THEORY OF ISOTHERMAL GALVANOMAGNETIC EFFECTS FOR SINGLE CRYSTALS

By

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PREFACE

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ABSTRACT

The isothermal galvanomagnetic effects bear various conventional names such as the transverse and the longitudinal magneto resistance, the Hall, the "planar Hall field," and the Corbino effect, corresponding to cases where the magnetic field is either normal or parallel to the current, or in the plane of the current and the Hall probes.

In the first part of this dissertation the isothermal galvanomagnetic effects are defined phenomenologically with the magnetic field, the electric field, and the current vectors arbitrarily oriented with respect to the crystal axes and to each other. Thus all the conventional studies cited above are included as special cases. The literature is inconsistent with regard to the parity properties of the galvanomagnetic effects as a function of the magnetic field $\underline{B}$. Some of these properties are here deduced from Onsager's relation and symmetry considerations. In particular, it is shown that the magneto resistance* is necessarily an even function of $\underline{B}$, while, contrary to convention, the Hall effect is in general neither an odd function (as is usually assumed) nor an even function of $\underline{B}$, but can be purely odd or purely even or zero under proper conditions.

These effects are then analyzed in terms of an ascending power series of the components of $\underline{B}$, whose coefficients are denoted by the "brackets." Prior to this work the crystallographic effects have never been taken into account comprehensively. An overall investigation of the effect of the 32 point groups upon the isothermal galvanomagnetic effects is attempted. A theorem is developed to deal generally with tensors of arbitrary rank under the restriction of an arbitrary N-fold axis of rotation.

*For convenience, we shall refer throughout to $\rho^{\lambda\mu}(\underline{B})$ as magneto resistance, and to $[\rho^{\lambda\mu}(\underline{B}) - \rho^{\lambda\mu}(\underline{B} = 0)]$ as magneto resistance change. Sometimes the latter is abbreviated by the former when no confusion is introduced.

The Corbino effect, which has not been previously studied in single crystals, is dealt with very briefly, and its relations with the magneto resistance and the Hall effect are established for special cases.

The brackets are then defined microscopically according to the conventional single-band model and according to a multiband model. This brings out a formal completion of the microscopic theory of the isothermal galvanomagnetic effects, developed by Jones and Zener (1934), Davis (1939), and Seitz (1950); by Sondheimer and Wilson (1947), and by Jones (1936). The multiband model includes the single band as well as the two-band and many-valley models as special cases.

A detailed discussion is presented of the conditions under which the even part of the galvanomagnetic tensor vanishes. This gives some criteria for avoiding one of the outstanding difficulties of the existing simple theories, viz., how to choose a simple microscopic model without yielding zero longitudinal magneto resistance.

INTRODUCTION

This dissertation consists of three parts:

I. A general definition of the isothermal galvanomagnetic effects is given, which includes most of the previous definitions as special cases, while rejecting some of them as inadequate. The magneto conductivity tensor is expanded in terms of an ascending power series of the constant magnetic field B, whose coefficients ("brackets") are analyzed. It is then possible to understand some experimental findings (at least qualitatively) and to compile experimental data more systematically.

II. A general theorem is developed to analyze the effect of an N-fold rotation axis upon an arbitrary even-rank tensor; thus explicit expressions for the galvanomagnetic effects corresponding to each of the 32 point groups are established.

III. "Brackets" pertaining to the galvanomagnetic effects are defined microscopically according to the band approximation. Thus by bringing together all previous efforts as well as the author's, we have the framework of a formally complete microscopic theory. Of special interest are some conditions for the vanishing of certain galvanomagnetic constants in terms of the functional forms of the energy and of the relaxation time of the "electron gas."

The first and second parts are presented in Chapters I and II, the third part in Chapter III. The motivation for this work is presented in this introduction. Appendix VI and Section 5 of Chapter I are recommended to those readers who wish to go immediately to the results.

Motivation.—Several names for special galvanomagnetic effects are familiar from the literature: the Hall effect, the longitudinal and transverse magneto resistance effect, the Corbino effect, and the 'planar Hall field.' We ask—

Question I. Can one define the effect in general in such a way that all these

effects are included as special cases?

Casimir[4] and others proposed to define the even and odd parts of the resistivity tensor in the presence of a magnetic field as the magneto resistance and Hall effect, respectively. There resulted some controversy in the literature regarding 'mixing of the magneto resistance in the Hall effect,'[15] and 'longitudinal Hall effect in the magneto resistance,'[17] which leads to—

Question II. Are the definitions of Casmir compatible with the physical measurements of the magneto resistance and the Hall effect?

The anisotropy of the galvanomagnetic effects of single crystals has never been discussed comprehensively. In 1950 Seitz proposed a formula for the current-field relation in the presence of an arbitrarily oriented weak magnetic field for cubic crystals.

Question III. Can one derive an equation, similar to Seitz's equation, which will hold generally for all crystal symmetries?

The most instructive findings come from experiments on the magneto resistance at low temperatures and high magnetic fields. Noting the strong and complicated anisotropy observed by Justi[8] and others on gold, Wilson[19] remarked in his book in 1953:

> It does not seem likely that any model simple enough to be tractable theoretically would give a magneto resistance curve of the complexity of those actually observed.

This remark provided the main motivation for the present thesis. The difficulty is reduced by one step if one can answer—

Question IV. What part of these complicated magneto resistance curves can be understood on the ground of symmetry considerations alone?

The phenomenological theory is developed in Chapters I and II to answer these four questions. It is estimated that a series up to the power of 24 or more is needed to interpret the magneto resistance curve of gold referred to above.

CHAPTER I

PHENOMENOLOGICAL THEORY: MAGNETO RESISTANCE AND HALL EFFECT

1. INTRODUCTION

Consider a volume element of an anisotropic isothermal* homogeneous single crystal of arbitrary shape placed in a homogeneous magnetic field $\underline{B}$. A constant current density $\underline{J}$ in the crystal is maintained by means of a suitable electric field $\underline{F}$ (see Figure 1).

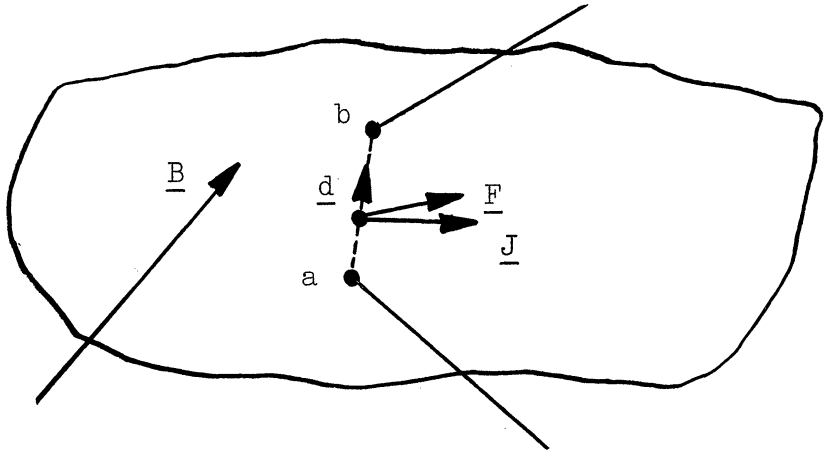


Figure 1. Orientation of vectors $\underline{J}$, $\underline{F}$, $\underline{B}$, and probes ab in an anisotropic single crystal.

Evidently $\underline{F}$ will be a vector function of $\underline{J}$ and $\underline{B}$,

$$\underline{F} = \underline{F}(\underline{J},\underline{B}) \quad . \tag{1}$$

The dependence of $\underline{F}$ on $\underline{B}$ represents the galvanomagnetic effect.** The crystal symmetry and other physical laws will, in general, restrict the possible forms of (1). It is the purpose of this chapter to find the proper description of $\underline{F}$ for all possible crystal symmetries, all orientations and magnitudes of $\underline{J}$ and $\underline{B}$ with respect to the symmetry axes of the crystal, under the restriction that Ohm's law is valid for fixed $\underline{B}$.

*Isothermal conditions are assumed throughout this paper without further explicit statement.

**Throughout this paper we restrict ourselves to nonferromagnetic substances.

The vector $\underline{F}$ can be determined experimentally for any given $\underline{J}$ and $\underline{B}$ by measuring the components $F^{1,2,3}$ of $\underline{F}$ in three independent directions. In a direction $\underline{d}$ one can measure F^d by measuring the potential difference V_{ab} between two probes a and b, without drawing current, and dividing by the distance ab. If $\underline{d}$ is taken along $\underline{J}$, the resulting dependence $F_{\parallel}(\underline{J},\underline{B})$ is called the magneto resistance effect; if $\underline{d}$ is normal to $\underline{J}$, then $F_{\perp}(\underline{J},\underline{B})$ is called a Hall effect. Both are special cases of the galvanomagnetic effect. Other special cases, such as the Corbino effect, imply a geometry and boundary conditions which are again different.

Historically, Lord Kelvin[1] first discovered the magneto resistance effect for Fe in 1856 and also predicted the Hall effect in 1851. After many attempts by various workers, Hall[1] discovered the effect named for him in 1879. The first empirical formula connecting the two effects was proposed by Beattie in 1896.[1] The name "galvanomagnetic effect" appeared in the literature, meaning the Hall, the magneto resistance effect, as well as some other effects such as the Corbino effect.

The dependence of the Hall effect on the magnetic field and on the temperature was studied by many investigators. In 1883 Righi[1] studied the influence of the crystal orientation of the Hall effect. Extensive summaries were given by Campbell[1] in 1923 and by Meissner[2] in 1935. Briefly, the findings[3] of all this work are that the Hall effect depends on the crystal orientation, and that it is not adequately described by a constant Hall coefficient. The Hall effect is not always an odd function of the magnetic field, contrary to a suggestion by Casimir[4] in 1945.

Numerous authors extended Lord Kelvin's work on magneto resistance to nonferromagnetic materials. Grunmach and Wiedert[1] published in 1906-07 the first extensive study for various elements at room temperature. In 1928-30 Kapitza[5] went to lower temperatures and higher magnetic fields. In 1897 Van Everdingen[1] had discovered the influence of the crystal orientation on the magneto resist-

ance. The effect was studied further by Schubnikow and de Haas,[6] Stierstadt,[7] Justi[8] and co-workers, Blom,[9] and others.[10] Schubnikow and de Haas, Stierstadt, and, more systematically, Blom, tried to analyze the angular dependence of the magneto resistance on the orientation of the magnetic field relative to the sample by a Fourier analysis. Briefly, findings[11] of all this work are that the magneto resistance depends markedly on the crystal orientation, especially at low temperatures; that for low magnetic fields (say less than 1 kilogauss) the magneto resistance is proportional to the square of the field, whereas at high fields the relation is a more complicated function of the field. According to most results, this function is even. In 1905 Voigt[12] laid the foundation for an appropriate description of the anisotropy of the Hall and magneto resistance effects. Further contributions to the phenomenological theory were made by Kohler,[13] Casmir,[4] Seitz.[14] Juretschke,[15] and other workers.

The ultimate aim of the theory of the galvanomagnetic effects is to describe the function (1) completely in terms of the electronic properties of the material concerned. This task can be divided into two parts. In the first or phenomenological part the function (1) is described in terms of a number—finite or infinite—of true isothermal galvanomagnetic constants that are characteristic for the material.[16] In the second or electron-theoretical part these constants are interpreted in terms of electronic properties.

The objective of the present chapter and the next is to give an explicit development and broadening of the phenomenological theory, leaving the electron-theoretical part to the last chapter. The plan of attack is as follows. In Section 2 the proper galvanomagnetic constants are defined, the dependence of $\underline{F}$ on the orientation of $\underline{J}$ and $\underline{B}$ is discussed, and some general relations are established. In Section 3 a general method is developed by means of which the effects of crystal symmetry are properly taken into account. In Section 4 formulas are given for the number of independent galvanomagnetic con-

stants for the various crystal classes. In Section 5 various explicit forms are given, particularly forms for $\underline{B}$ up to terms quadratic in the components of $\underline{B}$, for the various crystal symmetries, while the corresponding forms for higher powers can be elaborated from there on without essential difficulties. The significance of the results obtained is pointed out in Section 6.

2. DEFINITIONS AND GENERAL RELATIONS

a. Coordinate Systems.—Two sets of orthogonal coordinate systems will be used.

(1) The symmetry coordinates k_i ($i = 1,2,3$). These are adapted to the crystal symmetry* as follows:

For the groups C_1, S_1 the directions of the coordinate axes are arbitrary. For the groups S_2, S_4, S_6, C_2, C_3, C_4, C_6, C_{2h}, C_{3h}, C_{4h}, C_{6h}, the k_3 axis is taken along the axis of rotation;** the other axes have one degree of freedom.

For the groups T, T_h, T_d, the coordinate axes are taken along the twofold rotation axes.

For all other classes, k_3 is taken along the rotation axis of highest order, k_1 along a rotation axis** normal to k_3, and k_2 accordingly. Vector or tensor components with respect to these symmetry coordinates will carry Latin subscripts.

(2) The laboratory coordinates x^α ($\alpha = 1,2,3$) with x^1 along the current density $\underline{J}$, x^2 in the plane of $\underline{J}$ and $\underline{d}$, and x^3 accordingly. In the case of magneto resistance, $\underline{d}$ is along $\underline{J}$, allowing one degree of freedom for x^2 and x^3 in the plane normal to x^1. Vector and tensor components with respect to the laboratory coordinates will carry

*Only the macroscopic symmetry of the crystal, i.e., which one of the 32 crystallographic point groups it belongs to, need here be considered.

**The axis of an improper rotation is understood here as the normal to the corresponding reflection plane.

Greek superscripts. No confusion between superscripts and exponents should arise in practice.

