(7)}$	$\underline{\sigma}^{(2)}$
	<u>4/mmm</u>	<u>m</u> .4: <u>m</u>	422	4:2	$\sigma^{(2)}, \sigma^{(7)}$	$\underline{\sigma}^{(1)}$
	<u>4/mmm</u>	m.4: <u>m</u>	4mm	4.m	$\sigma^{(4)}, \sigma^{(7)}$	$\underline{\sigma}^{(1)}$
	<u>4/mmm</u>	m. <u>4</u> :m	<u>42m</u>	<u>4</u> .m	$\sigma^{(2)}, \sigma^{(8)}$	$\underline{\sigma}^{(1)}$
Trigonal	<u>3</u>	<u>6</u>	3	3	$\sigma^{(6)}$	$\underline{\sigma}^{(1)}$
	<u>32</u>	3: <u>2</u>	3	3	$\sigma^{(6)}$	$\underline{\sigma}^{(2)}$
	<u>3m</u>	3. <u>m</u>	3	3	$\sigma^{(6)}$	$\underline{\sigma}^{(4)}$
	<u>3m</u>	<u>6</u> .m	<u>3</u>	<u>6</u>	$\sigma^{(1)}, \sigma^{(6)}$	$\underline{\sigma}^{(2)}$
	<u>3m</u>	<u>6</u> .m	32	3:2	$\sigma^{(2)}, \sigma^{(6)}$	$\underline{\sigma}^{(1)}$
	<u>3m</u>	<u>6</u> .m	3m	3.m	$\sigma^{(4)}, \sigma^{(6)}$	$\underline{\sigma}^{(1)}$

Table 2 (Continued)

System	Symbol of Symmetry class and magnetic point group G'		Symbol of classical sub-group H		Generating matrices of group G'	
	International	Shubnikov	International	Shubnikov	Generating matrices of sub-group H	Additional generating matrix
Hexagonal	<u>6</u>	<u>6</u>	3	3	$\sigma^{(6)}$	$\underline{\sigma}^{(3)}$
	<u><math>\bar{6}</math></u>	3:m	3	3	$\sigma^{(6)}$	$\underline{\sigma}^{(5)}$
	<u>6/m</u>	<u>6:m</u>	$\bar{3}$	$\bar{6}$	$\sigma^{(1)}, \sigma^{(6)}$	$\underline{\sigma}^{(3)}$
	<u>6/m</u>	<u>6:m</u>	6	6	$\sigma^{(3)}, \sigma^{(6)}$	$\underline{\sigma}^{(1)}$
	<u>6/m</u>	<u>6:m</u>	$\bar{6}$	3:m	$\sigma^{(5)}, \sigma^{(6)}$	$\underline{\sigma}^{(1)}$
	<u>6 2 2</u>	<u>6:2</u>	32	3:2	$\sigma^{(2)}, \sigma^{(6)}$	$\underline{\sigma}^{(3)}$
	<u>6 2 2</u>	<u>6:2</u>	6	6	$\sigma^{(3)}, \sigma^{(6)}$	$\underline{\sigma}^{(2)}$
	<u>6mm</u>	<u>6.m</u>	3m	3.m	$\sigma^{(4)}, \sigma^{(6)}$	$\underline{\sigma}^{(3)}$
	<u>6mm</u>	<u>6.m</u>	6	6	$\sigma^{(3)}, \sigma^{(6)}$	$\underline{\sigma}^{(4)}$
	<u><math>\bar{6}2m</math></u>	<u>m.3:m</u>	32	3:2	$\sigma^{(2)}, \sigma^{(6)}$	$\underline{\sigma}^{(5)}$
	<u><math>\bar{6}m2</math></u>	<u>m.3:m</u>	3m	3.m	$\sigma^{(4)}, \sigma^{(6)}$	$\underline{\sigma}^{(5)}$
	<u><math>\bar{6}m2</math></u>	<u>m.3:m</u>	$\bar{6}$	3:m	$\sigma^{(5)}, \sigma^{(6)}$	$\underline{\sigma}^{(4)}$
	<u>6/mmm</u>	<u>m.6:m</u>	$\bar{3}m$	$\bar{6}.m$	$\sigma^{(1)}, \sigma^{(2)}, \sigma^{(6)}$	$\underline{\sigma}^{(2)}$
	<u>6/mmm</u>	<u>m.6:m</u>	6/m	6:m	$\sigma^{(1)}, \sigma^{(3)}, \sigma^{(6)}$	$\underline{\sigma}^{(2)}$
	<u>6/mmm</u>	<u>m.6:m</u>	622	6:2	$\sigma^{(2)}, \sigma^{(3)}, \sigma^{(6)}$	$\underline{\sigma}^{(1)}$
	<u>6/mmm</u>	<u>m.6:m</u>	6mm	6.m	$\sigma^{(3)}, \sigma^{(4)}, \sigma^{(6)}$	$\underline{\sigma}^{(1)}$
<u>6/mmm</u>	<u>m.6:m</u>	$\bar{6}m2$	m.3:m	$\sigma^{(2)}, \sigma^{(5)}, \sigma^{(6)}$	$\underline{\sigma}^{(1)}$	
Cubic	<u>m3</u>	$\bar{6}/2$	23	3/2	$\sigma^{(3)}, \sigma^{(9)}$	$\underline{\sigma}^{(1)}$
	<u>432</u>	3/4	23	3/2	$\sigma^{(3)}, \sigma^{(9)}$	$\underline{\sigma}^{(7)}$
	<u><math>\bar{4}3m</math></u>	3/4	23	3/2	$\sigma^{(3)}, \sigma^{(9)}$	$\underline{\sigma}^{(8)}$
	<u>m3m</u>	$\bar{6}/4$	m3	$\bar{6}/2$	$\sigma^{(1)}, \sigma^{(3)}, \sigma^{(9)}$	$\underline{\sigma}^{(7)}$
	<u>m3m</u>	$\bar{6}/4$	432	3/4	$\sigma^{(7)}, \sigma^{(9)}$	$\underline{\sigma}^{(1)}$
	<u>m3m</u>	$\bar{6}/4$	$\bar{4}32$	3/4	$\sigma^{(8)}, \sigma^{(9)}$	$\underline{\sigma}^{(1)}$

The symmetry of most of the magnetic materials (diamagnetic, paramagnetic, ferromagnetic, ferrimagnetic) can be described by the three types of Heesch-Shubnikov point groups, when the antisymmetry operator is identified with the magnetic moment (or spin) inversion operator (see, for example, Mackay, 1957). In that case a grey point group will contain the operation of magnetic moment inversion,  $\bar{A}$ , on its own; therefore if a spontaneous magnetic moment were to develop at any point within the crystal, described by that point group, the presence of  $\bar{A}$  would require that an equal magnetic moment should appear at the same point in the opposite direction. Therefore the symmetry of crystals with magnetic ordering cannot be described by a grey point group, but the symmetry of diamagnetic materials (in which the atoms or ions which constitute the crystal have zero magnetic moments) and paramagnetic materials in the absence of an external magnetic field (where the orientations of the magnetic moments of atoms or ions are random and the crystal can be considered as being invariant under the operation  $\bar{A}$ ) can be described by grey groups.

The symmetry of ferromagnetic crystals (which consist of atoms or ions with magnetic moments aligned along certain directions in the absence of an external magnetic field) and ferrimagnetic crystals (with some of the magnetic moments parallel to a particular direction and the rest anti-parallel to that direction in the absence of an external magnetic field) and some of the antiferromagnetic materials which possess a spontaneous net magnetic moment can be described by type I and type II Heesch-Shubnikov point group, where the magnetic moment inversion as a symmetry element on its own is absent. Application of these groups to magnetic structure determinations has been done by several groups of workers in this field (see, for example, Donnay et al, 1958 and le Corre, 1958).

## 5.6 The symmetry of magnetic crystals (II):

### Generalized symmetry

The symmetry of a large number of magnetically ordered materials can be described by using the Heesch-Shubnikov groups. However, there are some other magnetic materials whose symmetry cannot adequately be described by these groups. Examples of these are materials with helical or conical antiferromagnetic structures. The ordering of magnetic moments in these structures is such that there are more than two possible directions of magnetic moment present in the crystal. Therefore further generalization of classical point groups is necessary. One possible generalization is to consider the polychromatic point groups and space groups. But this cannot be used as a general approach, since the polychromatic groups can only describe the symmetry of magnetic materials where the angle between two successive spins is a discrete value ( $120^\circ$ ,  $90^\circ$  or  $60^\circ$ ) which is not always the case (see, for example, Cracknell 1975).

More comprehensive generalization can be achieved by using the spin groups developed by Litvin (1973). The idea of spin groups is closely related to the generalized magnetic groups defined by Naish (1963) and Kitz (1965), and is called 'spin space' groups by Brinkman and Elliot (1966). A symmetry operation in the generalized magnetic group, as it is called in this thesis, (or spin group) can be denoted by  $\{ R | R_1 | w_{1p} \}$ , where the rotation on the far left side in the bracket,  $R_p$ , acts only in spin space, that is, on the components of the spins, and the rotation,  $R_1$ , and translation,  $w_{1p}$ , act only in the geometrical space on the coordinates of the atoms. In special cases it is possible to have some symmetry operations that involve one rotational operation  $R_1$  for both the physical space coordinates and the spin space coordinates. Such a symmetry operation can be denoted by  $\{ R_1 | R_1 | w_1 \}$ . Further specification

of the generalized magnetic groups can be found in articles by Opechnowski (1971) and Opechowski and Dreyfus (1971).

### 5.7 Time inversion operation and magnetic groups

It has been shown (Section 5.5) that by identification of the magnetic moment inversion operator with the antisymmetry operator in Heesch-Shubnikov groups the structure of most magnetic materials can be put on a group theoretical basis. However, since the operation of time inversion, according to standard assumptions of the electromagnetic theory, has the effect of reversing the direction of magnetic moment (or spin), it has become a common practice to identify the time inversion operator,  $\theta$ , with the magnetic moment inversion operator (see, for example, Opechowski and Guccione 1965, Tavger and Zaitsev 1956, Birss 1966, Zoher and Török 1953, Dimmock 1963 a,b, Dimmock and Wheeler 1962 a,b, and Dimmock and Wheeler 1964). In this section it will be pointed out that this identification is not always correct and sometimes leads to incorrect results.

Time inversion operation has actually the effect of reversing the direction (or changing the sign) of every dynamic property which depends on time to an odd degree, i.e. time-antisymmetric properties including magnetic moment. Thus in adopting this operation as a symmetry operation of a magnetic crystal special care must be taken to make sure that there is no other time-antisymmetric property present in the crystal. In other words when a time-antisymmetric property, such as one of the transport properties (like current density), of a crystal is under consideration adopting time inversion operator imposes some restriction on the form of property which in actual fact should not be there. The way in which identification of the magnetic moment inversion operator with time inversion operator leads to incorrect results in the study of current

density in a magnetic crystal is discussed in Section 6.3.1.

The problems that arise as a result of identification of the magnetic moment inversion operator with the time inversion operator have been noticed by several workers: Birss (1966) suggests that the problem may arise because Neumann's principle does not hold for transport properties under the symmetry operations in space-time. This cannot be true because Neumann's principle is axiomatic in its nature. Pantula and Sudarshan (1970 a,b) have reached the conclusion that in the non-equilibrium steady state the crystal does not possess time-inversion symmetry. But then to remove the problem caused by time inversion they have only used the sub-group of time invariant operations of the appropriate group (Bhagacantam and Pantula 1967).

In addition to leading to wrong results, in some cases, the time inversion operator,  $\theta$ , proves to be inadequate to be identified with magnetic moment inversion operator in the sense that  $\theta$  can only provide two senses, while many magnetic crystals with complex magnetic ordering have more than two possible directions of magnetic moment (Section 5.6, thus more complex rotation-inversion operations on the spin (or magnetic moment) rather than just an inversion are needed to satisfy symmetry requirements (see, for example, Cracknell 1975, Litvin 1973 and Brinkman and Elliot 1966 a,b). In works on the symmetry of these magnetic materials some authors have considered time-inversion operator in combination with a full rotation group (including an inversion operation) on the spin arrangement (see, for example, Litvin 1973). Thus when using the generalized magnetic groups (or spin groups) worked out in their articles, it must be made quite clear that there is no time-antisymmetry property other than magnetic moment present in the calculations.

The symmetry and antisymmetry restrictions on the form of the transport tensors for materials with simple magnetic ordering have recently been established (Pourghazi, Saunders and Akgöz 1976) using the transformation law for field dependent tensors (equation 3.10). For reasons mentioned above, the use of the time inversion operator  $\theta$ , in that work has been avoided and the magnetic moment inversion operator has been employed.

#### 5.8 Generalized Neumann's principle

The effect of symmetry operations, corresponding to the transformation in physical space, on tensor properties of materials has been formulated through Neumann's principle (see Section 5.4). Equations (5.7) and (5.8) have been used by several authors to determine the symmetry restrictions on the form of field independent tensor properties of materials (see, for example, Birss 1966, Nye 1972, Bhagavantam 1966, and Wooster 1973). However in dealing with field dependent tensor properties of materials, when a symmetry operation corresponding to the transformation of field components is under consideration, there is some ambiguity in the validity and form of the Neumann's principle (see Birss 1966). We believe that this difficulty is due to the incorrect identification of the magnetic moment inversion operator with the time inversion operator, (see Section 5.7). Furthermore, since the transformation laws (3.10 and 3.11) should be used in constructing the analytical form of Neumann's principle for field dependent tensors, rather than the transformation laws (2.39), (2.41), Neumann's principle will have a slightly different analytical form for field dependent tensors. The transformation law for a field dependent tensor with  $t$  contravariant and  $s$  covariant indices ( $t + s = n$ ) and of weight  $\omega_1$  in subspace  $v$  (the physical space, for



example) and  $v$  contravariant and  $u$  covariant indices ( $v + u = \ell$ ) and of weight  $\omega_2$  in subspace  $M$  (the magnetic subspace or spin space for example) (see Section 3.7) can be written as (equation 3.11):

$$\begin{aligned}
 & \underbrace{B^{m_1 \dots m_v}}_{u} \underbrace{g_{m_1 \dots m_v}}_v \underbrace{r^{j_1 \dots j_t}}_t \underbrace{r^{k_1 \dots k_s}}_s (m'^a, r'^b) = \\
 & = \left| \frac{\partial m^g}{\partial m'^i} \right|^{\omega_1} \cdot \left| \frac{\partial r^j}{\partial r'^k} \right|^{\omega_2} \cdot \frac{g_1}{\alpha_1} \dots \frac{g_v}{\alpha_v} \cdot \frac{\beta_1}{\delta_1} \dots \frac{\beta_u}{\delta_u} \cdot \frac{j_1}{\gamma_1} \dots \frac{j_t}{\gamma_t} \\
 & \cdot \frac{\partial r^{\delta_1}}{\partial r'^{k_1}} \dots \frac{\partial r^{\delta_s}}{\partial r'^{k_s}} B^{m_1 \dots m_v} r^{j_1 \dots j_t} \left( \frac{\partial m'^a}{\partial m^\psi} m^\psi \cdot \frac{\partial r'^b}{\partial r^\mu} r^\mu \right) \quad (5.8)
 \end{aligned}$$

Now through Neumann's principle we can write

$$\underbrace{B^{m_1 \dots m_v}}_{u} \underbrace{g_{m_1 \dots m_v}}_v \underbrace{r^{j_1 \dots j_t}}_t \underbrace{r^{k_1 \dots k_s}}_s (m'^a, r'^b) = \underbrace{B^{m_1 \dots m_v}}_{u} \underbrace{g_{m_1 \dots m_v}}_v \underbrace{r^{j_1 \dots j_t}}_t \underbrace{r^{k_1 \dots k_s}}_s (m^a, r^b). \quad (5.9)$$

Substituting for  $\underbrace{B^{m_1 \dots m_v}}_{u} \underbrace{g_{m_1 \dots m_v}}_v \underbrace{r^{j_1 \dots j_t}}_t \underbrace{r^{k_1 \dots k_s}}_s (m'^a, r'^b)$  from equation (5.9)

into equation (5.8) we get:

$$\begin{aligned}
 & B \begin{matrix} g_1 & \dots & g_v \\ m_1 & \dots & m_v \end{matrix} \begin{matrix} j_1 & \dots & j_t \\ r_1 & \dots & r_t \end{matrix} (m^a, r^b) = \\
 & \begin{matrix} i_1 & \dots & i_u \\ m_1 & \dots & m_u \end{matrix} \begin{matrix} k_1 & \dots & k_s \\ r_1 & \dots & r_s \end{matrix} \\
 & = \left| \frac{\partial m^g}{\partial m'^i} \right|^{\omega_1} \cdot \left| \frac{\partial r^j}{\partial r'^k} \right|^{\omega_2} \cdot \frac{\partial m'^{g_1}}{\partial m^{\alpha_1}} \dots \frac{\partial m'^{g_v}}{\partial m^{\alpha_v}} \cdot \frac{\partial m^{\beta_1}}{\partial m'^{i_1}} \dots \frac{\partial m^{\beta_u}}{\partial m'^{i_u}} \cdot \frac{\partial r'^{j_1}}{\partial r^{\gamma_1}} \dots \\
 & \frac{\partial r'^{j_t}}{\partial r^{\gamma_t}} \cdot \frac{\partial r^{\delta_1}}{\partial r'^{k_1}} \dots \frac{\partial r^{\delta_s}}{\partial r'^{k_s}} B \begin{matrix} \alpha_1 & \dots & \alpha_v \\ m_1 & \dots & m_v \end{matrix} \begin{matrix} \gamma_1 & \dots & \gamma_t \\ r_1 & \dots & r_t \end{matrix} \left( \frac{\partial m'^a}{\partial m^\psi} m^\psi \cdot \frac{\partial r'^b}{\partial r^\mu} r^\mu \right)
 \end{aligned} \tag{5.10}$$

This is the most general, analytical form of Neumann's principle for field dependent tensors. Equation (5.10) can be equally well expressed in terms of operator form of the transformation matrices,  $\left( \frac{\partial m^i}{\partial m^j} \right)$  and  $\left( \frac{\partial r^i}{\partial r^j} \right)$ , i.e.  $\{ R_m | R_r \}$ , where  $R_m$  acts on the coordinates in M subspace and  $R_r$  acts on the coordinates in V subspace. That is for an unweighted tensor we can write:

$$\begin{aligned}
 & B \begin{matrix} g_1 & \dots & g_v \\ m_1 & \dots & m_v \end{matrix} \begin{matrix} j_1 & \dots & j_t \\ r_1 & \dots & r_t \end{matrix} (m^a, r^b) = \\
 & \begin{matrix} i_1 & \dots & i_u \\ m_1 & \dots & m_u \end{matrix} \begin{matrix} k_1 & \dots & k_s \\ r_1 & \dots & r_s \end{matrix} \\
 & = \{ R_m | R_r \} B \begin{matrix} \alpha_1 & \dots & \alpha_v \\ m_1 & \dots & m_v \end{matrix} \begin{matrix} \gamma_1 & \dots & \gamma_t \\ r_1 & \dots & r_t \end{matrix} (\{ R_m \} m^\psi, \{ R_r \} r^\mu) .
 \end{aligned} \tag{5.11}$$

In the special case where there is orthogonal linear transformation of coordinates in both subspaces to be considered, equation (5.10) can be written as:

$$B_{m_{i_1} \dots m_{i_n} r_{j_1} \dots r_{j_\ell}}(m_a, r_b) = |R_m|^p |R_r|^q \binom{(R_m)}{m_{i_1} \alpha_1} \dots \binom{(R_m)}{m_{i_n} \alpha_n} \binom{(R_r)}{r_{j_1} \beta_1} \dots \binom{(R_r)}{r_{j_\ell} \beta_\ell} \\ B_{m_{\alpha_1} \dots m_{\alpha_n} r_{\beta_1} \dots r_{\beta_\ell}} \left( \binom{(R_m)}{m_{\alpha_1} \psi}, \binom{(R_r)}{r_{\beta_1} \mu} \right) \quad (5.12)$$

where  $\binom{(R_m)}{m_{i_\alpha}}$  and  $\binom{(R_r)}{r_{j_\beta}}$  are the corresponding elements in the transformation matrices, and p and q are constants and have values zero or one according to the weight of tensor in each subspace (i.e. p = 0 if the tensor has even weight, that is if it is polar, in M and p = 1 if the tensor has odd weight, that is if it is axial in M).

Equations (5.10), (5.11) and (5.12) are different analytical forms of Neumann's principle for field dependent tensors defined upon spaces where the transformation operators can be divided into two parts, each acting on the coordinates in one subspace only. But there are some cases where the transformation operator cannot be divided in this fashion (see Section 3.8) because of the dependence of the coordinates of the field subspace on the coordinates of geometrical subspace. This will be investigated in the next section.

### 5.9 Neumann's principle for symmetry operations which act on the coordinates of both subspaces

To construct the analytical form of Neumann's principle for spatial symmetry operations which act on the coordinates in the field subspace, the appropriate transformation law should be chosen from one of the equations (3.18), (3.19) and (3.20).

#### 5.9.1 Example

As an example consider a space composed of two subspaces - field

subspace and geometrical subspace. In that space a field dependent tensor property B can now be considered which acts like a scalar function (zero rank tensor field) in the field subspace. Under a transformation of coordinates {A} in geometrical subspace, Neumann's principle can have one of the following forms depending on the nature of coordinates in the field subspace:

(a) when the coordinates in the field subspace behave like (covariant) vectors in geometrical subspace ,

$$B_{r_1 \dots r_t}^{k_1 \dots k_t} \left( \frac{\partial x^\alpha}{\partial x'^i} m_\alpha, \frac{\partial x'^g}{\partial x^\beta} r^\beta \right) = \frac{\partial x'^{j_1}}{\partial x^{\gamma_1}} \dots \frac{\partial x'^{j_t}}{\partial x^{\gamma_t}} \cdot \frac{\partial x^{\sigma_1}}{\partial x'^{k_1}} \dots \cdot \frac{\partial x^{\delta_s}}{\partial x'^s} B_{r_1 \dots r_t}^{\gamma_1 \dots \gamma_t} (m_\alpha, r^\beta), \tag{5.13}$$

where  $\frac{\partial x^i}{\partial x'^j}$  is the  $a_{ij}$  element of the transformation matrix (A) (equation 5.13) can equally well be written for fields which are contra-variant vectors in geometrical subspace, and also for weighted field vectors). For linear orthogonal transformation of coordinates (A) equation (5.13) can be written as:

$$B_{r_{k_1} \dots r_{k_s}} (\pm a_{i\alpha} m_\alpha, a_{j\beta} r^\beta) = a_{k_1 \gamma_1} \dots a_{k_s \gamma_s} B_{r_{\gamma_1} \dots r_{\gamma_s}} (m_\alpha, r^\beta), \tag{5.14}$$

where  $\pm$  signs in the bracket on the l.h.s. of equation correspond to whether the field is a polar or an axial vector.

(b) When the coordinates in the field subspace are second rank tensors in geometrical subspace ,

$$B_{r_1 \dots r_s}^{j_1 \dots j_t} \left( \frac{\partial r^{\alpha_1}}{\partial r'^{i_1}} \dots \frac{\partial r^{\alpha_2}}{\partial r'^{i_2}} m_{\alpha_1 \alpha_2}, \frac{\partial r^g}{\partial r^\beta} r^\beta \right) = \frac{\partial r'^{j_1}}{\partial r^{\gamma_1}} \dots \frac{\partial r'^{j_t}}{\partial r^{\gamma_t}} \cdot \frac{\partial r^{\delta_1}}{\partial r'^{k_1}} \dots \frac{\partial r^{\delta_s}}{\partial r'^{k_s}} B_{r_1 \dots r_s}^{\gamma_1 \dots \gamma_t} (m_{\alpha_1 \alpha_2}, r^\beta), \quad (5.15)$$

where  $m_{i_1 i_2}$  are the components of the field tensor along the coordinate axes in the geometrical subspace (the field tensor can have contravariant indices as well).

When a linear orthogonal transformation of coordinates, denoted by A - where there is no difference between covariant and contravariant indices - is considered equation (5.15) can be written as

$$B_{r_{k_1} \dots r_{k_s}}^{(\pm a_{i_1 \alpha_1} a_{i_2 \alpha_2} m_{\alpha_1 \alpha_2}, a_{j\beta} r^\beta)} = a_{k_1 \gamma_1} \dots a_{k_s \gamma_s} B_{r_{\gamma_1} \dots r_{\gamma_s}} (m_{\alpha_1 \alpha_2}, r^\beta), \quad (5.16)$$

where  $\pm$  signs in the bracket on the left-hand side of equation (5.16) refer to the field tensor being either a polar or an axial tensor.