The definition of the laboratory system implies

$$J^2 = J^3 = 0 \ . \tag{2}$$

Denoting the direction cosines between the two coordinate systems by ℓ_i^α and using the summation convention for repeated indices, we have

$$\left.\begin{aligned} J^\alpha &= J_i \ell_i^\alpha \\ J_i &= J^\alpha \ell_i^\alpha \\ F^\beta &= F_j \ell_j^\beta \\ F_j &= F^\beta \ell_j^\beta \ . \end{aligned}\right\} \tag{3}$$

b. Assumption I. Ohm's Law.—We assume Ohm's law to be valid for any constant applied magnetic field $\underline{B}$, i.e., the current density $\underline{J}$ is a homogeoeous linear vector function of $\underline{F}$. Thus, in symmetry coordinates:

$$\left.\begin{aligned} J_i &= \sigma_{ij}\,(\underline{B})\,F_j \\ F_j &= \rho_{ji}\,(\underline{B})\,J_i \ , \end{aligned}\right\} \tag{4}$$

where the conductivity tensor components σ_{ij} and the resistivity components ρ_{ji} are both functions of $\underline{B}$ and are related by

$$\rho_{ji} = \Delta_{ij}/\Delta \ . \tag{5}$$

Here Δ is the determinant of the σ_{ij} and Δ_{ij} is the cofactor of σ_{ij} in Δ. The functions $\sigma_{ij}(\underline{B})$ and $\rho_{ji}(\underline{B})$ are characteristic of the material at any given temperature and independent of the geometry of galvanomagnetic measurements. The effects of crystal symmetry are to place restrictions on these functions. However, the direction of current flow $\underline{J}$ has, in general, no particularly simple relation to the symmetry coordinates, and the results of measurements are most directly expressed in terms of laboratory coordinates. Ohm's law, restated in laboratory coordinates, is

$$F^{\alpha} = \rho^{\alpha 1}(\underline{B})J^{1}$$

where

$$\rho^{\alpha 1}(\underline{B}) = \rho_{ji}(\underline{B})\ell_j^{\alpha}\ell_i^{1} = \Delta_{ij}(\underline{B})\ell_i^{1}\ell_j^{\alpha}/\Delta(\underline{B}) \quad . \tag{6}$$

For $\alpha = 1$ these equations describe the magneto resistance effect; for $\alpha = 2$ or 3 they represent the Hall effect. The latter form expressed these galvanomagnetic effects in terms of the conductivity components in symmetry coordinates.

c. Assumption II. Onsager's Relations.—The validity of Onsager's relations is assumed:

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

Consequently,

$$\sigma_{ij}(\underline{B}) = \rho_{ij}(-\underline{B}) \tag{7}$$

and

$$\rho^{\alpha\beta}(\underline{B}) = \rho^{\beta\alpha}(-\underline{B}) \tag{8}$$

d. The Parity of the Magneto Resistance Effect.—Equation (8) states that

$$\rho^{11}(\underline{B}) = \rho^{11}(-\underline{B}) \quad , \tag{9}$$

which proves the theorem that the magneto resistance effect is even in $\underline{B}$. In the literature[17] there has been some controversy about the evenness of ρ^{11}, but the above argument shows that under the very broad assumptions stated, ρ^{11} must be an even function in $\underline{B}$ without exception.

e. Parity of the Hall Effect.—The Hall effect as defined by (6) with $\alpha \neq 1$ implies that the Hall electrodes are normal to the current. We shall adhere to this definition, though some experimenters prefer to define the Hall effect as measured with the Hall electrodes on an equipotential when $\underline{B} = 0$.

In general the Hall effect is neither an odd or an even function of $\underline{B}$. This is true for either definition. However, in a number of special configurations the crystal symmetry may impose a special parity on the Hall effect. The

complete list of such configurations is as follows. Consider the crystallographic point group, obtained from that of the crystal by augmenting it with an inversion center. The physical significance of this augmented group is explained in Section 3. Then one can easily prove with respect to this augmented group:

(1) If $\underline{B}$ lies along a 3-, 4-, or 6-fold axis and either $\underline{J}$ or $\underline{d}$ is normal to $\underline{B}$, then the Hall effect is odd.

(2) If $\underline{B}$ is normal to a 2-, 4-, or 6-fold axis and either $\underline{J}$ or $\underline{d}$ is along that axis, then the Hall effect is odd.

(3) If $\underline{B}$ lies along any 2-, 3-, 4-, or 6-fold rotation axis and is coplanar with $\underline{J}$ and $\underline{d}$, then the Hall effect is even.

(4) If $\underline{B}$, $\underline{J}$, and $\underline{d}$ are normal to the same 2-, 4-, or 6-fold axis, then the Hall effect is even.

(5) If $\underline{B}$ and either $\underline{J}$ or $\underline{d}$ lie along any 2-, 3-, 4-, or 6-fold rotation axis, then the Hall effect vanishes.

There are no other cases in which the Hall effect is purely even, odd, or zero as a function of $\underline{B}$. The "new" galvanomagnetic effect reported by Goldberg and Davis,[18] for example, is a case illustrating points (4) and (5). In their Figure 1 the slight discrepancy between the axis direction and the direction of zero Hall effect must be due to an experimental error of imperfect alignment.

f. Assumption III. Power Series Expansion of $\sigma_{ij}(\underline{B})$.—Most galvanomagnetic measurements suggest that $\sigma_{ij}(\underline{B})$ can be expanded as a series in powers of the components B_k. One of many typical examples is reproduced by A. H. Wilson[19] from work by Justi and Scheffers on gold. If a Fourier analysis of polar diagrams of this sort involves significant terms with arguments of the sines or cosines up to $n\phi$, then, it is easily shown, significant contributions to the conductivity components σ_{ij} arise from terms proportional to the n^{th} power of B and vice versa.

There is an observed limitation to the appropriateness of a power-

series expansion for galvanomagnetic effects. Experiments[20] have shown that the Hall voltage and the magneto resistance at low temperatures contain oscillating terms which presumably are connected with the van Alphen - de Haas effect and are proportional to B sin B_0/B. Such terms do not possess a derivative with respect to B at B = 0 and hence cannot be expanded in powers of B. Consequently, the development presented here does not apply to that part of the galvanomagnetic effects which arises from terms of such a nature.

As the third assumption, we write

$$\sigma_{ij}(\underline{B}) = \sum_{n=0}^{\infty} \sum_{m=0}^{n} \sum_{p=0}^{m} [m-p,p,n-m]_{ij} \; B_1^{m-p} B_2^{p} B_3^{n-m} \tag{10}$$

or, introducing the direction cosines γ_i of $\underline{B}$ with respect to the symmetry coordinates,

$$\sigma_{ij}(\underline{B}) = \sum_{n=0}^{\infty} B^n \sum_{m=0}^{n} \sum_{p=0}^{m} [m-p,p,n-m]_{ij} \; \gamma_1^{m-p} \gamma_2^{p} \gamma_3^{n-m} \; . \tag{10a}$$

The coefficients in this expansion are designated by the bracket symbols and are independent of $\underline{B}$. They are the true phenomenological material constants characterizing the galvanomagnetic behavior of any particular material. They are sums of components of tensors of rank 2n + 2 since the axial vector $\underline{B}$ is an antisymmetric tensor of rank two.*

Onsager's relations imply

$$[m-p,p,n-m]_{ij} = (-)^n \; [m-p,p,n-m]_{ji} \; . \tag{11}$$

Consequently, it is sufficient to consider ij values of 11, 22, 33, 23, 31, 12, only. This will always be done unless stated otherwise. Another consequence of (11) is that all brackets with n = odd and i = j vanish. Denoting by ω an arbitrary odd number:

*In order to set the tensor character in evidence, the brackets will sometimes be denoted by $[(23)^{m-p}, (31)^{p}, (12)^{n-m}]_{ij}$. The quantities (23), (31), (12) will be referred to as the pairs of inner indices and ij as the outer indices.

$$[m\text{-}p,p,\omega\text{-}m]_{ii} = 0 \quad . \tag{11a}$$

The restrictions imposed on the brackets by the crystal symmetry will be described in the next section. The fact that (6) is simpler in terms of ρ_{ij} then in terms of σ_{ij} would suggest a power-series expansion of the former. The latter was chosen since the brackets so obtained permit a simpler electron theoretical interpretation. However, the contents of all that follows are applicable without any modification to ρ-brackets and σ-brackets alike.

3. THE EFFECTS OF CRYSTAL SYMMETRY

a. Only Eleven Point Groups Need Analysis.—Tensor components that are material constants must be invariant under the operations of the crystallographic point group of the crystal considered. If the tensor components are of even rank, they transform identically into themselves under inversion. Consequently, all tensor components of even rank that are material constants must be invariant under the operations of the point group that is obtained by augmenting the point group of the crystal considered by an inversion center. This is obviously also true for the brackets. Any point group augmented by an inversion center becomes one of the eleven well-known crystallographic point groups which possess such a center. Thus, it suffices to analyze these eleven point groups. They can all be generated by at most two rotations in addition to the inversion center. We shall generate the eleven point groups by means of the elements shown in Table I. In the second row are listed the twenty-one point groups without inversion center which go over into those of the first row by the addition of an inversion center.

Under a general rotation each bracket is transformed into a linear combination of other brackets. If the rotation be a covering operation, and thus requires invariance of the bracket, then certain relations must hold between the brackets.

TABLE I

GENERATING THE ELEVEN POINT GROUPS

Point Group	S_2	C_{2h}	C_{3i}	C_{4h}	C_{6h}	D_{2h}	D_{3i}	D_{4h}	D_{6h}	T_h	O_h
Equivalent	C_1	C_2	C_3	C_4	C_{3h}	C_{2v}	C_{3v}	D_{2d}	D_{3h}	T	T_d
Point		C_s		S_4	C_6	D_2	D_3	C_{4v}	C_{6v}		O
Groups								D_4	D_6		
Generating* Elements											
axis along k_3	-	2	3	4	6	2	3	4	6	2	4
axis along k_1	-	-	-	-	-	2	2	2	2	-	-
axis along [111]	-	-	-	-	-	-	-	-	-	3	3

*If an axis is taken as a generating element, its multiplicity N is listed at the appropriate place. The inversion center which is a common generating element of all groups is not listed.

Under inversion each bracket is transformed identically into itself. Hence, no relations between brackets can be derived from the requirement of invariance under inversion.

b. A Theorem Concerning the Effect of an N-Fold Rotation Axis Along k_3.—The effects of an N-fold rotation axis along k_3 are covered by a theorem which states that certain linear equations must hold between the brackets. In order to express these combinations concisely, some notations are introduced. Let s be the number of non-threes among a given ij and let Θ be the number of twos minus the number of ones in ij. The numbers s,Θ define uniquely one of the six independent pairs of indices ij, and vice versa. Table II gives the relation explicitly for further reference. We write

$$[m\text{-}p,p,n\text{-}m]_{ij} \equiv [m\text{-}p,p,n\text{-}m]_{(s,\Theta)} \quad . \tag{12}$$

Let z denote a nonnegative integer $\leq$ s and w a nonnegative integer $\leq$ m. Each of the linear equations referred to by the theorem will be labeled by five integers n, m, s, z, w. All brackets occurring in one equation have the same n,m,s,

but may differ in p,Θ. The parameters z,w serve to label the various equations with the same n,m,s, involving the same brackets with different coefficients.

TABLE II

TABLE OF s AND Θ VALUES

ij	s	Θ
33	0	0
31	1	-1
23	1	+1
11	2	-2
12	2	0
22	2	+2

Theorem

For an N-fold rotation axis along k_3, the brackets satisfy the equations

$$\sum_{\Theta} \sum_{p=0}^{m} g(m,p,w)\, \epsilon(s,\Theta,z)\, [m-p,p,n-m]_{(s,\Theta)} = 0 \quad , \tag{13}$$

provided the inequality

$$h \equiv m+s - 2(w+z) \neq kN \qquad (k=0,\pm1,\pm2\ldots) \tag{14}$$

holds; in other words, h is not a multiple of N.

The summation over Θ is meant to include all ij combinations with constant s. The coefficient g(m,p,w) is defined in terms of binomial coefficients by

$$g(m,p,w) \equiv i^p \sum_{q=0} (-)^q \binom{m-p}{q}\binom{p}{w-q} \quad . \tag{15}$$

The factor $\epsilon(s,\Theta,z)$ is given in Table III for all values for which it is defined. The proof of this basic theorem is given in Appendix I. In Appendix II it is shown that the only solution for the complete set (13) for given n,m,s, is that all brackets involved vanish. A consequence is that the equations (13) with the condition (14) represent a complete description of the symmetry properties of the brackets.

For finding the relations between brackets of given n,m,s, one will first list all brackets of this set according to their p and Θ values, next es-

tablish their coefficients gϵ for all possible values of the parameters w,z, and finally write down one equation of the type (13) for each set of w,z values compatible with (14). Shortcuts to this procedure will be explained after some corollaries of the theorem have been proved.

TABLE III

THE VALUES OF $\epsilon(s,\theta,z)$

			n = even			n = odd		
s	θ	ij z →	0	1	2	0	1	2
0	0	33	1	-	-	-	-	-
1	-1	31	1	1	-	1	1	-
1	1	23	i	-i	-	-i	i	-
2	-2	11	1	1	1	-	-	-
2	0	12	2i	0	-2i	0	2i	0
2	2	22	-1	1	-1	-	-	-

c. Some Consequences of the Theorem.—In formulating the fundamental theorem a rotation axis was taken along k_3. It is simple to apply the theorem to a rotation axis along k_1 or k_2 by permutation of both inner and outer indices. The effect of a threefold axis along the [111] direction can be taken into account by requiring invariance for the brackets under cyclic permutation of the indices 1,2,3 both in and outside any bracket. Thus the effect of symmetry for the eleven point groups is completely described by the theorem with these generalizations.

However, in a number of cases the application of the theorem is greatly simplified by means of some corollaries.

Corollary I

For N = even (2,4,6) about k_3, all brackets for which the index 3 occurs an odd number of times (inside plus outside) are zero.

Proof

In any particular bracket, the index 3 occurs 2-s+m times. Thus it must be shown that all brackets with (m+s) odd vanish. If (m+s) is odd then h cannot be an integral multiple of the even number N. Thus all equations provided by the general theorem are valid. According to the theorem, given in Appendix II, all brackets concerned must now vanish.

q.e.d.