(c) When the coordinate in the field subspace act like tensors of ranks (u) higher than two ,

$$B_{r_1 \dots r_s}^{j_1 \dots j_t} \left( \frac{\partial r^{\alpha_1}}{\partial r'^{i_1}} \dots \frac{\partial r^{\alpha_u}}{\partial r'^{i_u}} m_{\alpha_1 \dots \alpha_u}, \frac{\partial r^g}{\partial r^\beta} r^\beta \right) = \frac{\partial r'^{j_1}}{\partial r^{\gamma_1}} \dots \frac{\partial r'^{j_t}}{\partial r^{\gamma_t}} \cdot \frac{\partial r^{\delta_1}}{\partial r'^{k_1}} \dots \frac{\partial r^{\delta_s}}{\partial r'^{k_s}} B_{r_1 \dots r_s}^{\gamma_1 \dots \gamma_t} (m_{\alpha_1 \dots \alpha_u}, r^\beta), \quad (5.17)$$

The field tensor can also have contravariant indices. When a linear transformation of coordinates axes in geometrical subspace is considered equation (5.17) can be written as

$$B_{r_{k_1} \dots r_{k_s}} (\pm a_{i_1 \alpha_1} \dots a_{i_u \alpha_u} m_{\alpha_1 \dots \alpha_u}, a_{j_\beta} r_\beta) =$$

$$a_{k_1 \gamma_1} \dots a_{k_s \gamma_s} B_{r_{\gamma_1} \dots r_{\gamma_s}} (m_{\alpha_1 \dots \alpha_u}, r_\beta), \quad (5.18)$$

where again the  $\pm$  signs, in the bracket on the left hand side of equation (5.18), refer to field tensor being a polar or an axial tensor.

Using equation (5.14), (5.16) and (5.18), the restrictions imposed by the ordinary crystal groups (i.e. type I Heesch-Shubnikov groups, where only spatial symmetry operations are present) on the field dependent tensor properties, which have been defined through transformation laws (3.18), (3.19) and (3.20), have been investigated in Appendix I. The results for field dependent tensors up to rank four in geometrical subspace, with zero and first and second rank field tensors are listed in Tables A3 to A14

### 5.9.2 The general case

We may generalize the concepts of Section 5.9.1 to write Neumann's principle for field dependent tensor properties which have ranks higher than zero in the field subspace, where field components are themselves tensors in the geometrical subspace. To do this the symmetry operations  $\{ R_m \}$  which act on the field components can be derived from equation (3.23), as:

$$\{ R_m \} = \frac{\partial x^i}{\partial x'^1} \dots \frac{\partial x^i}{\partial x'^u} , \quad (5.19)$$

where  $u$  is the rank of the field tensor in the geometrical subspace, and  $\partial x^i / \partial x'^{\alpha_1}$  is an element of the transformation operation  $\{ R_r \}$  which acts on the coordinates in the geometrical subspace. Now equation (5.10) can be used as Neumann's principle.

There is also the possibility that the symmetry operations in the field subspace can be a combination of the operations of the form derived from equation (5.19), and other operations which are defined only in the field subspace, where again Neumann's principle will have the form of equation (5.10) and the geometrical part of symmetry operation should be worked out from equation (5.19).

In addition to the restrictions imposed by the symmetry operations of the space under consideration, a field dependent tensor may exhibit intrinsic symmetry. In other words the physical nature of the property may dictate certain restrictions, on the field dependent tensor components. An example of intrinsic symmetry is provided by Onsager's theorem (Onsager 1931 a,b) which is based on thermodynamical arguments (for further details see any textbook on irreversible thermodynamics such as, for example, de Groot 1951). This theorem has been used to find the restrictions on the form of transport properties in the next chapter.

CHAPTER 6

FIELD DEPENDENT TENSOR PROPERTIES OF CRYSTALS

6.1 Introduction

The concepts of the last chapter reveal that when a field-dependent physical property, such as one of the transport properties, of a crystal is under consideration the usual form of Neumann's principle (equations 5.4 to 5.8) fails to give correct results as far as the symmetry operations of the field coordinates are concerned. In this chapter the magnetoresistivity tensor for magnetic materials is considered. First the ways other workers have tackled the problem of finding the effect that symmetry operations acting on the magnetic field coordinates can have on the magnetoresistivity tensor and the discrepancy in the results obtained are discussed. Then making use of the transformation law of field dependent tensors (equation 3.10) and the generalized form of Neumann's principle (equation 5.10) the restrictions on the form of the magnetoresistivity tensor have been found.

Furthermore, the forms of the magnetothermoelectric power tensor  $\alpha_{ij}(\mathcal{B})$  for each of the magnetic point groups have been obtained using the same method as for the magnetoresistivity tensor. In addition the way that the permittivity tensor behaves as a field dependent tensor in a magnetic material is described.

6.2 The conductivity of a crystal

When an electric field, described by a polar vector  $\vec{E}$ , acts in a conductor, an electric current of density  $\vec{J}$  flows. In an isotropic medium  $\vec{J}$  is parallel to  $\vec{E}$  and the relationship between their components



is given by (Ohm's law):

$$\vec{J} = \sigma \vec{E} , \tag{6.1}$$

where  $\sigma$  is called the conductivity of the medium. That is

$$J_1 = \sigma E_1 , \quad J_2 = \sigma E_2 , \quad J_3 = \sigma E_3 \tag{6.2}$$

where  $E_1, E_2, E_3$  and  $J_1, J_2, J_3$  are the components of the vectors  $\vec{E}$  and  $\vec{J}$  in a rectangular cartesian system of coordinate axes,  $Ox_1, Ox_2, Ox_3$ .

Now when the medium is a crystal the conductivity is not necessarily isotropic, the vectors  $\vec{E}$  and  $\vec{J}$  need no longer be parallel; the conductivity cannot be represented by a scalar. However usually each component of  $\vec{J}$  is still linearly related to all three components of  $\vec{E}$ , and Ohm's law (equation 6.1) may now be represented by

$$\begin{aligned} J_1 &= \sigma_{11} E_1 + \sigma_{12} E_2 + \sigma_{13} E_3 , \\ J_2 &= \sigma_{21} E_1 + \sigma_{22} E_2 + \sigma_{23} E_3 , \\ J_3 &= \sigma_{31} E_1 + \sigma_{32} E_2 + \sigma_{33} E_3 . \end{aligned} \tag{6.3}$$

Or

$$J_i = \sigma_{ij} E_j , \tag{6.4}$$

where each  $\sigma_{ij}$  is constant. Thus according to the quotient law (see Section 2.12),  $\sigma_{ij}$  is a second rank polar tensor (field independent). The symmetry operations of the crystal impose restrictions on the form of  $\sigma_{ij}$  (see Section 5.4). Moreover there exists a restriction imposed by the intrinsic symmetry dictated by Onsager reciprocity relation which can be shown by

$$\sigma_{ij} = \sigma_{ji} . \quad (6.5)$$

The spatial symmetry restricted form the conductivity tensor  $\sigma_{ij}$  is well known, see for example, Nye (1972), Birss (1966) and Bhagavantam (1966).

### 6.3 The magnetoconductivity property of a crystal

If one now considers either a crystal that exhibits spontaneous magnetic ordering or a nonmagnetic crystal that is subjected to an external magnetic field, the relationship between  $\vec{J}$  and  $\vec{E}$  is still linear but the conductivity  $\sigma_{ij}$  must be replaced in equation (6.4) by a tensor  $\sigma_{ij}(\vec{B})$  which depends on the direction of the magnetic induction vector,  $\vec{B}$ , so that

$$J_i = \sigma_{ij}(\vec{B}) E_j . \quad (6.6)$$

where  $\sigma_{ij}(\vec{B})$  is called the magnetoconductivity tensor, and is a second rank polar (magnetic) field dependent tensor. Ohm's law (equation 6.6) can equally well be expressed in the following form:

$$E_i = \rho_{ij}(\vec{B}) J_j , \quad (6.7)$$

where  $\rho_{ij}(\vec{B})$  is the magnetoresistivity tensor and is the inverse of the magnetoconductivity tensor. In this case the details of the application of Onsager's theorem (equation 6.5) and Neumann's principle (see Section 5.8) have to be re-examined. If a crystal is subjected to a magnetic field  $H$ , one that may be an external field or may arise as an internal field in the crystal, it is then possible to show (see Onsager 1931 a,b and DeGroot 1951) that equation (6.5) has to be replaced by

$$\sigma_{ij}(\vec{B}) = \sigma_{ji}(-\vec{B}) , \quad (6.8)$$

and as for the magnetoresistivity tensor, the Onsager reciprocity relation will dictate

$$\rho_{ij}(\vec{B}) = \rho_{ji}(-\vec{B}) . \quad (6.9)$$

In obtaining the restrictions imposed by the symmetry properties of crystals on the forms of the magnetoconductivity and the magnetoresistivity tensors through Neumann's principle there has been some controversy among different workers (see Birss 1963, 1966, Kleiner 1966, 1967, 1969, Cracknell 1969, 1973, 1975 and Akgöz and Saunders 1975a). In the next section we shall give a short review of each of the methods adopted by different workers and comment on them and at the end we shall give our own method.

#### 6.4 Magnetic symmetry restrictions on the forms of the magnetoresistivity and the magnetoconductivity tensors.

The symmetry of a magnetically ordered crystal or of a nonmagnetic crystal in an external magnetic field  $H$  can be described by some magnetic point group  $G'$  which can be written as (see Sections 5.5, 5.6, 5.7)

$$G' = H + /A (G - H)$$

where  $G$  is the corresponding classical (spatial) point group and  $H$  is one of its subgroups and  $/A$  is the anti-symmetry operator, which can be identified with the magnetic moment (spin) inversion operator. Previous workers have identified the magnetic moment inversion operator with the time-inversion operator. This together with the failure to treat the magnetoconductivity and the magnetoresistivity tensors as field-dependent tensors (see Akgöz and Saunders 1975a) has led the procedures adopted

by these workers (prescriptions A, B and C) to wrong result.

#### 6.4.1 Prescription A - By Birss

In this prescription Birss follows previous workers in the field (Juretschke 1955, Mason et al 1953, and others) to express the components of the magnetoresistivity tensor  $\rho_{ij}(\vec{B})$  as series expansions in ascending powers of  $\vec{H}$ , the magnetic field. That is (Birss 1966, p.112, equation 3.26)

$$E_i = \rho_{ij} J_j + R_{ijk} J_j H_k + \dots \quad (6.10)$$

Now  $\rho_{ij}$ ,  $R_{ijk}$ , ... are second, third, ... rank field independent tensors. To correspond with these expansion coefficients, the usual experimental practice is to restrict measurement to the low magnetic field region, so that terms higher than second order can then be neglected.

In dealing with the anti-symmetry operation, Birss first identifies this operation with the time-inversion operation on the ground that since electron spin is associated with angular momentum which is a time-antisymmetric property, time-inversion operation reverses the direction of spin and therefore the direction of magnetic moment (for more detail see Birss 1966, pp.74-78). Then he states that for crystals where transport properties are present there exists an intrinsically preferred direction of time, that is, transport properties are time-antisymmetric) the application of Neumann's principle yields the erroneous result that all transport effects are prohibited for non-magnetic (i.e. time-symmetric) crystals. Therefore he concludes that "Neumann's principle cannot be applied in space-time." Then Birss gives the following prescription (referred to as prescription A by Kleiner 1966) for finding the restrictions on the forms of transport property tensors, based on what has been said above.

- (i) Use Onsager's theorem, i.e.  $\rho_{ij}(\vec{H}) = \rho_{ji}(-\vec{H})$ ,
- (ii) use Neumann's principle only for the unitary elements of the magnetic point group (elements which do not contain time-inversion operators in any form),
- (iii) ignore the antiunitary elements of the magnetic point group (elements which contain time-inversion operator).