In preparation of Corollary II let two brackets be called "adjoint" with respect to k_3, if they can be obtained from one another by interchanging the indices 1 and 2*, both inside and outside, and writing the resulting pairs of indices in the conventional order. For example, the brackets

$$[m-p,p,n-m]_{23} \quad \text{and} \quad [p,m-p,n-m]_{31}$$

are adjoint. Indeed the first bracket can be written as $[(23)^{m-p},(31)^{p},(12)^{n-m}]_{23}$. Upon interchanging 1 and 2 this becomes $[(32)^{p},(13)^{m-p},(21)^{n-m}]_{13}$. All pairs must now be interchanged in order to appear in the conventional order. The n inner pairs each give a minus sign. The outer pair gives $(-)^n$ according to Onsager's relation (11). The result is always a plus sign. The resulting bracket is $[(23)^{p},(31)^{m-p},(12)^{n-m}]_{31}$, which is the same as $[p,m-p,n-m]_{31}$. Thus the adjoining operation with respect to k_3 transforms one bracket into another one, by interchanging p with m-p and θ with $-\theta$.

Corollary II

For N = 4 about k_3, nonvanishing adjoint brackets are either equal or opposite. They are equal if the number of occurrences of the index 2 is even, opposite if this number is odd.

Proof

Under a fourfold rotation about k_3, k_1 transforms into k_2' and k_2 into $-k_1'$. Thus the result of this rotation differs from the operation "adjoining"

*Similarly we define adjoint with respect to k_1 (or k_2) by interchanging the indices 2 and 3 (or 3 and 1).

only by a factor (-) to the power of the number of occurrences of the index 2. If the index 2 occurs an even number of times the factor is +1, otherwise -1. Since the fourfold rotation is a covering operation the corollary is proved.

q.e.d.

The indices 1 and 2 occur both even or both odd. Indeed the total number of indices 1, 2, and 3 is even, and the occurrence of the index 3 is even according to Corollary I. Thus the corollary is symmetric with respect to the indices 1 and 2.

Corollary III

If in an equation of the type (13) each bracket $[m-p,p,n-m]_{ij}$ is replaced by $[m-p,p,n'-m]_{ij}$, where n' has the same parity as n, the resulting equation also belongs to the set (13) and has the same h.

Proof

The corollary is essentially due to the fact that k_3 is the rotation axis. In equation (13) n occurs only in two places: in the brackets, all brackets in one equation having the same n, and in ϵ (see Table III). In the latter the influence of n enters only through its parity, hence different values of n with the same parity lead to similar equations. Since the definition (14) of h does not contain n, the h-values of such equations are equal.

q.e.d.

A consequence of this corollary is that a change from n to n' with the same parity in any bracket relation leads to another valid relation, i.e., bracket relations for given values of m,s need to be tabulated only for n = even and for n = odd, a fact which has permitted great simplification in the tables of bracket relations that follow.

Corollary IV

Two equations of the type (13) with equal n,m,s having parameter values w,z and w'=m-w, z'=s-z, i.e., h'=-h, are conjugate complex.

Proof

One must prove that the coefficient $g\epsilon$ is transformed into its conjugate complex by changing from w,z to w',z'. According to (15) it is easily shown that $g(m,p,w) = (-)^{m+p}\, g(m,p,m-w)$. Since the definition of g contains a factor i^p,

$$g(m,p,w) = (-)^m\, g^*(m,p,w') \ , \tag{16}$$

the asterisk denoting the complex conjugate. Likewise, Table III shows that

$$\epsilon(s,\theta,z) = \epsilon^*(s,\theta,z') \ . \tag{16a}$$

Thus by changing from w,z to w',z' the equation is multiplied through by the constant factor $(-)^m$ and each coefficient changes to its complex conjugate.

q.e.d.

The occurrence of the equations (13) in complex conjugate pairs permits a simplification in listing or surveying all such equations. If the real and imaginary part of each equation is taken separately, one need only consider one equation of each conjugate complex pair and maintain all self-conjugate equations. This can be done in two ways. In the first way one restricts the range of w to values satisfying the selection rule:

$$m - 2w \geq 0 \ ,$$

and leaving $0 \leq z \leq s$ free. In this way only equations with $h \geq 0$ are selected, and this procedure is most practical for the making of tables of bracket relations. In the second way one restricts the range of z to values satisfying the selection rule:

$$s - 2z \geq 0 \ ,$$

and leaving $0 \leq w \leq m$ free. This way is useful for proving some general relations, for example, those of Appendix III. It is evident that for self-conjugate equations

$$m - 2w = s - 2z = 0$$

is a necessary and sufficient condition. The number of real equations so obtained is equal to the number of original complex equations.

Corollary V

If in an equation of the type (13) each bracket is replaced by its adjoint, the resulting equation also belongs to the set (13) and has the same $|h|$.

Proof

Each equation (13) contains adjoint pairs of brackets, characterized by p,θ and $p'=m-p,\theta'=-\theta$, since summations over p and θ occur.

The coefficients of adjoint brackets in one equation are $g(m,p,w)\ \epsilon(s,\theta,z)$ and $g(m,p',w)\ \epsilon(s,\theta',z)$. Thus, replacing all brackets by their adjoints is equivalent to interchanging the above coefficients without changing the brackets. We shall prove that, apart from a constant factor, this change in coefficients transforms the equation into its conjugate complex, which according to Corollary IV also belongs to the set and has opposite h.

It follows directly from equation (15) that

$$g(m,p,w) = (-)^{m+w_i-m}\, g^*(m,p',w) \quad , \tag{17}$$

where $p'=m-p$. It is also easy to verify in Table III that

$$\epsilon(s,\theta,z) = (-)^{n+z_i s}\, \epsilon^*(s,\theta',z) \quad , \tag{17a}$$

where $\theta' = -\theta$. Thus by changing from p,θ to p',θ', the coefficients are multiplied by the constant factor $(-)^{n_i h}$ and change to their conjugate complex.

q.e.d.

A consequence of this corollary is: For any real relation between brackets its adjoint relation is also valid with the same coefficients. This fact is extensively used in constructing the tables of bracket relations which follow.

A number of other corollaries follow from the symmetry of g and ϵ. The principal ones are listed below, proofs being left to the reader. They are useful for checking relations among brackets.

Corollary VI

Any relation between brackets with s = 1 ($\Theta = \pm 1$) is invariant for the substitution $\Theta' = -\Theta$ followed by reversal of the sign of the coefficients of all terms with $\Theta' = -1$.

Corollary VII

Any relation between brackets with s = 2 is invariant for the substitution $\Theta' = -\Theta$ followed by reversal of the sign of the coefficients of all terms with $\Theta = 0$.

Corollary VIII

Any relation between brackets for s = 1, n = even, is transformed to a valid relation for n = odd by changing the sign of all brackets with $\Theta = +1$, and vice versa.

Corollary IX

For m = odd any relation between brackets is invariant for the substitution $m' = m-p$ followed by reversal of the sign of the coefficients of all terms with outer indices 31 and 12.

d. The Procedure for Tabulating the Bracket Relations.—It was stated that the brackets are linear combinations of components of tensors of even rank. Thus the analysis can be restricted to eleven out of thirty-two point groups. Moreover, Onsager's relations permit one to use only six pairs of indices ij, with equations (11) and (11a) valid for all point groups. The theorem, given by equations (13) and (14), allows complete tabulation of all bracket relations for all these groups. Often the application of the corollaries, especially I and II, is helpful in obtaining the tables for certain groups from those of other groups. The brackets of the group S_2 can be tabulated completely by using equations (11) and (11a) only. It is to be remembered that all the tables that follow are constructed according to the convention that k_3 is taken along the ro-

tation axis of highest order and k_1 along a rotation axis normal to k_3, if there be one.

TABLE IV

PROCEDURE FOR TABULATING BRACKET RELATIONS

Table of Group	+ Corollary I About k_3	+ Corollary I About k_1	+ Corollary II About k_3	+ Invariance Under Cyclic Permutation	Yields Table of Group
S_2	+				C_{2h}
C_{2h}		+			D_{2h}
C_{2h}			+		C_{4h}
D_{2h}			+		D_{4h}
D_{2h}				+	T_h
D_{4h}				+	O_h
C_{3i}		+			D_{3i}
C_{3i}	+				C_{6h}
C_{6h}		+			D_{6h}

The first six groups of the last column of Table IV are seen to be completely derivable from the Corollaries I and II and the invariance under cyclic permutation, as indicated by the + signs. The groups D_{3i}, C_{6h}, D_{6h} are based on C_{3i}, which required the direct application of the general theorem, assisted by the various corollaries. We have not found any simple rule yielding the complete tabulation for C_{3i}.

e. Bracket Relations for C_{2h} and D_{2h}.—Table V for C_{2h} and D_{2h} is constructed on the basis of Corollary I. The effect of symmetry is manifest entirely in the vanishing of certain brackets; all nonvanishing brackets are independent. Thus, we have used three symbols to indicate the state of a bracket whose inner part is given by the second column and whose outer indices

appear in the first row. The inner parts of brackets contain the symbols e for an arbitrary even number and ω for an arbitrary odd one.

+ means the bracket is independent both for C_{2h} and D_{2h}.

⊕ means the bracket is independent for C_{2h} but vanishes for D_{2h}.

0 means the bracket vanishes both for C_{2h} and for D_{2h}.

Examples: $[203]_{23}$ is found to be zero as shown by $[ee\omega]_{23}$ in the eighth row,

$[204]_{12}$ is found to be independent for C_{2h} and zero for D_{2h} as shown by [eee] in the first row.

The outer indices 11, 22, 33 cannot occur with n = odd, according to equation (11a). Table V is complete for all n.

TABLE V

BRACKET RELATIONS FOR C_{2h} AND D_{2h}

	ij →	23	31	12	11	22	33
n = even	[eee]	0	0	⊕	+	+	+
	[eωω]	+	⊕	0	0	0	0
	[ωeω]	⊕	+	0	0	0	0
	[ωωe]	0	0	+	⊕	⊕	⊕
n = odd	[ωωω]	0	0	⊕			
	[ωee]	+	⊕	0			
	[eωe]	⊕	+	0			
	[eeω]	0	0	+			

+ means bracket independent for C_{2h} and D_{2h}.
⊕ means bracket independent for C_{2h}, zero for D_{2h}.
0 means bracket zero for C_{2h} and D_{2h}.

f. Bracket Relations for C_{4h} and D_{4h}.—The effect of symmetry is manifested in two ways: either a bracket is zero or it is equal to plus or minus its

adjoint (as defined in Corollary II of the theorem). Of each such pair of adjoint brackets, one bracket can be chosen as independent. In the first, fourth, fifth, and eighth or last row self-adjoint brackets may occur. A self-adjoint bracket may be forced to vanish if it must be minus its adjoint. Thus it turns out that four symbols are needed, whose meaning is explained under the Table VI, which gives the complete bracket relations for all n.

Examples: $[202]_{12} = -[022]_{12}$ for C_{4h}, zero for D_{4h} (first row).

$[220]_{12}$ = self-adjoint and $-[220]_{12}$, hence zero for C_{4h} and D_{4h}.

$[202]_{11} = +[022]_{22}$; one of the pair is independent, both for C_{4h} and D_{4h}.

TABLE VI

BRACKET RELATIONS FOR C_{4h} AND D_{4h}

	ij →	23	31	12	11	22	33
n = even	[eee]	0	0	$\dot{\ominus}$	┼ ---	┼	┼
	[eαω]	┼	⊖	0	0	0	0
	[ωeω]	⊖	┼	0	0	0	0
	[αωe]	0	0	┼	⊖ ---	⊖	$\dot{\ominus}$
n = odd	[αωω]	0	0	$\dot{\ominus}$			
	[ωee]	┼	⊖	0			
	[eωe]	⊖	┼	0			
	[eeω]	0	0	┼			

┼ means bracket is one of an independent pair and equal to its adjoint for C_{4h} and D_{4h}.

⊖ means bracket is one of an independent pair and equal to minus its adjoint for C_{4h}, zero for D_{4h}.

$\dot{\ominus}$ means ⊖ and in addition zero if self-adjoint.

0 means zero for C_{4h} and for D_{4h}.

Dotted lines connect adjoint places.

g. Bracket Relations for T_h and O_h.—Table VII for these groups is derived from Table V for D_{2h} and Table VI for D_{4h} by requiring that brackets remain invariant under cyclic permutation of all indices. The six permutations of the indices 1,2,3 fall into two groups of three cyclic permutations. Brackets belonging to two such cyclic groups are pairwise adjoint with respect to k_1, k_2, and k_3. If adjoint brackets are to be equal, such as happens in O_h, or if brackets are pairwise self-adjoint, the two cyclic groups coincide. For example, we have for T_h a cyclic group of three equal brackets, obtained by cyclic interchange of inner and outer indices from the first one:

$$[202]_{11} = [220]_{22} = [022]_{33} .$$

The other cyclic group of three equal brackets can be obtained from these by a transposition of two indices. Thus by interchanging 1 and 2, i.e., adjoining with respect to k_3, one obtains:

$$[022]_{22} = [220]_{11} = [202]_{33} .$$

For O_h all six are equal. On the other hand, the bracket $[220]_{33}$ is self-adjoint with respect to k_3, hence there is only one cyclic group of three brackets derived from it and they are equal both for T_h and O_h, namely:

$$[220]_{33} = [022]_{11} = [202]_{22} .$$

h. The Bracket Relations for C_{3i}, D_{3i}, C_{6h}, D_{6h}.—No simple rules for the complete tabulation are available and the theorem plus corollaries will be used. In order to obtain the most compact form for the results, the following scheme has been adopted.

For any particular bracket we must first decide whether or not it is zero. For C_{3i} all zero brackets are listed in Table VIII. The proof that these brackets are zeros for C_{3i} is given in Appendix III. The groups D_{3i}, C_{6h}, and D_{6h} have the same zeros and the additional zeros listed in Table IX. The latter was obtained from Tables V, VI, and VII according to the procedure shown in Table IV.

TABLE VII

BRACKET RELATIONS FOR T_h AND O_h

	ij →	23	31	12	11	22	33
n = even	[eee]	0	0	0	+----	+---	--+
	[eωω]	+	0	0	0	0	0
	[ωeω]	0	+	0	0	0	0
	[ωωe]	0	0	+	0	0	0
n = odd	[ωωω]	0	0	0			
	[ωee]	+	0	0			
	[eωe]	0	+	0			
	[eeω]	0	0	+			

+ means nonvanishing bracket for T_h and for O_h.

0 means zero bracket for T_h and O_h.

In T_h + is one of an independent cyclic set of three equal brackets.

In O_h + is one of an independent permuted set of three or six equal brackets (three, if brackets are pairwise self-adjoint).

Dotted lines indicate places of brackets of the same set.

If a bracket does not vanish according to Tables VIII and IX, then its relations to other brackets are shown in Table X, up to m = 6 inclusive.

Table X is arranged in three parts, according to s = 0, 1, or 2. Each part consists of seven sub-tables for m = 0, 1, ... 6. The sub-tables, except the simplest ones, have the form of a core array of coefficients bordered by brackets. This arrangement represents a double-entry table, similar to the familiar trigonometric tables: brackets on the left are equal to the linear combinations of those at the top, with the listed coefficients, whereas brackets on the right use these same coefficients with those at the bottom. That this arrangement, in which adjoint brackets stand at opposite ends of

TABLE VIII

ZERO BRACKETS FOR C_{3i}, D_{3i}, C_{6h}, D_{6h}

	ij →	23	31	12	11	22	33
n = even	[eee]	[ooe]	[ooe]	[ooe]			
	[eωω]						[o1ω]
	[ωeω]						[1oω]
	[ωωe]						[11e]
							[31e]
							[13e]
n = odd	[ωωω]			[11ω]			
				[31ω]			
				[13ω]			
	[ωee]			[1oe]			
	[eωe]			[o1e]			
	[eeω]	[ooω]	[ooω]				

TABLE IX

ZERO BRACKETS FOR D_{3i}, C_{6h}, D_{6h}

	ij →	23	31	12	11	22	33
n = even	[eee]	$\dot{*}$	*Δ	$\dot{\Delta}$			
	[eωω]		Δ	*Δ	*	*	$\dot{*}$
	[ωeω]	Δ		*	*Δ	*Δ	*Δ
	[ωωe]	*Δ	*		Δ	Δ	$\dot{\Delta}$
n = odd	[ωωω]	*	*Δ	$\dot{\Delta}$			
	[ωee]		Δ	*Δ			
	[eωe]	Δ		$\dot{*}$			
	[eeω]	*Δ	$\dot{*}$				

Δ means zero bracket for D_{3i} and for D_{6h}.
* means zero bracket for C_{6h} and for D_{6h}.
· is a reminder to check Table VIII.

rows and columns, is possible is due to Corollary V. For example, for s = 1, m = 4 we have

$$[31e]_{23} = [40e]_{31} + 3[04e]_{31}$$

$$[13e]_{31} = 3[40e]_{23} + [04e]_{23}$$

The two equations are adjoint with respect to k_3.

TABLE X

RELATIONS FOR NONVANISHING BRACKETS FOR C_{3i}, D_{3i}, C_{eh}, D_{eh}

s = 0

m	
0	$[00e]_{33}$
1	---
2	$[20e]_{33} = [02e]_{33}$
3	$[12\omega]_{33} = -3[30\omega]_{33}$ $[21\omega]_{33} = -3[03\omega]_{33}$
4	$2[40e]_{33} = [22e]_{33} = 2[04e]_{33}$
5	$[50\omega]_{33}$ $[32\omega]_{33}$ -2 $[23\omega]_{33}$ $[14\omega]_{33}$ -3 $[41\omega]_{33}$ $[05\omega]_{33}$
6	$[60e]_{33}$ $[33e]_{33}$ $[06e]_{33}$ $[51e]_{33}$ 0 $-3/10$ 0 $[15e]_{33}$ $[42e]_{33}$ -6 0 9 $[24e]_{33}$ $[06e]_{33}$ $[33e]_{33}$ $[60e]_{33}$

TABLE X (Continued)

$s = 1 \quad n = \text{even}^*$

m	
0	---
1	$[1\omega]_{31} = [0\omega]_{23}$ $[0\omega]_{31} = -[1\omega]_{23}$
2	$2[2e]_{31} = -[1e]_{23} = -2[0e]_{31}$ $2[2e]_{23} = [1e]_{31} = -2[0e]_{23}$
3	$[3\omega]_{31} = [1\omega]_{31} = [2\omega]_{23} = [0\omega]_{23}$ $-[3\omega]_{23} = -[1\omega]_{23} = [2\omega]_{31} = [0\omega]_{31}$
4	$[4e]_{31}\ [0e]_{31}$ $[3e]_{23}\ 1\ 3\ [1e]_{31}$ $[2e]_{31}\ -3\ -3\ [2e]_{23}$ $[1e]_{23}\ -3\ -1\ [3e]_{31}$ $[0e]_{23}\ [4e]_{23}$
5	$[5\omega]_{31}\ [0\omega]_{23}$ | $[5\omega]_{23}\ [0\omega]_{31}$ $[4\omega]_{23}\ -2\ 3\ [1\omega]_{31}$ | $[4\omega]_{31}\ 2\ 3\ [1\omega]_{23}$ $[3\omega]_{31}\ -4\ 6\ [2\omega]_{23}$ | $[3\omega]_{23}\ -4\ -6\ [2\omega]_{31}$ $[0\omega]_{23}\ [5\omega]_{31}$ | $[0\omega]_{31}\ [5\omega]_{23}$
6	$[6e]_{31}\ [0e]_{31}$ $[5e]_{23}\ 1\ 3\ [1e]_{31}$ $[4e]_{31}\ -2\ -3\ [2e]_{23}$ $[3e]_{23}\ -2\ 2\ [3e]_{31}$ $[2e]_{31}\ -3\ -2\ [4e]_{23}$ $[1e]_{23}\ -3\ -1\ [5e]_{31}$ $[0e]_{23}\ [6e]_{23}$

*The same table can be used for n = odd if each bracket with outer indices 23 receives a minus sign, according to Corollary VII.

TABLE X (Continued)

$s = 2 \qquad n = \text{even}$

m	
0	$[ooe]_{11} = [ooe]_{22}$
1	$[1o\omega]_{11} = [o1\omega]_{12} = [1o\omega]_{22}$ $[o1\omega]_{22} = -[1o\omega]_{12} = [o1\omega]_{11}$
2	$[11e]_{12} = [2oe]_{11} - [2oe]_{22}$ $[o2e]_{11} = [2oe]_{22}$ $[o2e]_{22} = [2oe]_{11}$ $[11e]_{11} = -[11e]_{22} = 2[2oe]_{12} = -2[o2e]_{12}$

3

	$[3o\omega]_{11}$	$[3o\omega]_{22}$	
$[21\omega]_{12}$	-1/2	1/2	$[12\omega]_{12}$
$[12\omega]_{11}$	-1	-2	$[21\omega]_{22}$
$[12\omega]_{22}$	-2	-1	$[21\omega]_{11}$
$[o3\omega]_{12}$	-1/2	1/2	$[3o\omega]_{12}$
	$[o3\omega]_{22}$	$[o3\omega]_{11}$	

4

	$[4oe]_{11}$	$([o4e]_{11} + [4oe]_{22})$	$[o4e]_{22}$		$[4oe]_{12}$	$[o4e]_{12}$	
$[31e]_{12}$	-3/2	-1/2	5/2	$[13e]_{12}$	$[31e]_{11}$	1	3	$[13e]_{22}$
$[22e]_{11}$	-5/2	1/2	7/2	$[22e]_{22}$	$[31e]_{22}$	-1	-3	$[13e]_{11}$
$[o4e]_{11}$	1/2	1/2	-1/2	$[4oe]_{22}$	$[22e]_{12}$	-3	-3	$[22e]_{12}$
	$[o4e]_{22}$	$([4oe]_{22} + [o4e]_{11})$	$[4oe]_{11}$		$[o4e]_{12}$	$[4oe]_{12}$	

5

	$[5o\omega]_{11}$	$[o5\omega]_{12}$	$[5o\omega]_{22}$	
$[41\omega]_{12}$	1	3	-1	$[14\omega]_{12}$
$[32\omega]_{11}$	-3	-6	1	$[23\omega]_{22}$
$[32\omega]_{22}$	1	6	-3	$[23\omega]_{11}$
$[23\omega]_{12}$	-3	-4	3	$[32\omega]_{12}$
$[14\omega]_{11}$	0	2	-3	$[41\omega]_{22}$
$[14\omega]_{22}$	-3	-2	0	$[41\omega]_{11}$
	$[o5\omega]_{22}$	$[5o\omega]_{12}$	$[o5\omega]_{11}$	

TABLE X (Concluded)

6	$[6oe]_{11}$	$[6oe]_{22}$	$[oGe]_{11}$	$[oGe]_{22}$		$[6oe]_{12}$	$[oGe]_{12}$	$[33e]_{11}$	
	$[51e]_{12}$	-1	1	-3	3	$[15e]_{12}$	$[51e]_{11}$	2/5	18/5	-3/10	$[15e]_{22}$
	$[42e]_{11}$	-4	-2	3	6	$[24e]_{22}$	$[51e]_{22}$	-8/5	-12/5	-3/10	$[15e]_{11}$
	$[42e]_{22}$	-2	-4	6	3	$[24e]_{11}$	$[42e]_{12}$	-2	-3	0	$[24e]_{12}$
	$[33e]_{12}$	2	-2	-2	2	$[33e]_{12}$	$[33e]_{22}$	4	-4	1	$[33e]_{11}$
		$[oGe]_{22}$	$[oGe]_{11}$	$[6oe]_{22}$	$[6oe]_{11}$			$[oGe]_{12}$	$[6oe]_{12}$	$[33e]_{22}$	

s = 2 n = odd

m	
0	$[o\alpha\omega]_{12}$
1	---
2	$[o2\omega]_{12} = [2o\omega]_{12}$
3	$[21e]_{12} = -3[o3e]_{12}$ $[12e]_{12} = -3[3oe]_{12}$
4	$2[4o\omega]_{12} = [22\omega]_{12} = 2[o4\omega]_{12}$
5	$2[41e]_{12} = 3[23e]_{12} = -[o5e]_{12}$ $2[14e]_{12} = 3[32e]_{12} = -[5oe]_{12}$
6	$[51\omega]_{12} = -3/10[33\omega]_{12} = [15\omega]_{12}$ $[42\omega]_{12} = -6[6o\omega]_{12} + 9[o6\omega]_{12}$ $[24\omega]_{12} = 9[6o\omega]_{12} - 6[o6\omega]_{12}$

4. THE NUMBER OF NONVANISHING INDEPENDENT BRACKETS

Let I(n) be the number of nonvanishing independent brackets for each point group as a function of n; further let P(n) be the number of possible brackets, $E^*(n)$ the number of valid equations (13) between them, E(n) the number of equations (13), valid and nonvalid, and K(n) the number of nonvalid

equations (13) corresponding to h = kN. Then evidently

$$I(n) = P(n) - E^*(n) = P(n) - E(n) + K(n) \quad . \tag{18}$$

Case 1. Groups C_N (N = 1,2,3,4,6)

It will be shown in Appendix II that $P_C(n) = E_C(n)$ for a rotation axis along k_3, reducing (18) to

$$I_{C_N}(n) = K_{C_N}(n) \quad . \tag{19}$$

In order to evaluate $K_{C_N}(n)$, a counting diagram as shown in Figure 2 can be used. For any of the six allowed combinations of s,z when n is even (three when n is odd), each possible equation (13) is represented by a point in the h,m plane. The equations for a given value of n are represented by lattice points $m \leq n$. Since by definition $0 \leq w \leq m$, we have $-m + (s-2z) \leq h \leq + m + (s -2z)$; hence, for each s,z pair (subgraph), the points fill a triangular array. For purposes of counting it is convenient to think of each point as the center of a one-by-two rectangle, the rectangles filling the area. The points (equations) satisfying h = kN lie on a series of equidistant horizontal lines spaced by a distance N.

For the group C_1 all the points must be counted as a function of n, i.e., up to m = n inclusive, leading to

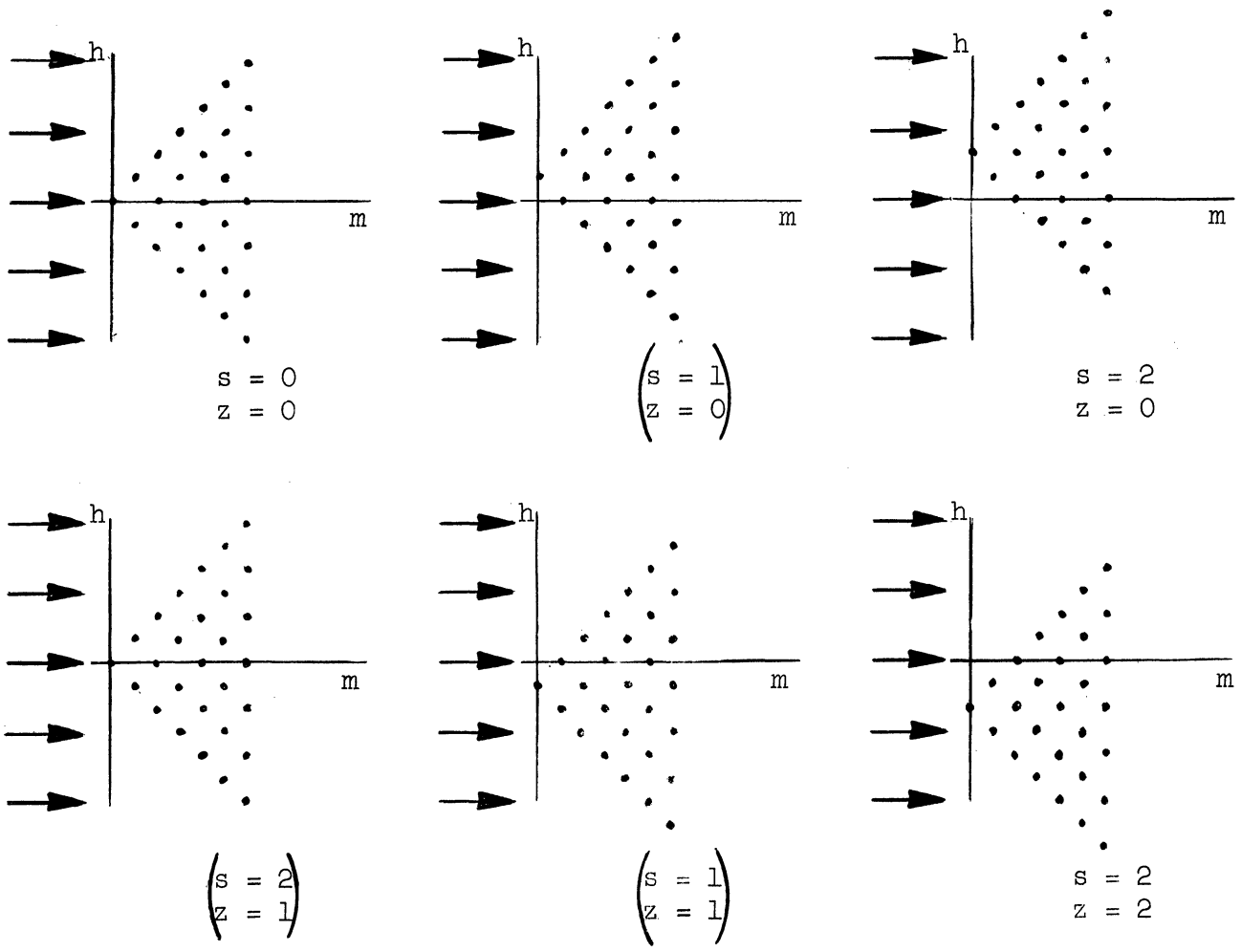
$$I_{C_1}(n) = P_C(n) = E_C(n) = K_{C_1}(n) = a_o n^2 + b_o n + c_o \quad , \tag{20}$$

where, for n = even, $a_o = 3$, $b_o = 9$, $c_o = 6$, and, for n = odd, $a_o = 3/2$, $b_o = 9/2$, $c_o = 3$.