The objections on this procedure are as follows:

- (a) Working with the low field coefficients (which are field-independent tensors) has some disadvantages, which are described in Section 3.3.
- (b) Kleiner (1966,1967,1969) objects to Birss' procedure on the grounds that by ignoring the anti-symmetry elements, it does not exploit the fully symmetry of the situation.
- (c) Identification of the spin-inversion operation with the time-inversion operation is not always correct (see Section 5.7), especially when there is some transport phenomenon present in the crystal. The way in which this identification leads to incorrect results for the conductivity tensor of a paramagnetic material will now be discussed here. Consider the current density  $\vec{J}$  in a paramagnetic crystal, subjected to an electric field  $\vec{E}$  in the absence of any external magnetic field (i.e.  $\vec{H} = 0$ ). Symmetry of the crystal will be described by one of the type II Heesch-Shubnikov point groups, in which  $\mathcal{A}$ , the magnetic moment (spin) inversion operator is a symmetry operator on its own as well as in combination  $\mathcal{A}\mathcal{S}$  with the spatial symmetry operators  $\mathcal{S}$  of the crystal point group. Now if  $\theta$  the operation of time inversion is identified with  $\mathcal{A}$ ,

in consequence of the fact that the current density  $\vec{J}$  is a time anti-symmetric property, then

$$\theta \vec{J} = -\vec{J} . \quad (6.11)$$

Taken this together with Neumann's principle ( $\vec{J} = \theta \vec{J}$ ) leads to

$$\vec{J} = \theta \vec{J} = -\vec{J} . \quad (6.12)$$

That is the current density is null. This cannot be true. From the point of view of the conductivity tensor, from Ohm's law ,

$$J_i = \sigma_{ij} E_j , \quad (6.13)$$

after the operation of  $\theta$  ,

$$\theta J_i = \theta \sigma_{ij} \theta E_j \quad (6.14)$$

$E_j$  is a time-symmetric property ,

$$\theta E_j = E_j . \quad (6.15)$$

Substituting from equations (6.11) and (6.15) into (6.14) we get

$$\theta \sigma_{ij} = -\sigma_{ij} . \quad (6.16)$$

But Neumann's principle dictates ,

$$\theta \sigma_{ij} = +\sigma_{ij} , \quad (6.17)$$

therefore

$$\sigma_{ij} = -\sigma_{ij} = 0 . \quad (6.18)$$

This indicates that all the paramagnetic crystals should be insulators in the absence of an external magnetic field. This is not true. Thus use of  $\theta$ , the operation of time-inversion does lead to the incorrect result that the conductivity tensor is null. We object to Birss' statement that Neumann's principle does not hold for transport phenomena in magnetic crystal ; further we consider that if application of Neumann's principle does lead to an incorrect result, then such a finding casts doubt not on Neumann's principle, but on the identification of the time-inversion operator,  $\theta$  with  $\mathcal{A}$ . Furthermore as the justification for identification of  $\theta$  with  $\mathcal{A}$ , Birss proves that the time-inversion operator has the effect of reversing the direction of the spin; however he does not prove that the two operations have exactly similar effects which is a necessary condition for such an identification. In fact the time-inversion operation has a much broader effect than the simpler operation of magnetic moment inversion:  $\theta$  actually changes the direction (or sign) of all the dynamic phenomena which depend on time to an odd degree.

#### 6.4.2 Prescription B: By Kleiner

Kleiner (1966,1967,1969) objects to the procedure adopted in prescription A on the grounds that no use is being made of the antisymmetry operations of the corresponding magnetic point group. He proposes a procedure which he calls "prescription B", in which he treats the problem on microscopic grounds and obtains the following equations.

$$\tau_{\mu\nu}^{B A}(\omega, \vec{B}) = \sum_K \sum_{\lambda} \tau_{K\lambda}^{B A}(\omega, \vec{B}) D^{(B)}(u)_{K\mu} D^{(A)}(u)_{\lambda\nu}, \quad (6.19)$$

for the spatial symmetry operators of the corresponding point group ,

and

$$\tau_{\mu\nu}^B A_{\lambda}^{\rightarrow}(\omega, \vec{B}) = \sum_K \sum_{\lambda} \tau_{\lambda}^{A+} B_{\mu}^+ K(\omega, \vec{B}_a) D^{(B)}(a)_{K\mu} \cdot D^{(A)}(a)_{\lambda\nu}^* \quad (6.20)$$

for the symmetry operators which involve  $\theta$ , the operation of time-inversion. In these equations  $\tau_{\mu\nu}^B A_{\lambda}^{\rightarrow}(\omega, \vec{B})$  are the components of a transport tensor,  $\omega$  is the angular frequency (which for Ohm's law is zero),  $\vec{B}$  is the magnetic field,  $D^{(A)}(a)_{\lambda\nu}$  and  $D^{(B)}(a)_{K\mu}$  are the transformation matrices corresponding to the unitary (spatial) symmetry operations, and  $D^{(A)}(a)_{\lambda\nu}^*$  and  $D^{(B)}(a)_{K\mu}$  are the ones corresponding to antiunitary symmetry operations (those which contain  $\theta$ ). Equation (6.19) is the same as the commonly accepted equation based on the definition of a field-independent second rank tensor and the use of Neumann's principle. Equation (6.20) differs from equation (6.19) in that the transformation matrices on the right-hand side of equation (6.20) are the complex conjugates of those in equation (6.19), and also the transposition of the suffixes on the right-hand side of equation (6.20) does not occur in equation (6.19). In Kleiner's procedure, relations between transport coefficients are found by using in equations (6.19) and (6.20) the unitary and antiunitary elements, respectively, that are contained in the group  $G'$  (or  $J$  or  $J(\vec{B})$  in Kleiner's notation):  $G'$  is the group of the operations which leave the Hamiltonian  $H(\vec{B})$  invariant ( $G'$  is called the Schrödinger group of the system and is usually the same as the magnetic point group or the magnetic space group of the crystal). It is possible to choose, on physical grounds, a Hamiltonian with more (not less) symmetry than  $G'$ , the magnetic point group. Considering this fact, in Kleiner's procedure, Onsager's theorem has been dealt with in a different way from that which Birss employs. Instead of using the group  $G'$  that includes only the operations which leave the Hamiltonian  $H(\vec{B})$  of the system



invariant, Kleiner constructs another group  $K(\vec{\mathfrak{B}})$ . In addition to the operations of the magnetic group  $G'$ ,  $K(\vec{\mathfrak{B}})$  also includes all the operations that send  $H(\vec{\mathfrak{B}})$  into  $H(-\vec{\mathfrak{B}})$ . By using the larger group  $K(\vec{\mathfrak{B}})$  instead of  $G'$ , Kleiner is able to derive the generalized Onsager reciprocal relations as a consequence of requiring the tensor to be invariant under the operations of the group  $K(\vec{\mathfrak{B}})$ . Therefore in prescription B, Onsager's reciprocity relations are not used, because they are assumed to be covered by the use of  $K(\vec{\mathfrak{B}})$ . The group  $K(\vec{\mathfrak{B}})$  having been contracted, prescription B consists of the following steps:

- (i) Use equation (6.19) for the unitary elements of  $K(\vec{\mathfrak{B}})$ .
- (ii) Use equation (6.20) for the antiunitary elements (those which contain  $\theta$ , the time-inversion operator) of  $K(\vec{\mathfrak{B}})$ .

The following objections can be made to this procedure:

(a) Cracknell (1973) objects to Kleiner's procedure in using the group  $K(\vec{\mathfrak{B}})$  and states that: in using the group  $K(\vec{\mathfrak{B}})$  instead of  $G'$ , Kleiner assumes that only even terms in  $\vec{\mathfrak{B}}$  appear in  $H(\vec{\mathfrak{B}})$ , the Hamiltonian of the crystal. This is not justified, since the only physical reason for this assumption is the modified Onsager relation

$$\sigma_{ij}(\vec{\mathfrak{B}}) = \sigma_{ji}(-\vec{\mathfrak{B}}) \quad (6.21)$$

which means that the diagonal components of the electrical conductivity tensor are even functions of  $\vec{\mathfrak{B}}$ . This is certainly a different condition from the assumption that all the components be even functions of  $\vec{\mathfrak{B}}$ .

Furthermore Cracknell finds the assumption "prescription B leads to correct simplifications of a transport tensor property of a crystal with symmetry described by one of the magnetic point group, because the requirement of invariance of the tensor under  $H(\vec{\mathfrak{B}})$  leads to the right answer for

the generalized Onsager reciprocity relation" unjustified.

(b) We have the further objection to the procedure adopted by Kleiner that in constructing the magnetic point group  $G'$ ,  $\theta$ , the operation of time-inversion, has been identified with the operation of magnetic moment inversion operation (for more detail on why this identification is not correct see Section 6.4.1(c)).

#### 6.4.3 Prescription C : by Cracknell

Cracknell (1973) follows Birss' macroscopic approach to the problem, and he also assumes without any proof that the magnetic moment-inversion operator can be identified with  $\theta$ , the time-inversion operator. Then in dealing with the antiunitary operations which do involve  $\theta$ , he adopts the following procedure:

I. Consider Ohm's law in the absence of any magnetic field (internal or external)

$$J_i = \sigma_{ij} E_j . \quad (6.22)$$

$\theta$  will reverse the sign of  $\vec{J}$ , but will leave  $\vec{E}$  unaltered; that is  $\vec{J}$  is a c tensor (i.e. a tensor which changes sign under the operation of  $\theta$ ) of rank one and  $\vec{E}$  is an i tensor (i.e. a tensor which remains invariant under  $\theta$ ) of rank one. Therefore, from (6.22),  $\sigma_{ij}$  is a c tensor of rank two,

$$\theta \sigma_{ij} = - \sigma_{ij} \quad (6.23)$$

From this Cracknell comes to the conclusion that  $\theta$  cannot be a symmetry operation of the complete configuration of specimen  $+\vec{J} + \vec{E}$ . Then he regards the specimen as a "black box" which contains some material entities and a magnetic field  $\vec{H}$ , and considers a crystal for which  $\theta$  is a symmetry

operation. Now since  $\theta$  is a symmetry operation of the black box, then

$$\theta \sigma_{ij} = \sigma_{ij} \quad (6.24)$$

Then Cracknell claims that equations (6.24) and (6.23) are not in conflict because equation (6.24) applies if the symmetry of the specimen is described by one of the grey groups, and if it is assumed that Neumann's principle still holds for  $\theta$ , while equation (6.23) refers to the application of  $\theta$  to a larger system of which  $\theta$  is not a symmetry operation. Therefore if equation (6.24) holds, then equation (6.23) cannot hold, because  $\sigma_{ij}$  would then be null.

II. Now if  $\vec{H} \neq 0$ , that is, when the black box consists of a magnetically ordered crystal or consists of a non-magnetic crystal situated in an applied magnetic field,  $\theta$  is not a symmetry operation on its own. But there are certain antiunitary operations of the form  $\theta S$ , where  $S$  is a spatial point group operation, which are symmetry operations of the black box. Then Cracknell supposes that Neumann's principle still holds (despite Birss' argument) for these operations  $\theta S$ . That is,

$$(\theta S) \sigma_{ij}(\vec{H}) = \sigma_{ij}(\vec{H}) . \quad (6.25)$$

Now to make use of the transformation properties of the tensor under these antiunitary operations, the result of the application of  $\theta$  to  $\sigma_{ij}(\vec{H})$  must be determined. For this Cracknell states that "the effect of  $\theta$  on the motions of all the particles in the black box will be to reverse the directions of their velocities and, therefore, the Lorentz forces  $\mu \mu_0 e (\vec{v} \times \vec{H})$ ; therefore, the Hamiltonian will only remain invariant if  $H$  is also reversed. Consequently, the current  $J_i$  flowing in a given direction as a result of the application of an electric field  $E_j$  will be

unaltered if the direction of  $\vec{B}$  is also reversed; that is

$$\theta \sigma_{ij}(\vec{B}) = \sigma_{ij}(-\vec{B}) . \quad (6.26)$$

Cracknell describes equation (6.26) to be simply a statement of the fact that the compound operation of time-reversal plus changing the sign of  $\vec{B}$  is a symmetry operation of the system in the black box. Equations (6.26) and (6.24) only apply when direct current is under consideration. For alternating current, Cracknell defines the following equations to replace equations (6.24) and (6.26) respectively ,

$$\theta \sigma_{ij} = \sigma_{ij}^* \quad (6.27)$$

and

$$\theta \sigma_{ij}(\vec{B}) = \sigma_{ij}^*(-\vec{B}) \quad (6.28)$$

Then substituting from equation (6.28) into equation (6.25) Cracknell gives the following treatment ,

$$\begin{aligned} \sigma_{ij}(\vec{B}) &= \theta S \sigma_{ij}(\vec{B}) = S \theta \sigma_{ij}(\vec{B}) \\ &= S \sigma_{ij}^*(-\vec{B}) . \end{aligned}$$

That is ,

$$\sigma_{ij}(\vec{B}) = S_{ip} S_{jq} \sigma_{pq}^* [S^{-1}(-\vec{B})] \quad (6.29)$$

or

$$\sigma_{ij}(\vec{B}) = S_{ip} S_{jq} \sigma_{pq}^*(\vec{B}) , \quad (6.30),$$

i.e.,

$$\sigma_{ij}(\vec{B}) = S_{ip} S_{jq} \sigma_{pq}^*(\vec{B}) \quad (6.31)$$

Cracknell, therefore, arrives at the following procedure, for finding the restrictions on the form of magnetoconductivity tensor, imposed by magnetic symmetry of the crystal, (which he calls prescription C):

- (i) Use equations (6.5) and (6.8) based on Onsager's theorem,
- (ii) use

$$\sigma_{ij} = R_{ip} R_{jq} \sigma_{pq} \quad (6.32)$$

based on Neumann's principle for the unitary elements  $R$  of  $G'$ , the magnetic point group, and

- (iii) use equation (6.29), based on a modified form of Neumann's principle, for the antiunitary elements  $\theta S$ , of  $G'$ .