For $C_N(N > 1)$ the number of points lying on the horizontal lines h = kN must be counted and is easily seen to be of the form $an^2 + bn + c$, where

$$a = a_o/N \tag{21}$$

stems from the main triangle area covered by these lines (i.e., the rectangles of the lattice points on these lines) while



Points represent E-equations (13) in h,m plane for the various possible combinations of s and z. Arrows indicate K-equations for which h = kN. The case illustrated is N = 3. For n = even all six diagrams are valid; for n = odd, only those with parentheses.

Figure 2. Counting diagram.

$$\left.\begin{aligned} b &= b_o/N && \text{for } N = \text{odd} \\ b &= (b_o + 1)/N && \text{for } N = \text{even},\ n = \text{even} \\ b &= (b_o + 1/2)/N && \text{for } N = \text{even},\ n = \text{odd} \end{aligned}\right\} \quad (22)$$

stems from circumference points with h = kN whose rectangle areas stick out beyond the main triangle area. The values of c are most easily evaluated in practice by solving for c for some low value of n for which I_{C_N} has been counted. In this way the formulas of Table XI for the C classes result.

Case 2. Groups D_N (N = 2,3,4,6)

The quantities on the right-hand side of (18) will now be interpreted after the effect of a binary axis along k_1 has been taken into account. This effect is manifest in two ways: certain brackets vanish, reducing P(n), and certain equations about k_3 must be dropped, reducing E(n), as will now be shown.

According to Corollary I, all brackets for which the index 1 occurs an odd number of times vanish. In any bracket the index 1 occurs p + n - m times inside and 1/2(s - θ) times outside, together p + n - m + 1/2 (s - θ) times. On the other hand, any equation (13) about k_3 contains brackets with the same n,m,s, but different p,θ. The coefficient gε of any such bracket is $i^{p+1/2(s-\theta)}\, i^s$ times a real factor. Thus, if n - m + s is even, then all brackets with imaginary coefficients in the equations (13) about k_3 vanish due to the binary axis about k_1, while if n - m + s is odd, those with real coefficients vanish. Thus, every equation (13) about k_3 becomes equivalent to its complex conjugate, and in order to find $E^*_{D_N}(n)$ it is only necessary to count points h ≠ kN for which h > 0, i.e., the upper half of the counting diagram of Figure 2. Consequently

$$E^*_{D_N}(n) = 1/2\ E^*_{C_N}(n) \quad . \qquad (23)$$

The number of possible brackets after introducing the binary axis k_1 is clearly

$$P_{D_N}(n) = I_{C_{2h}}(n) \quad , \qquad (23a)$$

or wit (18) and (20)

$$I_{D_N}(n) = I_{C_{2h}}(n) - 1/2\,[I_{C_1}(n) - I_{C_N}(n)] \quad . \tag{24}$$

Substituting the results found under Case 1 for $I_{C_{2h}}$ and I_{C_1}, we have for

$$n = \text{even} \qquad I_{D_N}(n) = 1/2\, I_{C_N}(n) + 1/2\, n + 1 \tag{24a}$$

$$n = \text{odd} \qquad I_{D_N}(n) = 1/2\, I_{C_N}(n) + 1/4\, n + 1/4 \tag{24b}$$

Case 3. Groups T_h, O_h

For the class T_h, analysis of the effect of cyclic permutations leads immediately to

$$I_{T_h} = 1/3\, I_{D_{2h}} \quad ,$$

while for O_h case various simple ways of counting yield the results of Table XI.

Case 4. Isotropic Case

For an isotropic sample, one can always take the 3-axis along the applied constant magnetic field. The number of nonvanishing independent brackets would be just that corresponding to the crystal classes C_N with N being infinite. Therefore, every equation given by (13) and (14) is valid except those pertaining to h = 0. Since m = 0 always, the number of such equations is given by

$$\left.\begin{aligned} &a = b = 0 \\ &c = \begin{cases} 1 & \text{if } n = \text{odd or zero} \\ 2 & \text{if } n = \text{even} > \text{zero.} \end{cases} \end{aligned}\right\} \tag{24c}$$

Note that the first line of equation (24c) agrees with equations (21) and (22).

5. EXPLICIT FORMS OF THE GALVANOMAGNETIC TENSOR

It was shown in Section 2.b that

$$\rho^{\alpha 1}(\underline{B}) = \rho_{ji} \ell_j^{\alpha} \ell_i^1 = \Delta_{ij} \ell_i^1 \ell_j^{\alpha} / \Delta \tag{25}$$

where Δ_{ij} is the cofactor of σ_{ij} in $\Delta = \det \sigma_{ij}$, and ℓ_i^{α} is the direction cosine of the laboratory coordinates axis α with respect to the symmetry coordinate i. For $\alpha = 1$ the equation represents the magneto resistance, for $\alpha \neq 1$ the Hall effect,

TABLE XI

THE NUMBER OF NONVANISHING INDEPENDENT BRACKETS $an^2 + bn + c$

Group	n	a	b	c
$C_1=S_2$	even	3	9	6
	odd	3/2	9/2	3
C_{2h}	even	3/2	5	4
	odd	3/4	5/2	7/4
C_{3i}	even	1	3	2
	odd	1/2	3/2	1
C_{4h}	even	3/4	5/2	2
	4k+1	3/8	5/4	11/8
	4k-1	3/8	5/4	7/8
C_{6h}	6k-2	} 1/2	} 5/3	4/3
	6k			2
	6k+2			8/3
	6k-1	} 1/4	} 5/6	7/12
	6k+1			23/12
	6k+3			5/4
D_{2h}	even	3/4	3	3
	odd	3/8	3/2	9/8
D_{3i}	even	1/2	2	2
	odd	1/4	1	3/4
D_{4h}	even	3/8	7/4	2
	4k+1	3/16	7/8	15/16
	4k-1	3/16	7/8	11/16
D_{6h}	6k-2	} 1/4	} 4/3	5/3
	6k			2
	6k+2			7/3
	6k-1	} 1/8	} 2/3	13/24
	6k+1			29/24
	6k+3			7/8
T_h	even	1/4	1	1
	odd	1/8	1/2	3/8
O_h	even	1/8	3/4	1
	4k+1	1/16	3/8	9/16
	4k-1	1/16	3/8	5/16

and this is true for all that follows. Substituting the expansions of all σ_{ij} into (25) we obtain

$$\rho^{\alpha_1}(\underline{B}) = \left(\sum_{\eta=0} P_{2\eta}^{\alpha_1} B^{2\eta} + \sum_{\eta=0} Q_{2\eta+1}^{\alpha_1} B^{2\eta+1}\right) \Big/ \sum_{\eta=0} M_{2\eta} B^{2\eta} \quad . \qquad (26)$$

The explicit expressions of $P_{2\eta}^{\alpha_1}$, $Q_{2\eta+1}^{\alpha_1}$, and $M_{2\eta}$ in terms of the brackets and the two sets of direction cosines can be readily obtained from (25) and (26) since M is the expansion of Δ and P and Q are expansions of $(\Delta_{ij} \ell_i^{\alpha} \ell_j^1)$.

There are three classes of special cases of equation (26) that are of interest for both historical and practical reasons. The first class, which is valid for some crystal symmetries, pertains to special geometrical configurations. The second class, valid for an arbitrarily oriented magnetic field, pertains to isotropic substances only. The third class, valid for all crystal symmetries, pertains to a small, but arbitrarily oriented, magnetic field.

a. Galvanomagnetic Tensor for Special Orientations*.—This class of special cases applies to all crystal symmetries except S_2 and C_{2h}. The 3-axis is taken either along a rotational axis of three-, four-, or six-fold symmetry or along a two-fold axis if it is accompanied by another two-fold axis normal to it. This class is divided into two subclasses according to the relative orientations of the magnetic field and the current.

Case 1. Transverse Field

Assume

(1) Laboratory coordinates are along symmetry coordinates, i.e.,

$$\ell_1^1 = \ell_2^2 = \ell_3^3 = 1 \ .$$

(2) The magnetic field is along the k_3-axis, i.e., $\gamma_3 = 1$.

(3) The current flows along the k_1-axis.

According to the results of Section 3, under condition (2) there are only two kinds

*In most papers on the theory of galvanomagnetic effects the formulas for this class up to the second power of B are used instead of equation (26).

of nonvanishing brackets, $[oo\omega]_{12}$, $[ooe]_{ii}$, which will be abbreviated by $[\omega]_{12}$, $[e]_{ii}$, i = 1,2,3. It follows that

$$\rho^{11}(\underline{B}) - \rho^{11}(\underline{B} = 0) = - \sum_{\eta=1} B^{2\eta} U_{2\eta} \Big/ [o]_{11} \sum_{\eta=0} B^{2\eta} N_{2\eta} \tag{27}$$

$$\rho^{21}(\underline{B}) = - \sum_{\eta=0} B^{2\eta+1} [2\eta + 1]_{12} \Big/ [o]_{11} \sum_{\eta=0} B^{2\eta} N_{2\eta} \tag{28}$$

$$\rho^{31}(\underline{B}) = 0 \; ; \tag{29}$$

where

$$\sum_{\eta=0} B^{2\eta} N_{2\eta} = \sum_{\eta=0} B^{2\eta} [o]_{11} [2\eta]_{22} + \sum_{\eta=1} B^{2\eta} U_{2\eta} \tag{30}$$

$$U_{2\eta} = \sum_{q=0}^{\eta-1} \left\{ [2(\eta - q)]_{11} [2q]_{22} + [2q + 1]_{12} [2\eta - 2q - 1]_{12} \right\} . \tag{31}$$

Case 2. Longitudinal Field

Assume

(1) Laboratory coordinates are along symmetry coordinates, i.e.,

$$\ell_1^1 = \ell_2^2 = \ell_3^3 = 1 .$$

(2) The magnetic field is along the k_3-axis, i.e., $\gamma_3 = 1$.

(3) The current flows along the k_3-axis.

Then

$$\rho^{33}(\underline{B}) - \rho^{33}(\underline{B}=0) = - \sum_{\eta=1} B^{2\eta} [2\eta]_{33} \Big/ [o]_{33} \sum_{\eta=0} B^{2\eta} [2\eta]_{33} \tag{32}$$

$$\rho^{13}(\underline{B}) = \rho^{23}(\underline{B}) = 0 . \tag{33}$$

Note that equations (27-33) have the same parity as predicted in Section 2.d, from which one can in fact write down equations (29) and (33) directly.

b. Explicit Expression of $\rho^{\lambda\mu}(\underline{B})$ for Isotropic Substances.—Upon the introduction of a magnetic field, an isotropic sample behaves anisotropically as if it posesses a rotation axis of infinite-fold order along the direction of the magnetic field. In this case one can always take the 3-axis along the magnetic field direction; thus only brackets of the form $[oon]_{ij}$, or $[n]_{ij}$, are involved. There are only three kinds of nonvanishing brackets: $[ooe]_{11}$, $[ooe]_{33}$, and $[oo\omega]_{12}$. Therefore, remembering that $[ooo]_{11} = [ooo]_{33}$, the explicit forms of $P_{2\eta}^{\lambda\mu}$, $Q_{2\eta+1}^{\lambda\mu}$, and $M_{2\eta}$ contained in equation 26 can be readily written out as follows:

$$P_{2\eta}^{\lambda\mu} = \delta_{\lambda\mu} \sum_{q=0}^{\eta} [2(\eta - q)]_{11} [2q]_{33} + \ell_3^{\lambda} \ell_3^{\mu} \left\{ \sum_{q=0}^{\eta} [2(\eta - q)]_{11} ([2q]_{11} - [2q]_{33}) + \right.$$
$$\left. + \sum_{q=0}^{\eta-1} [2q + 1]_{12} [2(\eta - q) + 1]_{12} \right\} \tag{34}$$

$$Q_{2\eta+1} = -\ell_3^{\nu} \sum_{q=0}^{\eta} [2(\eta - q)]_{33} [2q + 1]_{12} \tag{35}$$

$$M_{2\eta} = \sum_{r=0}^{\eta} [2(\eta - r)]_{33} \left\{ \sum_{q=0}^{r} [2(r - q)]_{11} [2q]_{11} + \sum_{q=1}^{r} [2(r - q) + 1]_{12} [2q - 1]_{12} \right\}, \tag{36}$$

where ℓ_k^{ν} has been used as an abbreviation defined by

$$\ell_k^{\nu} \equiv \ell_i^{\lambda} \ell_j^{\mu} - \ell_j^{\lambda} \ell_i^{\mu} .$$

Thus, if $\lambda = \mu$, ℓ_k^{ν} automatically vanished in agreement with the evenness of the magneto resistance, while if $\lambda \neq \mu$, the subscripts ijk must be a permutation of 123 of the same parity as the superscripts $\lambda\mu\nu$. In that case ℓ_k^{ν} is the direction cosine between the symmetry axis k and the laboratory axis ν. Note that if λ- , μ- , and 3-axis are orthogonal to each other, then $\rho^{\lambda\mu}(\underline{B})$ is a purely odd function of $\underline{B}$. This result conforms with the prediction of Section 2.e.

c. Galvanomagnetic Effects for Low Values of the Magnetic Field.— This class applies to cases with arbitrary orientation of the sample and of the magnetic field with respect to the crystal axes for all crystal structures. For the practical purpose of reading off the explicit form of the galvanomagnetic tensor components $\rho^{\alpha 1} = F^{\alpha}/J^{1}$ in terms of the brackets, tables have been compiled for all except that for S_2, which is omitted for simplicity.