Prescription A and prescription C will always lead to the same results, except that, as a result of part (iii), prescription C may lead to some further simplification on the form of  $\sigma_{ij}$  beyond that achieved by prescription A.

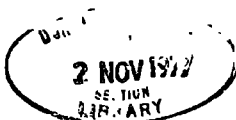
We have the following objections to this prescription:

- (a) In part (ii) of prescription C magnetoconductivity tensor components have been treated like field-independent tensor components, which is not correct (see Akgöz and Saunders 1975a).
- (b) Identification of the time-inversion operation with the magnetic-moment inversion operation is not correct (see Section 6.3.1 for more detail), and this leads to the following weaknesses in Cracknell's discussion to justify his prescription; in part I of his discussion despite Cracknell's claim we believe that equation (6.23) is in conflict with equation (6.24), because equation (6.23) always holds and  $\sigma_{ij}$  is always a second rank polar c tensor (which changes sign under the operation of

time-inversion) and if  $\theta$  is the symmetry operation of the system  $\sigma_{ij}$  is a null tensor. Furthermore in part II, we find the discussion on the effect of  $\theta$  on  $\sigma_{ij}(\vec{B})$  which leads to equation (6.26) unsatisfactory. Firstly because it says that as a result of the operation of  $\theta$  on the system, the velocity  $\vec{v}$  (and therefore the current density  $\vec{J}$ ) will be reversed, and for the Lorentz force, and therefore the Hamiltonian, to remain invariant under  $\theta$ ,  $\vec{B}$  the magnetic field should also be reversed. Then it says that as a result of reversing the direction of  $\vec{B}$ ,  $\vec{J}$  the current density will remain unaltered. These two statements are contradictory. Then there is the further objection to Cracknell's procedure in deriving equation (6.31) that: in writing equation (6.29) Cracknell, without any discussion, recognizes the need to operate the symmetry operation on the argument of  $\sigma_{ij}(\vec{B})$  as well as on its components, but in writing equation (6.30) he replaces  $S^{-1}(-\vec{B})$  by  $(\vec{B})$  which may be correct for certain symmetry operations, but is not true for others.

#### 6.4.4 Prescription D : Present work

A major weakness of the earlier prescription is that they all suffer from the lack of their authors to appreciate  $\sigma_{ij}(\vec{B})$  is a field-dependent tensor. A new prescription has therefore been developed in which the magnetoconductivity tensor components are treated as the components of a field-dependent tensor, and the generalized Neumann's principle (see Section 5.8) is employed to find the symmetry and antisymmetry restrictions on the form of  $\sigma_{ij}(\vec{B})$ . Furthermore the antisymmetry operator,  $A$ , is not identified with  $\theta$ , the time inversion operator. To find the effect of  $A$  on  $\sigma_{ij}(\vec{B})$  we must ensure the invariance of Ohm's law under this operation. Ohm's law for direct current in the presence of a magnetic field can be written as ,



$$J_i(\vec{B}) = \sigma_{ij}(\vec{B}) E_j . \quad (6.33)$$

Under the operation of magnetic moment inversion (the antisymmetry operation), this becomes

$$\mathcal{A} J_i(\vec{B}) = \mathcal{A} \sigma_{ij}(\vec{B}) \mathcal{A} E_j . \quad (6.34)$$

To find the effect of  $\mathcal{A}$  on  $\sigma_{ij}(\vec{B})$ , it is required to know the effect of  $\mathcal{A}$  on  $J_i(\vec{B})$  and  $E_j$ . The electric field vector  $E_j$  is invariant under  $\mathcal{A}$ ,

$$\mathcal{A} E_j = E_j . \quad (6.35)$$

The effect of  $\mathcal{A}$  on  $\vec{B}$  is defined as ,

$$\mathcal{A} \vec{B} = -\vec{B} \quad (6.36)$$

when the operator  $\mathcal{A}$  acts on a system containing a magnetic moment and a current density  $J_i(\vec{B})$ , the only effect is to alter the direction of  $\vec{B}$  and so ,

$$\mathcal{A} J_i(\vec{B}) = J_i(\mathcal{A}\vec{B}) = J_i(-\vec{B}) . \quad (6.37)$$

For Ohm's law to hold in the system under the operation of magnetic moment inversion, substitution from (6.35) and (6.37) into (6.34) leads to ,

$$\mathcal{A} \sigma_{ij}(\vec{B}) = \sigma_{ij}(-\vec{B}) \quad (6.38)$$

For the symmetry operations  $\mathcal{A} \mathcal{R}$  , Neumann's principle demands that ,

$$\mathcal{A} \mathcal{R} \sigma_{ij}(\vec{B}) = \sigma_{ij}(\mathcal{A} \mathcal{R} \vec{B}) , \quad (6.39)$$

or

$$\mathcal{R} \mathcal{A} \sigma_{ij}(\vec{B}) = \sigma_{ij}(\mathcal{R} \mathcal{A} \vec{B}) , \quad (6.40)$$

since  $A \mathbb{R} = \mathbb{R} A$ , substituting for  $A \sigma_{ij}(\vec{B})$  from (6.38) into (6.40), we obtain

$$\mathbb{R} \sigma_{ij}(-\vec{B}) = \sigma_{ij}(\mathbb{R} A \vec{B}) = \sigma_{ij}(-\mathbb{R} \vec{B}).$$

Therefore

$$\mathbb{R} \sigma_{ij}(\vec{B}) = \sigma_{ij}(\mathbb{R} \vec{B}). \quad (6.41)$$

Thus we obtain

$$\sigma_{ij}(|\mathbb{R}|R_{1q} \mathbb{B}_q, |\mathbb{R}|R_{2q} \mathbb{B}_q, |\mathbb{R}|R_{3q} \mathbb{B}_q) = R_{im} R_{jn} \sigma_{mn}(\mathbb{B}_1, \mathbb{B}_2, \mathbb{B}_3). \quad (6.42)$$

Therefore, the analytical form of Neumann's principle for  $\sigma_{ij}(\vec{B})$  (or  $\rho_{ij}(\vec{B})$ ) applies to crystals belonging to any of the three types (I, II, III) of Heesch-Shubnikov point groups, for both kinds of spatial symmetry operations (the ones which are elements of the magnetic point group on their own, and the ones which in combination with  $A$ , the operation of magnetic moment inversion, are elements of the magnetic point group). When  $\vec{H} \neq 0$ , the form of  $\sigma_{ij}(\vec{B})$  does not depend on whether the specimen consists of a non-magnetic crystal (paramagnetic and diamagnetic and some antiferromagnetic crystals) in an applied magnetic field or of a magnetically ordered crystal. Furthermore since  $\sigma_{ij}$  is a second rank polar tensor and  $\vec{B}$  a first rank axial tensor they are both invariant under the operation of inversion in the space (see Table A.1).

Therefore our prescription D for finding the forms of  $\sigma_{ij}(\vec{H})$  for a crystal belonging to a magnetic point group is as follows:

- (i) Find the corresponding classical point group  $G$  of the magnetic point group  $G'$ , noting that  $G'$  depends upon the direction of  $\vec{B}$ ,



(ii) take the enantiomorphous point group of this classical point group and use its generating elements in equation (6.42), which is based on the transformation law for field dependent tensors and generalized Neumann's principle, to distinguish the non-zero components for a chosen magnetic direction, and

(iii) apply equation (6.8) based on Onsager's theorem.

Thus we have concluded that the symmetry restricted forms of  $\sigma_{ij}(\vec{H})$  for crystals belonging to magnetic point group  $G'$  are identical to those of the crystals belonging to the corresponding point group  $G$ . The latter have been listed for  $\vec{H}$  directed along the major crystallographic axes by Akgöz and Saunders (1975a).

### 6.3 Symmetry restrictions on the forms of other transport properties

In a magnetic crystal or a non-magnetic crystal in an external magnetic field the electrical and heat current densities  $\vec{j}$  and  $\vec{q}$  are related to the electromotive force  $\vec{E}$  and the temperature gradient  $\vec{\nabla}T$  by the phenomenological linear transport equations

$$E_i = \rho_{ij}(\vec{H}) J_j + \alpha_{ij}(\vec{H}) \nabla_j T \quad (6.43)$$

$$q_i = \pi_{ij}(\vec{H}) J_j - \kappa_{ij}(\vec{H}) \nabla_j T \quad (6.44)$$

where each component of the second rank transport tensors - the magneto-resistivity  $\rho_{ij}(\vec{H})$  (the reverse of the magnetoconductivity  $\sigma_{ij}(\vec{H})$ ), the magnetothermoelectric power  $\alpha_{ij}(\vec{H})$ , the magneto-Peltier effect  $\pi_{ij}(\vec{H})$  and the magnetothermal conductivity  $\kappa_{ij}(\vec{H})$  - depends on the magnetic field. Thus these transport properties should be dealt with as field-dependent tensors. The spatial and magnetic symmetry restrictions on the forms of

all these tensors are the same as those on the magnetoconductivity tensor. The only difference is the intrinsic symmetry dictated by Onsager's theorem, which is not the same for all these properties. That is

$$\sigma_{ij}(\vec{B}) = \sigma_{ji}(-\vec{B}), \quad (6.45)$$

$$\rho_{ij}(\vec{B}) = \rho_{ij}(-\vec{B}), \quad (6.46)$$

$$\kappa_{ij}(\vec{B}) = \kappa_{ij}(-\vec{B}), \quad (6.47)$$

and

$$(1/T) \pi_{ij}(\vec{B}) = \alpha_{ji}(-\vec{B}) \quad (6.48)$$

Therefore the magnetoresistivity tensor  $\rho_{ij}(\vec{B})$  and the magnetothermal conductivity tensor  $\kappa_{ij}(\vec{B})$  take the same forms as  $\sigma_{ij}(\vec{B})$ . The forms of the magnetothermoelectric power  $\alpha_{ij}(\vec{B})$  and the magneto-Peltier effect  $\pi_{ij}(\vec{B})$  for crystals belonging to the magnetic point group  $G'$  are the same as those of crystals belonging to the corresponding classical point group  $G$ , in a magnetic field; they are different from  $\sigma_{ij}(\vec{B})$ . These forms have been tabulated by Akgöz and Saunders (1975b).

### 6.6 The permittivity of a crystal

In an anisotropic body, the magnetic field intensity  $\vec{H}$  (field strength) and the magnetic induction  $\vec{B}$  (flux density) are connected by the relation (see Nye 1957) ,

$$B_i = \mu_{ij} H_j, \quad (6.49)$$

where  $\mu_{ij}$  is called the permittivity of the body and is a second rank polar tensor with respect to spatial transformations. But, as considered in Section (3.7), there are cases where we have to deal with more

complicated transformation operators of the kind  $\{R_p | R_i | w_{ip}\}$ , with  $R_p$  operating only on the spin (magnetic) space coordinates. Therefore the behaviour of  $\mu_{ij}$  has to be investigated in this space, and to do this the tensorial behaviour of  $\vec{B}$  and  $\vec{H}$  in that space have to be found.

Magnetic field is a vector (first rank tensor) in the magnetic subspace and so is the magnetic induction. Therefore, using the quotient law (Section 4.6), it can be shown that permittivity must be a second rank tensor in the magnetic subspace as well as in the physical subspace. This means that in the combined space of magnetic and physical subspaces magnetic field and magnetic induction will each have nine components (each of the three components in the physical, or geometrical, subspace will have three components in the magnetic subspace). Therefore the permittivity tensor will have eighty one components in this combined space. Equation (6.49) may now be written

$$(B_i)_\alpha = (\mu_{ij})_{\alpha\beta} (H_j)_\beta \quad (6.50)$$

where  $\alpha$  and  $\beta$  refer to the coordinate axis in the magnetic subspace and  $i$  and  $j$  to the coordinate axis in the geometrical subspace.

A linear relationship between the magnetic induction,  $\vec{B}$ , and the magnetic field  $\vec{H}$  does not hold for all the substances. There are some cases where permittivity depends on the magnitude of the applied magnetic field. In the ordinary physical subspace this may be shown by

$$B_i = \mu_{ij}(\vec{H}) H_j \quad (6.51)$$

In this case permittivity can be dealt with as a field dependent tensor field and every transformation operator will operate on the components of its argument  $(\vec{H})$  as well as on its own components.

APPENDIX I

SPATIAL SYMMETRY RESTRICTED FORMS OF FIELD DEPENDENT

TENSORS OF RANK ZERO IN THE FIELD SUBSPACE, WHERE

FIELD COMPONENTS ARE THEMSELVES TENSORS IN

GEOMETRICAL SUBSPACE

A.1 Introduction

In dealing with the field dependent tensor properties of solids, the situation where the field components have some kind of tensorial dependence on the coordinate axes in geometrical subspace is frequently encountered. The magnetoresistivity tensor in magnetic crystals is an example of such physical properties, where the components of resistivity tensor depend on the magnetic field which itself is a first rank tensor in geometrical subspace. Here the transformation operations of the coordinate axes in geometrical subspace will affect the coordinate axes of the field subspace too (see Section 5.9), unless otherwise stated. Inserting symmetry operations of this kind in Neumann's principle (equation 5.18), the general forms of these field dependent tensors for each of the 32 classical crystallographic point groups have been obtained in this appendix. Three-dimensional rotation groups have been employed as the instrument for identification of the non-zero components. The forms of field dependent tensors up to fourth rank in the matter tensor and second rank in the field tensor (the argument of the field dependent tensor) are tabulated at the end of this appendix.

To avoid writing long sentences we use 'field dependent tensor' to mean "field dependent tensors of rank zero (scalar function) in the field subspace" in the rest of this appendix.

A.2 Application of Neumann's Principle

Transformation law of a field dependent tensor (equation 3.20) requires that both the tensor components and the field components (the argument of the tensor) be transformed. Therefore Neumann's principle (equation 5.18) based on this transformation law for an orthogonal transformation of coordinates (in the geometrical subspace)  $x_i' = \sigma_{ij} x_j$  can be written as

$$B_{ijk...} (|\sigma|^c \sigma_{mn} \sigma_{op} \dots F_{np}) = |\sigma|^d \sigma_{ir} \sigma_{js} \sigma_{kt} \dots B_{rst...} (F_{mo...}) \quad (A.1)$$

where all the indices refer to the coordinates in geometrical subspace, field components are denoted by  $F_{mo...}$ ,  $\sigma_{ij}$ 's are the elements of the transformation matrix, and  $|\sigma|$  its determinant. Both the field dependent tensor (matter tensor) components  $B_{ijk...}$  and the arguments (field tensor)  $F_{mo...}$  can transform either as polar (zero c and d in equation A.1) or axial (c and d equal one in equation A.1) tensors. This results in four different kinds (labelled  $\alpha, \beta, \gamma, \delta$ ) of field dependent tensors which can be described by the following equation for the analytical form of Neumann's principle:

tensor type  $\alpha$  - polar matter tensor ( $d = 0$ ) dependent upon polar field tensor ( $c = 0$ ).

$$B_{ijk...} (\sigma_{mn} \sigma_{op} \dots F_{np}) = \sigma_{ir} \sigma_{js} \sigma_{kt} \dots B_{rst...} (F_{mo...}) \quad (A.2)$$

tensor type  $\beta$  - polar matter tensor ( $d = 0$ ) dependent upon axial field tensor ( $c = 1$ )

$$B_{ijk...} (|\sigma| \sigma_{mn} \sigma_{op} \dots F_{np}) = \sigma_{ir} \sigma_{js} \sigma_{kt} \dots B_{rst...} (F_{mo...}) \quad (A.3)$$

tensor type  $\gamma$  - axial matter tensor ( $d = 1$ ) dependent upon polar field tensor ( $c = 0$ )

$$B_{ijk\dots}(\sigma_{mn} \sigma_{op\dots} F_{np\dots}) = |\sigma| \sigma_{ir} \sigma_{js} \sigma_{kt\dots} B_{rst} (F_{mo\dots}) \quad (A.4)$$

tensor type  $\delta$  - axial matter tensor ( $d = 1$ ) dependent upon axial field tensor ( $c = 1$ )

$$B_{ijk\dots}(|\sigma| \sigma_{mn} \sigma_{op\dots} F_{np\dots}) = |\sigma| \sigma_{ir} \sigma_{js} \sigma_{kt\dots} B_{rst\dots} (F_{mo\dots}) \quad (A.5)$$

The matter and field tensors can be further classified into those of even and odd rank to give the following nomenclature:

tensor of kind a - even rank matter tensor and even rank field tensor;

tensor of kind b - odd rank matter tensor and even rank field tensor;

tensor of kind c - even rank matter tensor and odd rank field tensor;

tensor of kind d - odd rank matter tensor and odd rank field tensor.

Combination of this nomenclature with the  $\alpha, \beta, \gamma, \delta$  classification leads to sixteen distinct types of tensor labelled  $\alpha a, \dots, \delta d$ .

To find the maximum simplification in the forms of these sixteen types of tensor the set of generating matrices used by Birss (1966) (see Section 5.4) has been employed in equations (A.2), (A.3), (A.4) and (A.5). During this substitution of generating matrices, certain equalities or relationships have been found between tensors of the same rank for different point groups. These will now be listed.

1. The forms of the tensors for crystals belonging to centrosymmetrical point groups are affected by the fact that  $\sigma^{(1)}$  is a generating element; for  $\sigma^{(1)}$

$$\sigma_{ip} = \begin{cases} -1 & \text{if } i = p \\ 0 & \text{if } i \neq p \end{cases}$$

and the determinant  $|\sigma^{(1)}|$  is -1. In general

$$B_{ijk...} (\pm \sigma_{mm} \sigma_{oo...} F_{mo...}) = \pm \sigma_{ii} \sigma_{jj} \sigma_{kk} \dots B_{ijk...} (F_{mo...}) \quad (\text{A.6})$$

where the + sign corresponds to polar and the - sign to axial tensors.

This can be written as

$$B_{ijk...} (\pm (-1)^n F_{mo...}) = \pm (-1)^m B_{ijk...} (F_{mo...}) \quad (\text{A.7})$$

where m and n are respectively the ranks of the matter and field tensors.

Thus four different sets of equations, which depend upon both the rank and polarity of the tensor, result:

$$(i) \quad B_{ijk....} (F_{mo...}) = B_{ijk....} (F_{mo....}) \quad (\text{A.8a})$$

for this case,  $\sigma^{(1)}$  does not introduce any simplification and therefore the appropriate enantiomorphous point group generating elements are sufficient to produce the maximum simplification of the tensor.

$$(ii) \quad B_{ijk....} (F_{mo...}) = -B_{ijk....} (F_{mo....}) = 0 \quad (\text{A.8b})$$

hence the matter tensor is null .

$$(iii) \quad B_{ijk\dots}(-F_{mo\dots}) = B_{ijk\dots}(F_{mo\dots}) \quad (A.8c)$$

the matter tensor components are even functions of the field tensor components,

$$(iv) \quad B_{ijk\dots}(-F_{mo\dots}) = -B_{ijk\dots}(F_{mo\dots}) \quad (A.8d)$$

the matter tensor components are odd functions of the field tensor components. Inspection of equations (A. 8) for each of the sixteen different types of tensor leads to the general result shown in Table A.1.

2. For those point groups which contain only the generating elements  $\sigma^{(0)}$ ,  $\sigma^{(2)}$ ,  $\sigma^{(3)}$ ,  $\sigma^{(6)}$ ,  $\sigma^{(7)}$  and  $\sigma^{(9)}$  whose determinants are unity, the forms of all the field dependent tensors of the same rank for a given point group are identical for both the polar and axial matter tensors; this is independent of the polar or axial nature of the field tensor.

3. The generating matrices  $\sigma^{(3)}$  and  $\sigma^{(5)}$  are such that  $\sigma^{(3)} = -\sigma^{(5)}$  and  $|\sigma^{(3)}| = 1 = -|\sigma^{(5)}|$ . Therefore

$$\begin{aligned} \{-1\}^n \sigma_{ir}^{(3)} \sigma_{js}^{(3)} \sigma_{kt}^{(3)} \dots B_{rst\dots}(F_{mo\dots}) &= \\ &= \pm \sigma_{ir}^{(5)} \sigma_{js}^{(5)} \sigma_{kt}^{(5)} \dots B_{rst\dots}(F_{mo\dots}) \end{aligned} \quad (A.9)$$

where n is the rank of matter tensor. Thus for even rank polar or odd rank axial field tensors, the two generating elements  $\sigma^{(3)}$  and  $\sigma^{(5)}$  have the same effect on the even rank polar or odd rank axial matter tensors.

### A.3 Tabulation of the forms of the field dependent tensors

The equalities and other relationships between the field dependent tensors between and within point groups are shown in Table 2. Null tensors



are also shown where they occur. To make matters easier, the plan used in construction of the table is based upon that used by Birss (1966), in his similar table (4a) for constant tensors. Where tensors are labelled with a different capital letter, their forms are dissimilar (some capital letters have bars on them. This is to increase the supply of letters and has no other special meaning). The subscripts  $m$  (for even numbers) and  $n$  (for odd numbers) show the rank of the matter tensors.  $(F_p)$  and  $(F_q)$  represent the field tensor, here  $p$  shows an even rank and  $q$  an odd rank tensor; where they occur the superscripts  $o$  and  $e$  show that only odd or even functions of the field components are present. The significance of a dash on the letters  $B$  or  $C$  representing the matter tensor is that there is in this case a simple relationship between the pairs of forms  $B$  and  $B'$  or  $C$  and  $C'$ , namely that if even or odd terms are present in the dashed letter they are absent in the un-dashed one and vice versa. Thus, if a component of  $B$  is an even function of the field components, then that component of  $B'$  is an odd function. Furthermore, if a component of  $B$  contains both odd and even terms, then that component of  $B'$  is zero and vice versa.

The complete forms of the tensors represented symbolically in Table A.2 are detailed in Tables A.3 to A.14. The forms of the field dependent tensors up to fourth rank ( $m = 0, 2, 4; n = 1, 3$ ) for the matter tensor and up to second rank ( $p = 0, 2; q = 1$ ) for the argument have been obtained by systematic substitution of the generating matrices for each point group into equations (A.2) - (A.5). The matter tensor components are represented by  $X, Y, Z$  and of course for higher rank tensors in combination such as  $XY$ . The field tensor components are shown as  $x, y, z$ , also in combinations such as  $xy$  for a second rank field tensor. Each column shows a particular tensor component and a

row shows all the components of a particular tensor; certain components exist only as either an even or an odd function of the field tensor - this is indicated directly. When an equality between components occurs then it is shown by writing in its place that term (or even or odd part of the term) in the same row to which it is equal. To reduce the size of the tables a system of permutation of the matter tensor component suffices (similar to that used by Birss (1966)) for constant tensors has been adopted. Thus the notations of the type XZ(2) show permutations which apply to every component in the column and the number in brackets gives the number of distinct components obtained. In addition the field dependent tensors require a similar permutation xy2 and yz2 of the suffices for the field tensor. The forms presented in tables A.3 - A.14 provide the basis for studies of the anisotropy of the field dependent properties of crystals.

A.4 Use of the tabulation to find  $T_2(F_1)$  for the point group  $\bar{3}m$

To exemplify the use of these tables let us extract the form of a second rank polar matter tensor which depends upon a first rank axial field tensor for the point group  $\bar{3}m$ . In Table A.2 this type of tensor occurs as  $T_{m q}(F_1)$  in the tenth column in the  $\bar{3}m$  row. This is one of those tensors which obeys case (1) (equation A.8a) and so has the same form in this chosen point group ( $\bar{3}m$ ) as it does for the corresponding enantiomorphous point group (32). The ranks of the tensor sought lead to  $T_2(F_1)$  and the form can therefore be obtained from the section for  $m = 2$  and  $q = 1$  in Table A.7. In the even and odd terminology (see for example, Akgöz and Saunders 1975 a, Akgöz and Saunders 1975 b, Sümengen and Saunders 1972)

$$\begin{array}{c}
 \text{even} \qquad \qquad \qquad \text{odd} \\
 T_{ij}(F_1) = \begin{bmatrix} T_{11}(F_1) & \cdot & T_{13}(F_1) \\ \cdot & T_{22}(F_1) & \cdot \\ T_{31}(F_1) & \cdot & T_{33}(F_1) \end{bmatrix} + \begin{bmatrix} \cdot & T_{12}(F_1) & \cdot \\ T_{21}(F_1) & \cdot & T_{23}(F_1) \\ \cdot & T_{32}(F_1) & \cdot \end{bmatrix} \\
 \\
 T_{ij}(F_2) = \begin{bmatrix} T_{11}(F_2) & \cdot & T_{13}(F_2) \\ \cdot & T_{22}(F_2) & \cdot \\ T_{31}(F_2) & \cdot & T_{33}(F_2) \end{bmatrix} + \begin{bmatrix} T_{11}(F_2) & \cdot & T_{13}(F_2) \\ \cdot & T_{22}(F_2) & \cdot \\ T_{31}(F_2) & \cdot & T_{33}(F_2) \end{bmatrix} \\
 \\
 T_{ij}(F_3) = \begin{bmatrix} T_{11}(F_3) & \cdot & \cdot \\ \cdot & T_{11}(F_3) & \cdot \\ \cdot & \cdot & T_{33}(F_3) \end{bmatrix} + \begin{bmatrix} \cdot & T_{12}(F_3) & \cdot \\ -T_{12}(F_3) & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{bmatrix}
 \end{array}$$

(A.12)

A.5 Conclusion

The forms of the tensors shown in Table A.3 have been obtained by reference only to the symmetry restrictions imposed by the point group operations. In addition a field dependent tensor may exhibit further symmetry intrinsic to the physical nature of the property it describes. Then the tensor will be simplified further.