If only terms up to B^2 are considered, then equation (26) becomes

$$\rho^{\alpha 1} = \left\{ P_o^{\alpha 1} + Q_1^{\alpha 1} B + (P_2^{\alpha 1} - P_o^{\alpha 1} M_2/M_o) B^2 + \ldots \right\}/M_o \quad . \tag{37}$$

Table XII gives M_o. Table XIII gives the coefficients of $l_i^1 \, l_j^{\alpha}$ in $P_o^{\alpha 1}$. Table XIV gives the coefficients of γ_k, the direction cosines of $\underline{B}$ in the crystal coordinate system, resulting in $Q_1^{\alpha 1}$. For the purpose of tabulating the coefficient of B^2 we write

$$P_2^{\alpha 1} - P_o^{\alpha 1} M_2/M_o = R_2^{\alpha 1} = R_{k\ell}^{\alpha 1} \gamma_k \gamma_\ell \, . \tag{38}$$

Tables XV, XVI, and XVII give the $R_{k\ell}^{\alpha 1}$ for the various classes. Coefficients for higher powers than B^2 can be obtained similarly if needed. These tables are useful, for example, in determining what measurements must be made in order to determine all the independent brackets (material constants). In principle, the number of measurements must be at least equal to the number of independent brackets. It must be emphasized that a complete set of brackets cannot be determined from magneto resistance measurements alone, even allowing variation of the l's and γ's. At least some Hall measurements are also required.

6. DISCUSSION

The anisotropy of galvanomagnetic effects, first studied by Righi in 1883, appeared in many works from time to time. However, the crystallographic effects have never been taken into account comprehensively. An overall investigation of the crystallographic effects of the 32 point groups upon the iso-

TABLE XII

THE EXPLICIT FORM OF M_o

C_{2h}	$[ooo]_{33}\,([ooo]_{11}\,[ooo]_{22} - [ooo]_{12}^2)$
D_{2h}	$[ooo]_{33}\,[ooo]_{11}\,[ooo]_{22}$
C_{3i}, D_{3i}, C_{4h} D_{4h}, C_{6h}, D_{6h}	$[ooo]_{33}\,[ooo]_{11}^2$
T_h, O_h	$[ooo]_{11}^3$

TABLE XIII

THE EXPLICIT FORM OF $P_o^{\alpha 1}$

	$\overset{1}{\ell_1}\ \overset{\alpha}{\ell_1}$	$\overset{1}{\ell_2}\ \overset{\alpha}{\ell_2}$	$\overset{1}{\ell_3}\ \overset{\alpha}{\ell_3}$	$\overset{1}{\ell_1}\ \overset{\alpha}{\ell_2} + \overset{1}{\ell_2}\ \overset{\alpha}{\ell_1}$
C_{2h}	$[ooo]_{22}[ooo]_{33}$	$[ooo]_{33}[ooo]_{11}$	$[ooo]_{11}[ooo]_{22} - [ooo]_{12}^2$	$-[ooo]_{33}[ooo]_{12}$
D_{2h}	$[ooo]_{22}[ooo]_{33}$	$[ooo]_{33}[ooo]_{11}$	$[ooo]_{11}[ooo]_{22}$	
C_{3i}, D_{3i} C_{4h}, D_{4h} C_{6h}, D_{6h}	$[ooo]_{11}[ooo]_{33}$	$[ooo]_{11}[ooo]_{33}$	$[ooo]_{11}^2$	
T_h, O_h	$[ooo]_{11}^2$	$[ooo]_{11}^2$	$[ooo]_{11}^2$	

TABLE XIV

THE EXPLICIT FORM OF $Q_1^{\alpha_1}$

	γ_1	γ_2	γ_3
C_{2h}	$\left\{ \begin{array}{l} \ell_1^\beta([100]_{23}[000]_{11}+[100]_{31}[000]_{12}) \\ +\ell_2^\beta([100]_{31}[000]_{22}+[100]_{23}[000]_{12}) \end{array} \right.$	$\ell_1^\beta([010]_{23}[000]_{11}+[010]_{31}[000]_{12})$ $+\ell_2^\beta([010]_{31}[000]_{22}+[010]_{23}[000]_{12})$	$\ell_3^\beta[001]_{12}[000]_{33}$
D_{2h}	$\ell_1^\beta[100]_{23}[000]_{11}$	$\ell_2^\beta[010]_{31}[000]_{22}$	$\ell_3^\beta[001]_{12}[000]_{33}$
C_{3i}, C_{4h}, C_{6h}	$\ell_1^\beta[100]_{23}[000]_{11}-\ell_2^\beta[010]_{23}[000]_{11}$	$\ell_1^\beta[010]_{23}[000]_{11}+\ell_2^\beta[100]_{23}[000]_{11}$	$\ell_3^\beta[001]_{12}[000]_{33}$
D_{3i}, D_{4h}, D_{6h} T_h, O_h	$\left\{ \begin{array}{l} \\ \ell_1^\beta[100]_{23}[000]_{11} \\ \\ \end{array} \right.$	$\ell_2^\beta[100]_{23}[000]_{11}$	$\ell_3^\beta[001]_{12}[000]_{33}$

TABLE XV

THE EXPLICIT FORM OF R_2 FOR C_{2h}, D_{2h} ♯

$-R^{\alpha\alpha}_{11}$	$t^{\alpha}_1 t^{1}_1 \{([000]_{33}[200]_{11} + [100]^{2*}_{31})\,A/B + 2([100]_{23}[100]_{31} - [000]_{33}[200]_{12})\,A + ([000]_{33}[200]_{22} + [100]^{2}_{23})\,AB\} +$ $+ t^{\alpha}_2 t^{1}_2 \{([000]_{33}[200]_{22} + [100]^{2}_{23})\,B/A + 2([100]_{23}[100]_{31} - [000]_{33}[200]_{12})\,B + ([000]_{11}[200]_{33} + [100]^{2}_{31})\,AB\} +$ $+ t^{\alpha}_3 t^{1}_3 \{[000]_{11}[000]_{22}[200]_{33} + [000]_{11}[100]^{2}_{23} + [000]_{22}[100]^{2*}_{31} + (2[100]_{23}[100]_{31} - [000]_{12}[200]_{33})(1 - AB)[000]^{*}_{12}\}/[000]_{33} +$ $+ (t^{\alpha}_1 t^{1}_2 + t^{\alpha}_2 t^{1}_1)\{([000]_{33}[200]_{12} - [100]_{23}[100]_{31})(1 + AB) - ([000]_{33}[200]_{11} + [100]^{2}_{31})\,A - ([000]_{33}[200]_{22} + [100]^{2}_{23})\,B\}^{*}$
$-R^{\alpha\alpha}_{22}$	$t^{\alpha}_1 t^{1}_1 \{([000]_{33}[020]_{11} + [010]^{2}_{31})\,A/B + 2([010]_{31}[010]_{23} - [000]_{33}[020]_{12})\,A + ([000]_{33}[020]_{22} + [010]^{2}_{23})\,AB\} +$ $+ t^{\alpha}_2 t^{1}_2 \{([000]_{33}[020]_{22} + [010]^{2*}_{23})\,B/A + 2([010]_{31}[010]_{23} - [000]_{33}[020]_{12})\,B + ([000]_{11}[020]_{33} + [010]^{2}_{31})\,AB\} +$ $+ t^{\alpha}_3 t^{1}_3 \{([000]_{22}[020]_{33}[000]_{11} + [000]_{11}[010]^{2*}_{23} + [000]_{22}[010]^{2}_{31}) + (2[010]_{23}[010]_{31} - [000]_{12}[020]_{33})(1 - AB)[000]^{*}_{12}\}/[000]_{33} +$ $+ (t^{\alpha}_1 t^{1}_2 + t^{\alpha}_2 t^{1}_1)\{([000]_{33}[020]_{12} - [010]_{31}[010]_{23})(1 + AB) - ([000]_{33}[020]_{11} + [010]^{2}_{31})\,A - ([000]_{33}[020]_{22} + [010]^{2}_{23})\,B\}^{*}$
$R^{\alpha\alpha}_{33}$	$t^{\alpha}_1 t^{1}_1 \{([000]_{22}[002]_{11} + [001]^{2}_{12}) / [000]_{11} - 2[002]_{12}\,A + [002]_{22}\,AB\}[000]_{33} +$ $+ t^{\alpha}_2 t^{1}_2 \{([000]_{11}[002]_{22} + [001]^{2}_{12}) / [000]_{22} - 2[002]_{12}\,B + [002]_{11}\,AB\}[000]_{33} +$ $+ t^{\alpha}_3 t^{1}_3 (1 - AB)^{2}[002]_{33}[000]_{11}[000]_{22} / [000]_{33} +$ $+ (t^{\alpha}_1 t^{1}_2 + t^{\alpha}_2 t^{1}_1)\{(1 + AB)[002]_{12} - ([000]_{22}[002]_{11} + [000]_{11}[002]_{22} + [001]^{2}_{12})\,A / [000]_{22}\}^{*}[000]_{33}$
$-(R^{\alpha\alpha}_{23} + R^{\alpha\alpha}_{32})$	$(t^{\alpha}_2 t^{1}_3 + t^{\alpha}_3 t^{1}_2)([000]_{11}[011]_{23} - [001]_{12}[010]_{31} - [000]_{12}[011]^{*}_{31}) + (t^{\alpha}_3 t^{1}_1 + t^{\alpha}_1 t^{1}_3)([000]_{22}[011]_{31} - [001]_{12}[010]_{23} - [000]_{12}[011]_{23})^{*}(1 - AB)$
$-(R^{\alpha\alpha}_{31} + R^{\alpha\alpha}_{13})$	$(t^{\alpha}_2 t^{1}_3 + t^{\alpha}_3 t^{1}_2)([000]_{11}[101]_{23} - [001]_{12}[100]_{31} - [000]_{12}[101]_{31})^{*} + (t^{\alpha}_3 t^{1}_1 + t^{\alpha}_1 t^{1}_3)([000]_{22}[101]_{31} - [001]_{12}[100]_{23} - [000]_{12}[101]^{*}_{23})(1 - AB)$
$-(R^{\alpha\alpha}_{12} + R^{\alpha\alpha}_{21})$	$t^{\alpha}_1 t^{1}_1 \{([000]_{33}[110]_{11} + 2[010]_{31}[100]_{31})\,A/B + (2[100]_{23}[010]_{31} + 2[010]_{23}[100]_{31} - [000]_{33}[110]_{12})\,A +$ $+ ([000]_{22}[110]_{33} + [000]_{33}[110]_{22} + 2[100]_{23}[010]_{23})\,AB\}^{*} +$ $+ t^{\alpha}_2 t^{1}_2 \{([000]_{33}[110]_{22} + 2[100]_{23}[010]_{23})\,B/A + (2[100]_{23}[010]_{31} + 2[010]_{23}[100]_{31} - [000]_{33}[110]_{12})\,B +$ $+ ([000]_{11}[110]_{33} + [000]_{33}[110]_{11} + 2[100]_{31}[010]_{31})\,AB\}^{*} +$ $+ t^{\alpha}_3 t^{1}_3 \{([000]_{22}[110]_{33}[000]_{11} + 2[000]_{22}[100]_{31}[010]_{31} + 2[100]_{23}[010]_{23}[000]_{11}) +$ $+ (2[100]_{23}[010]_{31} + 2[010]_{23}[100]_{31} - [000]_{12}[110]_{33})(1 - AB)[000]_{12}\}^{*}/[000]_{33} +$ $+ (t^{\alpha}_1 t^{1}_2 + t^{\alpha}_2 t^{1}_1)\{([000]_{33}[110]_{12} - [100]_{23}[010]_{31} - [010]_{23}[100]_{31})(1 + AB) -$ $- ([000]_{33}[110]_{11} + 2[010]_{31}[100]_{31})\,A - ([000]_{33}[110]_{22} + 2[100]_{23}[010]_{23})\,B\}$

$A = [000]^{*}_{12}/[000]_{11}$ $\quad A/B = 1/(B/A) = [000]_{22}/[000]_{11}$

$B = [000]^{*}_{12}/[000]_{22}$ $\quad$ * means zero for D_{2h}

♯ The whole table should be divided by a factor $(1 - AB)$.