Table A1

<p>even rank matter tensor even rank field tensor (a)</p>	<p>Polar matter tensor polar field tensor (<math>\alpha</math>)</p>	<p>Polar matter tensor axial field tensor (<math>\beta</math>)</p>	<p>Axial matter tensor polar field tensor (<math>\gamma</math>)</p>	<p>Axial matter tensor axial field tensor (<math>\delta</math>)</p>
<p>odd rank matter tensor even rank field tensor (b)</p>	<p>enantiomorphous point Group Generating elements are sufficient Case (ii) (null tensor)</p>	<p>matter tensor components are even functions of field tensor components</p>	<p>enantiomorphous point Group Generating elements are sufficient</p>	<p>matter tensor components are odd functions of field tensor components</p>
<p>even rank matter tensor odd rank field tensor (c)</p>	<p>matter tensor components are even functions of field tensor components</p>	<p>enantiomorphous point Group Generating elements are sufficient</p>	<p>matter tensor components are even functions of field tensor components</p>	<p>matter tensor components are odd functions of field tensor components</p>
<p>odd rank matter tensor odd rank field tensor (d)</p>	<p>matter tensor components are odd functions of field tensor components</p>	<p>Case (ii) (null tensor)</p>	<p>enantiomorphous point Group Generating elements are sufficient</p>	<p>Case (ii) (null tensor)</p>

Table A1



Table A3

The forms of field dependent tensors of zeroth rank (m=0) in the matter tensor

$l = 0$	$X(x)$	$l = 1$	$X(x)$	$X(y)$	$X(z)$	$p = 2$	$X(xx)$	$X(yy)$	$X(zz)$	$X(xy)$	$X(yx)$	$X(xz2)$	$X(yz2)$
$F_0^0$	$X(x)$	$A_0(F_1)$	$X(x)$	$X(y)$	$X(z)$	$A_0(F_2)$	$X(xx)$	$X(yy)$	$X(zz)$	$X(xy)$	$X(yx)$	$X(xz)$	$X(yz)$
$F_0^1$	$X(x)$	$B_0(F_1)$	even	even	$X(y)$	$B_0(F_2)$	$X(xx)$	$X(yy)$	$X(zz)$	$X(xy)$	$X(yx)$	even	even
$F_0^2$	—	$\tilde{B}_0(F_1)$	odd	odd	—	$\tilde{B}_0(F_2)$	—	—	—	—	—	odd	odd
$F_0^3$	even	$C_0(F_1)$	$X(x)$	$X(y)$	even	$C_0(F_2)$	even	even	even	even	even	$X(xz)$	$X(yz)$
$F_0^4$	$X(x)$	$D_0(F_1)$	even	even	even	$D_0(F_2)$	$X(xx)$	$X(yy)$	$X(zz)$	even	even	even	even
$F_0^5$	even	$E_0(F_1)$	even	even	$X(z)$	$E_0(F_2)$	even	even	even	$X(xy)$	$X(yx)$	even	even
$F_0^6$	—	$F_0(F_1)$	—	—	odd	$F_0(F_2)$	—	—	—	odd	odd	—	—
$F_0^7$	odd	$G_0(F_1)$	—	—	—	$G_0(F_2)$	odd	odd	odd	—	—	—	—
$F_0^8$	$X(x)$	$H_0(F_1)$	even	$X^2(x)$	$X(z)$	$H_0(F_2)$	$X(xx)$	$X(zz)$	$X^2(xz)$	$X(xy)$	$X(-xy)$	even	$X^2(xz)$
$F_0^9$	even	$I_0(F_1)$	even	$X^2(x)$	even	$I_0(F_2)$	$X(xx)$	$X(-xx)$	even	$X(xy)$	$X(xy)$	even	$X^2(xz)$
$F_0^{10}$	—	$J_0(F_1)$	even	$-X^2(x)$	—	$J_0(F_2)$	$X(xx)$	$-X(xx)$	—	$X(xy)$	$-X(-xy)$	even	$-X^2(xz)$
$F_0^{11}$	odd	$K_0(F_1)$	even	$-X^2(x)$	odd	$K_0(F_2)$	$X(xx)$	$-X(-xx)$	odd	$X(xy)$	$-X(xy)$	even	$-X^2(xz)$
$F_0^{12}$	$X(x)$	$L_0(F_1)$	even	$X^2(x)$	even	$L_0(F_2)$	$X(xx)$	$X(zz)$	$X(zz)$	even	$X^2(xy)$	even	$X^2(xz)$
$F_0^{13}$	even	$M_0(F_1)$	even	$X^2(x)$	$X(z)$	$M_0(F_2)$	even	$X^2(xx)$	even	$X(xy)$	$X(-xy)$	even	$X^2(xz)$
$F_0^{14}$	—	$N_0(F_1)$	—	—	odd	$N_0(F_2)$	—	—	—	odd	$-X^2(xy)$	—	—
$F_0^{15}$	odd	$O_0(F_1)$	—	—	—	$O_0(F_2)$	odd	odd	odd	—	—	—	—
$F_0^{16}$	even	$P_0(F_1)$	even	$X^2(x)$	even	$P_0(F_2)$	$\lambda(xx)$	$\lambda(-xx)$	even	even	$X^2(xy)$	even	$X^2(xz)$
$F_0^{17}$	—	$Q_0(F_1)$	even	$-X^2(x)$	—	$Q_0(F_2)$	$X(xx)$	$-X(xx)$	—	even	$-X^2(xy)$	even	$-X^2(xz)$
$F_0^{18}$	odd	$R_0(F_1)$	even	$-X^2(x)$	—	$R_0(F_2)$	$X(xx)$	$-X(-xx)$	odd	even	$-X^2(xy)$	even	$-X^2(xz)$
$F_0^{19}$	$X(x)$	$S_0(F_1)$	$X(x)$	$X(y)$	$X(z)$	$S_0(F_2)$	$X(xx)$	$X(yy)$	$X(zz)$	$X(xy)$	$X(yx)$	$X(xz)$	$X^2(yz)$
$F_0^{20}$	$X(x)$	$T_0(F_1)$	even	$X(y)$	even	$T_0(F_2)$	$X(xx)$	$X(yy)$	$X(zz)$	even	even	$X(xz)$	even
$F_0^{21}$	even	$U_0(F_1)$	$X(x)$	even	$X(z)$	$U_0(F_2)$	even	even	even	$X(xy)$	$X(yx)$	even	$X(yz)$
$F_0^{22}$	—	$V_0(F_1)$	odd	—	odd	$V_0(F_2)$	—	—	—	odd	odd	—	odd
$F_0^{23}$	odd	$W_0(F_1)$	—	odd	—	$W_0(F_2)$	odd	odd	odd	—	—	odd	—
$F_0^{24}$	$X(x)$	$\tilde{A}_0(F_1)$	even	even	$X(z)$	$\tilde{A}_0(F_2)$	$X(xx)$	$X(yy)$	$X(zz)$	$X(xy)$	$X(yx)$	even	even
$F_0^{25}$	even	$\tilde{B}_0(F_1)$	$X(x)$	$X(y)$	even	$\tilde{B}_0(F_2)$	even	even	even	even	even	$X(xz)$	$X(yz)$
$F_0^{26}$	—	$\tilde{C}_0(F_1)$	odd	odd	—	$\tilde{C}_0(F_2)$	—	—	—	—	—	odd	odd
$F_0^{27}$	odd	$\tilde{D}_0(F_1)$	—	—	odd	$\tilde{D}_0(F_2)$	odd	odd	odd	odd	odd	—	—
$F_0^{28}$	$X(x)$	$\tilde{E}_0(F_1)$	even	even	even	$\tilde{E}_0(F_2)$	$\lambda(xz)$	$X^2(yx)$	$X(zz)$	even	even	even	even
$F_0^{29}$	even	$\tilde{F}_0(F_1)$	even	even	$X(z)$	$\tilde{F}_0(F_2)$	even	even	even	$X(xy)$	$X(yx)$	even	even
$F_0^{30}$	—	$\tilde{G}_0(F_1)$	—	—	odd	$\tilde{G}_0(F_2)$	—	—	—	odd	odd	—	—
$F_0^{31}$	odd	$\tilde{H}_0(F_1)$	—	—	—	$\tilde{H}_0(F_2)$	odd	odd	odd	—	—	—	—
$F_0^{32}$	even	$\tilde{I}_0(F_1)$	even	$X(y)$	even	$\tilde{I}_0(F_2)$	even	even	even	even	even	$X(xz)$	even
$F_0^{33}$	—	$\tilde{J}_0(F_1)$	—	odd	—	$\tilde{J}_0(F_2)$	—	—	—	—	—	odd	—
$F_0^{34}$	odd	$\tilde{K}_0(F_1)$	—	—	—	$\tilde{K}_0(F_2)$	odd	odd	odd	—	—	—	—
$F_0^{35}$	$X(x)$	$\tilde{L}_0(F_1)$	even	$X^2(x)$	$X^2(x)$	$\tilde{L}_0(F_2)$	$X(xx)$	$X(zz)$	$X(zz)$	even	even	$X^2(yx)$	$X^2(yx)$
$F_0^{36}$	$X(x)$	$\tilde{M}_0(F_1)$	even	$X^2(x)$	$X^2(x)$	$\tilde{M}_0(F_2)$	$X(zz)$	$X(zz)$	$X(zz)$	even	$X^2(xy)$	$X^2(xy)$	$X^2(xy)$
$F_0^{37}$	even	$\tilde{N}_0(F_1)$	even	$X^2(x)$	$X^2(x)$	$\tilde{N}_0(F_2)$	even	$X^2(xx)$	$X^2(xx)$	even	$X^2(xy)$	$X^2(xy)$	$X^2(xy)$
$F_0^{38}$	—	$\tilde{O}_0(F_1)$	—	—	—	$\tilde{O}_0(F_2)$	—	—	—	even	$-X^2(xy)$	$-X^2(xy)$	$X^2(xy)$
$F_0^{39}$	odd	$\tilde{P}_0(F_1)$	—	—	—	$\tilde{P}_0(F_2)$	odd	$X^2(xx)$	$X^2(xx)$	even	$-X^2(xy)$	$-X^2(xy)$	$X^2(xy)$

The forms of field dependent tensors of Fink die ( $n = 1$ ) for the matter tensor and ranks zero ( $p = 0$ ) and one ( $q = 1$ ) for the field tensor.