TABLE XVI

THE EXPLICIT FORM OF R_2 FOR C_{3i}, C_{4h}, C_{6h}, D_{3i}, D_{4h}, D_{6h}

$-R_{11}^{\alpha\alpha}$	$l_1^\alpha l_1^1([200]_{11}[000]_{33} + [100]_{31}^{2*}) + (l_2^\alpha l_3^1 + l_3^\alpha l_2^1)[000]_{11}[200]_{23}^{\Delta}$ $+ l_2^\alpha l_2^1([200]_{22}[000]_{33} + [100]_{23}^{2}) + (l_3^\alpha l_1^1 + l_1^\alpha l_3^1)[000]_{11}[200]_{31}^{\Delta*}$ $+ l_3^\alpha l_3^1([200]_{33}[000]_{11} + [100]_{23}^{2} + [100]_{31}^{2*})[000]_{11}/[000]_{33} + (l_1^\alpha l_2^1 + l_2^\alpha l_1^1)([000]_{33}[200]_{12} - [100]_{23}[100]_{31})^*$
$-R_{22}^{\alpha\alpha}$	$l_1^\alpha l_1^1([200]_{22}[000]_{33} + [100]_{23}^{2}) - (l_2^\alpha l_3^1 + l_3^\alpha l_2^1)[000]_{11}[200]_{23}^{\Delta}$ $+ l_2^\alpha l_2^1([200]_{11}[000]_{33} + [100]_{31}^{2*}) - (l_3^\alpha l_1^1 + l_1^\alpha l_3^1)[000]_{11}[200]_{31}^{\Delta*}$ $+ l_3^\alpha l_3^1([200]_{33}[000]_{11} + [100]_{23}^{2} + [100]_{31}^{2*})[000]_{11}/[000]_{33} - (l_1^\alpha l_2^1 + l_2^\alpha l_1^1)([000]_{33}[200]_{12} - [100]_{23}[100]_{31})^*$
$-R_{33}^{\alpha\alpha}$	$(l_1^\alpha l_1^1 + l_2^\alpha l_2^1)([002]_{11}[000]_{33} + [001]_{12}^{2}[000]_{33}/[000]_{11}) + l_3^\alpha l_3^1[002]_{33}[000]_{11}^{2}/[000]_{33}$
$-(R_{23}^{\alpha\alpha} + R_{32}^{\alpha\alpha})$	$(l_1^\alpha l_1^1 - l_2^\alpha l_2^1)[000]_{33}[011]_{11}^{\Delta} + (l_2^\alpha l_3^1 + l_3^\alpha l_2^1)([011]_{23}[000]_{11} - [100]_{23}[001]_{12})$ $+ (l_3^\alpha l_1^1 + l_1^\alpha l_3^1)([011]_{31}[000]_{11} + [100]_{31}[001]_{12})^* - (l_1^\alpha l_2^1 + l_2^\alpha l_1^1)[000]_{33}[101]_{11}^{\Delta*}$
$-(R_{31}^{\alpha\alpha} + R_{13}^{\alpha\alpha})$	$(l_1^\alpha l_1^1 - l_2^\alpha l_2^1)[000]_{33}[101]_{11}^{\Delta*} - (l_2^\alpha l_3^1 + l_3^\alpha l_2^1)([011]_{31}[000]_{11} + [100]_{31}[001]_{12})^*$ $+ (l_3^\alpha l_1^1 + l_1^\alpha l_3^1)([011]_{23}[000]_{11} - [100]_{23}[001]_{12}) + (l_1^\alpha l_2^1 + l_2^\alpha l_1^1)[000]_{33}[011]_{11}^{\Delta}$
$-(R_{12}^{\alpha\alpha} + R_{21}^{\alpha\alpha})$	$l_1^\alpha l_1^1([000]_{33}[110]_{11}^{\dagger} + 2[100]_{23}[100]_{31})^* + (l_1^\alpha l_2^1 + l_2^\alpha l_1^1)([000]_{33}[110]_{12}^{\ddagger} - [100]_{23}^{2} + [100]_{31}^{2*})$ $- l_2^\alpha l_2^1([000]_{33}[110]_{11} + 2[100]_{23}[100]_{31})^* - 2(l_2^\alpha l_3^1 + l_3^\alpha l_2^1)[000]_{11}[200]_{31}^{\Delta*} + 2(l_3^\alpha l_1^1 + l_1^\alpha l_3^1)[000]_{11}[200]_{23}^{\Delta}$

* means zero for D_{3i}, D_{4h}, D_{6h}.

Δ means zero for C_{4h}, C_{6h}, D_{4h}, D_{6h}.

$\dagger$ means $[110]_{11} = -2[200]_{12}$

$\ddagger$ means $[110]_{12} = [200]_{11} - [200]_{22}$

} for C_{3i}, C_{6h}, D_{3i}, D_{6h}.

TABLE XVII

THE EXPLICIT FORM OF R_2 FOR T_h AND O_h

$-R_{11}^{\alpha 1}$	$\ell_1^1\ell_1^\alpha\,[200]_{11}\,[000]_{11} + \ell_2^1\ell_2^\alpha\,([200]_{22}\,[000]_{11} + [100]_{23}^2) + \ell_3^1\ell_3^\alpha\,([200]_{33}^*\,[000]_{11} + [100]_{23}^2)$
$-R_{22}^{\alpha 1}$	$\ell_1^1\ell_1^\alpha\,([200]_{33}^*\,[000]_{11} + [100]_{23}^2) + \ell_2^1\ell_2^\alpha\,[200]_{11}\,[000]_{11} + \ell_3^1\ell_3^\alpha\,([200]_{22}\,[000]_{11} + [100]_{23}^2)$
$-R_{33}^{\alpha 1}$	$\ell_1^1\ell_1^\alpha\,([200]_{22}\,[000]_{11} + [100]_{23}^2) + \ell_2^1\ell_2^\alpha\,([200]_{33}^*\,[000]_{11} + [100]_{23}^2) + \ell_3^1\ell_3^\alpha\,[200]_{11}\,[000]_{11}$
$-(R_{23}^{\alpha 1}+R_{32}^{\alpha 1})$	$(\ell_2^1\ell_3^\alpha + \ell_3^1\ell_2^\alpha)([011]_{23}\,[000]_{11} - [100]_{23}^2)$
$-(R_{31}^{\alpha 1}+R_{13}^{\alpha 1})$	$(\ell_3^1\ell_1^\alpha + \ell_1^\alpha\ell_3^1)([011]_{23}\,[000]_{11} - [100]_{23}^2)$
$-(R_{12}^{\alpha 1}+R_{21}^{\alpha 1})$	$(\ell_1^1\ell_2^\alpha + \ell_2^\alpha\ell_1^1)([011]_{23}\,[000]_{11} - [100]_{23}^2)$

For O_h * means $[200]_{33} = [200]_{22}$

For O_h Table XVII can be reduced to the following simplified form:

$$-R_2 = ([200]_{22}\,[000]_{11} + [100]_{23}^2)\,\delta^{\alpha 1} - ([100]_{23}^2 - [011]_{23}\,[000]_{11})\left(\sum_{i=1,2,3}\gamma_i\ell_i^\alpha\right)\left(\sum_{j=1,2,3}\gamma_j\ell_j^1\right)$$
$$+ [000]_{11}\,([200]_{11} - [200]_{22} - [011]_{23})\sum_{i=1,2,3}\gamma_i^2\ell_i^\alpha\ell_i^1$$

with $\delta^{\alpha 1} = \begin{cases} 1 \text{ if } \alpha = 1 \\ 0 \text{ otherwise} \end{cases}$.

When $\alpha = 1$, this simplified form becomes identical, except a multiplying constant, to equation (5) given by Pearson and Suhl (Ref. 11); see Table XVIII.

thermal galvanomagnetic effects is attempted in this chapter. The results include as special cases the work of Voigt and of Juretschke concerning the tables of brackets, the work of Seitz, Pearson and Suhl, and Goldberg and Davis concerning the formulas for cubic crystals, and some of the work of Kohler, insofar as it is concordant with Onsager's relations.

For D_{3i} and $m \leq 4$, Juretschke's[15] results agree completely with ours presented in Table X, except for a different notation. In order to facilitate the comparison of our bracket notation with the notations used by Seitz and by Pearson and Suhl for the case O_h, Table XVIII has been prepared.

TABLE XVIII

NOTATIONS OF VARIOUS AUTHORS

Seitz's Notation	Pearson and Suhl's Notation	Bracket Notation
$\sigma_o = 1/\rho_o$		$[000]_{11}$
α		$[100]_{23} = [001]_{12}$
β		$[200]_{22} = [002]_{11}$
γ		$[011]_{23} = [110]_{12}$
$\beta + \gamma + \sigma$		$[200]_{11} = [002]_{33}$
	a	$[100]_{23}/[000]_{11}$
	b	$([200]_{22}[000]_{11}+[100]^2_{23})/[000]^2_{11}$
	c	$-([100]^2_{23}-[011]_{23}[000]_{11})/[000]^2_{11}$
	d	$([200]_{11}-[200]_{22}-[011]_{23})/[000]_{11}$

Many investigators limit themselves to cases where the magnetic field is either parallel or normal to the current, or in the plane of the current and the Hall probes. Such limitations seem unnecessary with the broadened definitions of the galvanomagnetic effects, which permit the magnetic field to be arbitrarily oriented (Seitz did this for the magneto resistance of cubic crystals

including terms up to B^2). Therefore all the galvanomagnetic effects bearing various conventional names, such as the transverse and longitudinal magneto resistance, the Hall effect, the "planar Hall field," and the Corbino effect, are included as special cases. They can all be analyzed in terms of an ascending power series of the magnetic field; the only known exception is the oscillatory behavior at very low temperatures. The Corbino effect, about which, to the best of our knowledge no work has been done on single crystals, will be dealt with in Chapter II.

We have also brought to light certain properties regarding the parity of the galvanomagnetic effects, about which a certain lack of consistency is to be found in the literature. In particular, the magneto resistance is necessarily an even function of the magnetic field, while, contrary to the odd-Hall-effect convention, it was proved here that the Hall effect is in general neither an odd nor an even function of B, but can be purely odd or purely even or zero when proper conditions are satisfied. These contentions are firmly supported by experiments, for example by Logan and Marcus, and by Goldberg and Davis.

In testing a theory of the galvanomagnetic effects, one only needs to compare the theoretical and experimental values of the brackets. But this procedure has not been followed by all investigators. For example, as implied by Seitz's work, for $n \leq 2$ Table VII for O_h gives five independent brackets, i.e.,

$$[000]_{11},\ [001]_{12},\ [002]_{11},\ [110]_{12},\ [002]_{33}\ .$$

All empirical data prior to 1951 are incomplete. In 1951 Pearson and Suhl measured the first complete set of experimental brackets on germanium for terms up to B^2. Likewise, for $n \leq 2$, Tables VIII to X for D_{3i} give 12 independent brackets:

$$[000]_{11},\ [000]_{33};\ [100]_{23},\ [001]_{12},$$
$$[200]_{11},\ [200]_{22},\ [200]_{33},\ [002]_{11},$$
$$[200]_{23},\ [002]_{33}\ \ [011]_{11},\ [011]_{23},\ .$$

Experimentally, all data prior to 1956 are incomplete for materials of this group. Complete data were recently published by Okada (1956) and in part by Abeles and Meiboom (1954) for bismuth. Abeles and Meiboom, by taking $[ooo]_{11}$ and $[oo1]_{12}$ as given, made a complete set of quantitative calculations, against which the measurements of Pearson and Suhl were compared. Unfortunately, the comparisons were not made completely in terms of the brackets. In trying to bring this into order we analyzed the experimental data given by Tables I and II of Pearson and Suhl. We found that the data are not self-consistent. This might be due to experimental errors, or more likely to the uncorrected high-power terms and misalignment of the claimed geometry. The most serious inconsistency appeared in Table II of Pearson and Suhl, in which the values of b, c, and d, for α, β, and δ, for p-type Ge at 77°K give a negative sum. But according to their own Table I, the sum is positive, and it will be shown in general in Chapter III that the sum of b, c, and d, for the bracket $-[oo2]_{33}$, is always nonnegative.

CHAPTER II

PHENOMENOLOGICAL THEORY: THE CORBINO EFFECT*

1. GALVANOMAGNETIC EFFECTS AS BOUNDARY VALUE PROBLEMS

In the previous chapter the phenomenological theory of the isothermal galvanomagnetic effects for single crystals was developed quite generally insofar as Ohm's law is valid,** i.e.,

$$\underline{F}^{\alpha} = \rho^{\alpha\beta}\,\underline{J}^{\beta} \qquad (\alpha,\beta = 1,2,3) \quad . \tag{2.1}$$

In order to obtain $\rho^{\alpha\beta}$ the general practice is to employ samples of convenient geometry such that the solutions of the equations

$$\text{Curl } \underline{F}\ (\underline{B}) = 0 \tag{2.2}$$

$$\text{Div } \underline{J}\ (\underline{B}) = 0 \tag{2.3}$$

satisfy certain boundary conditions. Note that the vectors $\underline{J}$ and $\underline{F}$ are now functions of the constant external magnetic field $\underline{B}$.

In Chapter I, we used the boundary conditions

$$J^2 = J^3 = 0 \quad . \tag{2.4}$$

The physical realization of (4) limits us to samples of special geometry. Boundary conditions other than (4) have also been used, related to the various sample geometries employed (described in Table XIX).

Volterra,[21] in 1915, made a rather extensive study of the galvanomagnetic boundary value problems for isotropic samples. For single crystals the problem in general becomes much more complicated. Since the final aim of studying the galvanomagnetic effects is to obtain the material constants, or brackets, it does not seem efficient to adopt an awkward geometry involving in-

*The material presented in this chapter can be regarded as an immediate extension of the late Prof. W. W. Sleator's work (reference 48). Prof. Sleator's paper was brought to my attention by Prof. O. Laporte just before the final draft was put to print.

**This excludes the problems of "hot electron," superconductivity, oscillatory diamagnetism, and of the galvanomagnetic effects pertaining to ferromagnetic substances.

TABLE XIX

VARIOUS GEOMETRIES EMPLOYED*

Geometry	Author
Rectangular plate	Hall, 1879
Split rectangular plate	Righi, 1883
Cruciform	Righi, 1883
Semicircular plate	Ettingshausen and Nernst, 1886
Circular plate with a radial saw cut	Ettingshausen and Nernst, 1886
Circular plate with circular electrodes	Corbino, 1911
Circular plate with point electrodes	Alimenti 1915; Bordonavo, 1915
Square plate with two perpendicular sets of arms	Heaps, 1918
Circular cylinder with planar radial field	Poppelbaum, 1953

*See references 21 to 23.

inconvenient boundary conditions. Nevertheless, a simple case will be investigated in this chapter for historical and practical reasons. The case involves a circular disk bounded by two concentric circular electrodes. Such an arrangement is known as a Corbino disk. It was employed by Corbino for the first time in 1911.[22] In the literature,[23] however, the 'Corbino effect' has been used quite loosely to include galvanomagnetic measurements pertaining to cases where a current (rather than a voltage) transverse to the magnetic field is measured irrespective of the geometry of the sample*

In the next section it will be shown that a simple relation exists between the Corbino effect and the other galvanomagnetic effects, for isotropic samples or properly cut single-crystal samples with a suitably oriented magnetic field.