$n = 1$				$n = 1$									
$p = 0$	$X(x)$	$Y(x)$	$Z(x)$	$q = 1$	$X(x)$	$X(y)$	$X(z)$	$Y(x)$	$Y(y)$	$Y(z)$	$Z(x)$	$Z(y)$	$Z(z)$
$A_1(F_0)$	$X(x)$	$Y(x)$	$Z(x)$	$A_1(F_1)$	$X(x)$	$X(y)$	$X(z)$	$Y(x)$	$Y(y)$	$Y(z)$	$Z(x)$	$Z(y)$	$Z(z)$
$B_1(F_0)$	—	—	$Z(x)$	$B_1(F_1)$	odd	odd	—	odd	odd	—	even	even	$Z(z)$
$\bar{B}_1(F_0)$	$X(x)$	$Y(x)$	—	$\bar{B}_1(F_1)$	even	even	$X(z)$	even	even	$Y(z)$	odd	odd	—
$C_1(F_0)$	odd	odd	even	$C_1(F_1)$	—	—	odd	—	—	odd	$Z(x)$	$Z(y)$	even
$D_1(F_0)$	—	—	—	$D_1(F_1)$	odd	—	—	—	odd	—	—	—	odd
$E_1(F_0)$	—	—	odd	$E_1(F_1)$	—	odd	—	odd	—	—	—	—	—
$F_1(F_0)$	—	—	$Z(x)$	$F_1(F_1)$	—	odd	—	odd	—	—	even	even	even
$G_1(F_0)$	—	—	even	$G_1(F_1)$	odd	—	—	—	odd	—	even	even	$Z(z)$
$H_1(F_0)$	—	—	$Z(x)$	$H_1(F_1)$	odd	odd	—	$-X^0(y)$	$X^0(x)$	—	even	$Z^0(x)$	$Z(z)$
$I_1(F_0)$	—	—	even	$I_1(F_1)$	odd	odd	—	$X^0(y)$	$-X^0(x)$	—	even	$Z^0(x)$	even
$J_1(F_0)$	—	—	—	$J_1(F_1)$	odd	odd	—	$X^0(y)$	$-X^0(x)$	—	even	$-Z^0(x)$	—
$K_1(F_0)$	—	—	odd	$K_1(F_1)$	odd	odd	—	$-X^0(y)$	$X^0(x)$	—	even	$-Z^0(x)$	odd
$L_1(F_0)$	—	—	—	$L_1(F_1)$	odd	—	—	—	$X^0(x)$	—	—	—	odd
$M_1(F_0)$	—	—	odd	$M_1(F_1)$	—	odd	—	$-X^0(y)$	—	—	—	—	—
$N_1(F_0)$	—	—	$Z(x)$	$N_1(F_1)$	—	odd	—	$-X^0(y)$	—	—	even	$Z^0(x)$	even
$O_1(F_0)$	—	—	even	$O_1(F_1)$	odd	—	—	—	$X^0(x)$	—	even	$Z^0(x)$	$Z(z)$
$P_1(F_0)$	—	—	—	$P_1(F_1)$	odd	—	—	—	$-X^0(x)$	—	—	—	—
$Q_1(F_0)$	—	—	—	$Q_1(F_1)$	odd	—	—	—	$-X^0(x)$	—	—	—	—
$R_1(F_0)$	—	—	—	$R_1(F_1)$	odd	—	—	—	$X^0(x)$	—	—	—	odd
$S_1(F_0)$	—	—	$Z(x)$	$S_1(F_1)$	$X(x)$	$X(y)$	—	$Y(x)$	$Y(y)$	—	$Z(x)$	$Z(y)$	$Z(z)$
$T_1(F_0)$	—	—	—	$T_1(F_1)$	odd	—	—	even	$Y(y)$	—	odd	—	odd
$U_1(F_0)$	—	—	odd	$U_1(F_1)$	—	odd	—	$Y(x)$	even	—	—	odd	—
$V_1(F_0)$	—	—	$Z(x)$	$V_1(F_1)$	even	$X(y)$	—	odd	—	—	even	$Z(y)$	even
$W_1(F_0)$	—	—	even	$W_1(F_1)$	$X(x)$	even	—	—	odd	—	$Z(x)$	even	$Z(z)$
$\bar{A}_1(F_0)$	—	—	$Y(x)$	$\bar{A}_1(F_1)$	odd	odd	—	odd	odd	—	even	even	$Z(z)$
$\bar{B}_1(F_0)$	—	—	even	$\bar{B}_1(F_1)$	—	—	—	—	—	—	$Z(x)$	$Z(y)$	even
$\bar{C}_1(F_0)$	—	—	—	$\bar{C}_1(F_1)$	even	even	—	even	even	—	odd	odd	—
$\bar{D}_1(F_0)$	—	—	odd	$\bar{D}_1(F_1)$	$X(x)$	$X(y)$	—	$Y(x)$	$Y(y)$	—	—	—	odd
$\bar{E}_1(F_0)$	—	—	—	$\bar{E}_1(F_1)$	odd	—	—	—	odd	—	—	—	odd
$\bar{F}_1(F_0)$	—	—	odd	$\bar{F}_1(F_1)$	—	odd	—	odd	—	—	—	—	—
$\bar{G}_1(F_0)$	—	—	$Z(x)$	$\bar{G}_1(F_1)$	—	odd	—	odd	—	—	even	even	even
$\bar{H}_1(F_0)$	—	—	even	$\bar{H}_1(F_1)$	odd	—	—	—	odd	—	even	even	$Z(z)$
$\bar{I}_1(F_0)$	—	—	—	$\bar{I}_1(F_1)$	—	—	—	—	—	—	odd	—	—
$\bar{J}_1(F_0)$	—	—	—	$\bar{J}_1(F_1)$	—	—	—	even	even	—	odd	—	—
$\bar{K}_1(F_0)$	—	—	—	$\bar{K}_1(F_1)$	odd	—	—	even	$Y(y)$	—	—	—	odd
$\bar{L}_1(F_0)$	—	—	—	$\bar{L}_1(F_1)$	odd	—	—	—	$X^0(x)$	—	—	—	$X^0(x)$
$\bar{M}_1(F_0)$	—	—	—	$\bar{M}_1(F_1)$	odd	—	—	—	$X^0(x)$	—	—	—	$X^0(x)$
$\bar{N}_1(F_0)$	—	—	—	$\bar{N}_1(F_1)$	—	—	—	—	—	—	—	—	—
$\bar{O}_1(F_0)$	—	—	—	$\bar{O}_1(F_1)$	—	—	—	—	—	—	—	—	—
$\bar{P}_1(F_0)$	—	—	—	$\bar{P}_1(F_1)$	odd	—	—	—	$X^0(x)$	—	—	—	$X^0(x)$





Table A6

m = 2

P = 0	XX(x)	YY(x)	ZZ(x)	XY(x)	YX(x)	XZ(2)(x)	YZ(2)(x)
A <sub>2</sub> (F <sub>0</sub> )	XX(x)	YY(x)	ZZ(x)	XY(x)	YX(x)	XZ(x)	YZ(x)
B <sub>2</sub> (F <sub>0</sub> )	XX(x)	YY(x)	ZZ(x)	XY(x)	YX(x)	—	—
B <sub>2</sub> <sup>i</sup> (F <sub>0</sub> )	—	—	—	—	—	XZ(x)	YZ(x)
C <sub>2</sub> (F <sub>0</sub> )	even	even	even	even	even	odd	odd
D <sub>2</sub> (F <sub>0</sub> )	XX(x)	YY(x)	ZZ(x)	—	—	—	—
E <sub>2</sub> (F <sub>0</sub> )	even	even	even	odd	odd	—	—
F <sub>2</sub> (F <sub>0</sub> )	—	—	—	XY(x)	YX(x)	—	—
G <sub>2</sub> (F <sub>0</sub> )	odd	odd	odd	even	even	—	—
H <sub>2</sub> (F <sub>0</sub> )	XX(x)	XX(x)	ZZ(x)	XY(x)	-XY(x)	—	—
I <sub>2</sub> (F <sub>0</sub> )	XX(x)	XX(-x)	even	XY(x)	-XY(-x)	—	—
J <sub>2</sub> (F <sub>0</sub> )	XX(x)	-XX(x)	—	XY(x)	XY(x)	—	—
K <sub>2</sub> (F <sub>0</sub> )	XX(x)	-XX(-x)	odd	XY(x)	XY(-x)	—	—
L <sub>2</sub> (F <sub>0</sub> )	XX(x)	XX(x)	ZZ(x)	—	—	—	—
M <sub>2</sub> (F <sub>0</sub> )	even	XX <sup>p</sup> (x)	even	odd	-XY <sup>q</sup> (x)	—	—
N <sub>2</sub> (F <sub>0</sub> )	—	—	—	XY(x)	-XY(x)	—	—
O <sub>2</sub> (F <sub>0</sub> )	odd	XX <sup>q</sup> (x)	odd	even	-XY <sup>p</sup> (x)	—	—
P <sub>2</sub> (F <sub>0</sub> )	XX(x)	XX(-x)	even	—	—	—	—
Q <sub>2</sub> (F <sub>0</sub> )	XX(x)	-XX(x)	—	—	—	—	—
R <sub>2</sub> (F <sub>0</sub> )	XX(x)	-XX(-x)	odd	—	—	—	—
S <sub>2</sub> (F <sub>0</sub> )	XX(x)	XX(x)	ZZ(x)	XY(x)	-XY(x)	—	—
T <sub>2</sub> (F <sub>0</sub> )	XX(x)	XX(x)	ZZ(x)	—	—	—	—
U <sub>2</sub> (F <sub>0</sub> )	even	XX <sup>q</sup> (x)	even	odd	-XY <sup>p</sup> (x)	—	—
V <sub>2</sub> (F <sub>0</sub> )	—	—	—	XY(x)	-XY(x)	—	—
W <sub>2</sub> (F <sub>0</sub> )	odd	odd	odd	even	-XY <sup>p</sup> (x)	—	—
A <sub>2</sub> <sup>-</sup> (F <sub>0</sub> )	XX(x)	XX(x)	ZZ(x)	XY(x)	-XY(x)	—	—
B <sub>2</sub> <sup>-</sup> (F <sub>0</sub> )	even	XX <sup>q</sup> (x)	even	even	-XY <sup>p</sup> (x)	—	—
C <sub>2</sub> <sup>-</sup> (F <sub>0</sub> )	—	—	—	—	—	—	—
D <sub>2</sub> <sup>-</sup> (F <sub>0</sub> )	odd	XX <sup>q</sup> (x)	odd	odd	-XY <sup>p</sup> (x)	—	—
E <sub>2</sub> <sup>-</sup> (F <sub>0</sub> )	XX(x)	XX(x)	ZZ(x)	—	—	—	—
F <sub>2</sub> <sup>-</sup> (F <sub>0</sub> )	even	XX <sup>q</sup> (x)	even	odd	-XY <sup>p</sup> (x)	—	—
G <sub>2</sub> <sup>-</sup> (F <sub>0</sub> )	—	—	—	XY(x)	-XY(x)	—	—
H <sub>2</sub> <sup>-</sup> (F <sub>0</sub> )	odd	XX <sup>q</sup> (x)	odd	even	-XY <sup>p</sup> (x)	—	—
I <sub>2</sub> <sup>-</sup> (F <sub>0</sub> )	even	XX <sup>q</sup> (x)	even	—	—	—	—
J <sub>2</sub> <sup>-</sup> (F <sub>0</sub> )	—	—	—	—	—	—	—
K <sub>2</sub> <sup>-</sup> (F <sub>0</sub> )	odd	XX <sup>q</sup> (x)	odd	—	—	—	—
L <sub>2</sub> <sup>-</sup> (F <sub>0</sub> )	XX(x)	XX(x)	XX(x)	—	—	—	—
M <sub>2</sub> <sup>-</sup> (F <sub>0</sub> )	XX(x)	XX(x)	XX(x)	—	—	—	—
N <sub>2</sub> <sup>-</sup> (F <sub>0</sub> )	even	XX <sup>q</sup> (x)	XX <sup>q</sup> (x)	—	—	—	—
O <sub>2</sub> <sup>-</sup> (F <sub>0</sub> )	—	—	—	—	—	—	—
P <sub>2</sub> <sup>-</sup> (F <sub>0</sub> )	odd	XX <sup>q</sup> (x)	XX <sup>q</sup> (x)	—	—	—	—











































(1) (2) (3) (4) (5) (6) (7) (8) (9) (10) (11) (12) (13) (14) (15) (16) (17) (18) (19) (20) (21) (22) (23) (24) (25) (26) (27) (28) (29) (30) (31) (32) (33) (34) (35) (36) (37) (38) (39) (40) (41) (42) (43) (44) (45) (46) (47) (48) (49) (50) (51) (52) (53) (54) (55) (56) (57) (58) (59) (60) (61) (62) (63) (64) (65) (66) (67) (68) (69) (70) (71) (72) (73) (74) (75) (76) (77) (78) (79) (80) (81) (82) (83) (84) (85) (86) (87) (88) (89) (90) (91) (92) (93) (94) (95) (96) (97) (98) (99) (100)
(1) (2) (3) (4) (5) (6) (7) (8) (9) (10) (11) (12) (13) (14) (15) (16) (17) (18) (19) (20) (21) (22) (23) (24) (25) (26) (27) (28) (29) (30) (31) (32) (33) (34) (35) (36) (37) (38) (39) (40) (41) (42) (43) (44) (45) (46) (47) (48) (49) (50) (51) (52) (53) (54) (55) (56) (57) (58) (59) (60) (61) (62) (63) (64) (65) (66) (67) (68) (69) (70) (71) (72) (73) (74) (75) (76) (77) (78) (79) (80) (81) (82) (83) (84) (85) (86) (87) (88) (89) (90) (91) (92) (93) (94) (95) (96) (97) (98) (99) (100)

Table A13 (Cont.)



































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