*It is clear that the earlier controversy (see reference 1, p. 127) regarding the relative significance of the Hall and Corbino effects becomes meaningless. They, as well as the magneto resistance effect, are special cases of the general galvanomagnetic effect.

2. CORBINO EFFECT FOR SINGLE CRYSTALS

Consider a circular disk cut from a single crystal such that the normal is along a three-, four-, or six-fold axis of rotation. Suppose a constant radial current is maintained at constant temperature through two concentric circular electrodes by means of an electric field. When a constant magnetic field is applied normally to the disk, either of the following two equations can be used as boundary conditions,

$$F^{\phi} = J^{z} = 0 \tag{2.5}$$

$$F^{\phi} = F^{z} = 0 , \tag{2.6}$$

with ϕ, r, z denoting a cylindrical laboratory-coordinate system such that the z-axis is along the 3-axis and along the normal. Either (2.5) or (2.6) lead to

$$J^{z} = F^{z} = 0 \tag{2.7}$$

$$J^{r} = \frac{F^{r}\rho_{11}}{\rho_{11}^{2} + \rho_{12}^{2}} = F^{r}\,\sigma_{11} \tag{2.8}$$

$$J^{\phi} = \frac{F^{r}\rho_{12}}{\rho_{11}^{2} + \rho_{12}^{2}} = -F^{r}\,\sigma_{12} , \tag{2.9}$$

or in terms of the brackets directly:

$$J^{r} = F^{r} \sum_{\eta=0} B^{2\eta}\,[oo2\eta]_{11} \tag{2.10}$$

$$J^{\phi} = -F^{r} \sum_{\eta=0} B^{2\eta+1}\,[oo(2\eta+1)]_{12} \tag{2.11}$$

Note that the symmetry of the problem permits one to take any two perpendicular axes in the plane of the disk as the 1- and 2-axes; thus the first halves of equations (2.8) and (2.9) reveal general relations between the Corbino measurements J^{r}, J^{ϕ}, F^{r}, the magneto resistance ρ_{11}, and the Hall effect ρ_{12}. From these

relations or equations (2.10) and (2.11) one can immediately draw the following conclusions for a Corbino disk:

(1) The radial current J^r is always an even function of the normal magnetic field B.

(2) The circular current J^{ϕ} (which is usually known as the "Corbino current") is always an odd function of the magnetic field B.

These conclusions are also valid for isotropic samples. Experimental confirmation can be found in references 21 to 23.

The simplicity of equations (2.10) and (2.11) is noteworthy. They afford direct measurements of the brackets, which can then be used to test the microscopic theories much more readily than the usual magneto resistance and the Hall measurements. However, they involve only a limited number of brackets, and they cannot be used to determine a complete set of brackets.

One might think that another set of boundary conditions such as

$$F^z = J^z = 0 \qquad (2.12)$$

would be as effective as (2.5) or (2.6). But this is not the case, because of the way equations (2.1) are coupled.

CHAPTER III

MICROSCOPIC THEORY

1. INTRODUCTION

In order to survey the various parts of this dissertation, the following block diagram (Fig. 3) was prepared.

In the previous two chapters we studied the phenomenological part of the diagram; in this last chapter we shall study the microscopic part.

In essence, the main purpose of Chapter III is to give a general definition of the brackets according to the quantum theory of solids. This will be done in two ways: (1) according to the usual single-band model, (2) according to the multiband model.

a. Early Microscopic Theories of the Galvanomagnetic Effects.—[1,19] Five years after the discovery of the Hall effect, Lord Kelvin in 1884 praised Hall's work as the 'most important' since the days of Faraday. Many physicists, including such leading figures as Lord Kelvin, Stokes, Boltzmann, Lorentz, and J. J. Thompson, tried to give a microscopic interpretation to both the Hall effect and the magneto resistance.[1] It was in their efforts that the present theory of solids had its genesis.

The first successful theory was given by Drude in 1900; he assumed that a metal consists of a gas of electrons which possess an average velocity and pursue random motions through the metal. The metal ions, owing to their large mass, can be considered immobile. Drude's theory has an attractive simplicity and is able to predict the Wiedmann-Franz law, but his picture is known to give incorrect numerical results.

In 1904 Lorentz reinvestigated the problem by using the Maxwell-Boltzmann statistics and also investigated the dynamics of the collision process more carefully. It was found that Lorentz's theory made no improvement in the final results and in some cases was even worse than Drude's theory.

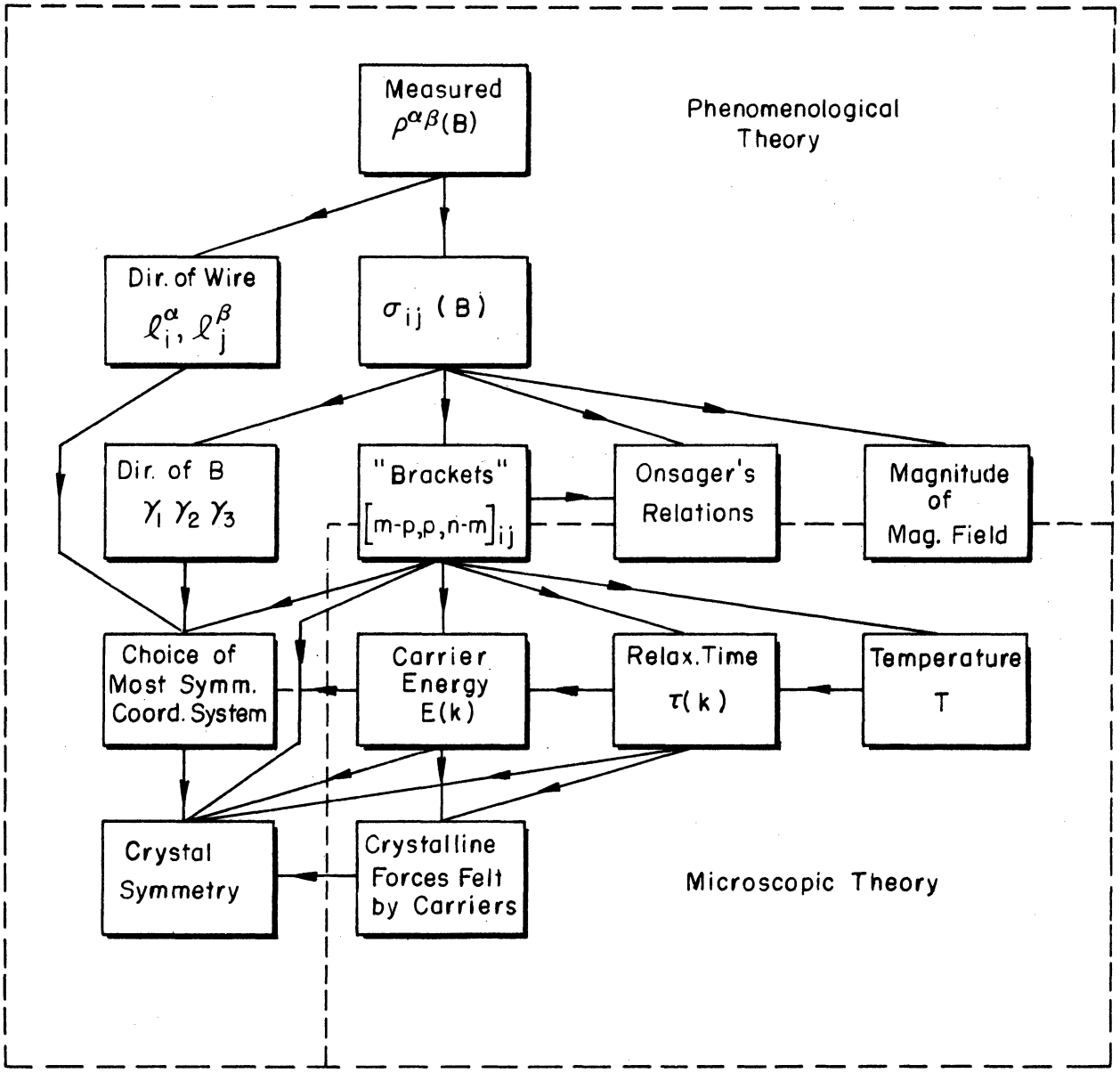


Figure 3. Block diagram of logical relations between various factors determining galvanomagnetic effects. Arrows show dependence of one block on another.

A great improvement in the situation was brought about in 1928 by Sommerfeld who introduced the Fermi statistics. He imagined a metal consisting of a number of electrons, without interaction, moving in a region of constant negative potential energy. The motion of these electrons in the metal is determined by the Schroedinger equation. In spite of its successes, Sommerfeld's theory fails to account for many facts such as the difference of metals and insulators, the two signs in the observed Hall effect, the cohesion energy of metals, and the fact that the calculated values of the magneto resistance are about 10^4 times smaller than the observed ones.

These and many other things can be nicely rectified, at least qualitatively, by the band theory of metals, which is an approximation based on the Schroedinger equation and the periodicity of the crystal structure. The band theory was essentially developed by Bloch. Jones and Zener (1934) were the first to obtain an order-of-magnitude agreement between their calculated values and the experimental data for lithium.

Thus during the years of 1928-1934, in the hands of Sommerfeld, Bloch, Peierls, Jones and Zener, Wilson, and others, the electronic theory of conduction phenomena in solids was established in its present form. Since then the theory has been advanced from the qualitative stage of the 1930's to the quantitative stage of today through the efforts of many investigators. The vast development made in the field of semiconductors after World War II has contributed greatly. However, nothing <u>fundamentally</u> new has been added since 1934.

The inherent difficulties of the band theory are: the justification of the one-electron approximation upon which the band theory is built; the assignment of a distribution function for the carriers in solids; the existence of a relaxation time; and the validity of a simple form of the Boltzmann equation of transport. Detailed accounts of these developments since the days of Drude and

difficulties can be found in standard text books,[19,24] and in the literature.*

b. Survey of the Restrictions of Existing Theories.—All the existing microscopic theories[19,28] can be conveniently classified into two categories: the single-band model and the multiband model.** All models make the following fundamental assumptions.

(A) Ohm's law is valid, i.e.,

$$J_i = \sigma_{ij}(\underline{B})\, F_j \qquad (i,j = 1,2,3) \ , \tag{3.1}$$

where summation over the repeated indices is implied. For the multiband model with q noninteracting bands the conductivity tensor components $\sigma_{ij}(\underline{B})$ are composed additively of the corresponding components of all bands:

$$\sigma_{ij}(\underline{B}) = \sum_{\lambda=1}^{q} \sigma_{ij}^{(\lambda)}(\underline{B}) \ . \tag{3.1a}$$

(B) According to the Bloch scheme, the charge carriers within each of the q noninteracting energy bands are associated with a group velocity

$$\underline{v}^{(\lambda)} = \nabla_{\underline{k}} E^{(\lambda)}/\hbar \ , \qquad \lambda = 1,2,\ldots,q \ , \tag{3.2}$$

where $\underline{k}$ is the quasi-momentum and $\hbar$ is Dirac's constant. When $\lambda = 1$, the superscript will be omitted for the single-band model here and in all that follows.

(C) The number of electrons or holes per unit volume in the λ-th band whose wave vector $\underline{k}$ lies within the range $\underline{k}$ to $\underline{k} + d\underline{k}$ is

$$\frac{1}{4\pi^3} f^{(\lambda)}(\underline{k},t)\, d\underline{k} \ . \tag{3.3}$$

The distribution function $f^{(\lambda)}(\underline{k},t)$ becomes $f_o^{(\lambda)}(E)$ when $\underline{B} = \underline{F} = 0$. The latter function is defined by the Fermi-Dirac distribution and the distribution of energy levels.

*For example, see references 25, 26, 27, and 28.

**The two-band model and the many-valley model encountered in the literature are special cases of the multiband model to be worked out presently. The same is true for the single-band model.

(D) In the presence of an electric field $\underline{F}$ and a magnetic field $\underline{B}$, $f^{(\lambda)}$ obeys the Boltzmann transport equation:

$$-\frac{e}{\hbar}\left[\underline{F}+\frac{1}{c}\underline{V}^{(\lambda)}\times\underline{B}\right]\cdot\nabla_{\underline{k}}f^{(\lambda)}(\underline{k},t)+\left[f^{(\lambda)}(\underline{k},t)-f_o{}^{(\lambda)}(E)\right]/\tau^{(\lambda)}(\underline{k})=0, \quad (3.4)$$

-e and c being the electron charge and the speed of light. $\tau^{(\lambda)}(\underline{k})$ is the relaxation time pertaining to the λ-th band whose existence is assumed. The noninteraction of the bands is expressed by the fact that no coupling exists between the equations for different values of λ (different bands).*

These assumptions are used in all theories of electron conduction in solids. For their validity, see references 19, and 24 to 28.

The single band model ($\lambda = q = 1$) was used by Jones and Zener in 1934, and improved by Davis in 1939 and by Seitz in 1950. It can be expected to be a reasonable approximation only for alkaline metals and for low concentration n-type or p-type semiconductors. Even for p-type Ge and Si its validity is limited because of the degeneracy of the valence bands. Davis' and Seitz's treatments of the single-band model are restricted as follows.

Restriction 1: Validity is limited to special orientations of the magnetic field and current relative to each other and to the crystallographic axes (Davis).

Restriction 2: Validity is limited to low values of the magnetic field (Seitz).

Restriction 3: Validity is limited to special classes of crystal symmetry (Seitz and Davis).

Although the idea can be traced back to Riecke[31] in 1898, the two-band

*To be more specific, let us consider the case of a rather empty s-band that overlaps nearly full p-band having slow holes and fast holes. By assumption, the electrons in the s-band are the first kind of carriers, the slow and the fast holes in the p-band are the second and the third kinds of carriers respectively; these carriers are moving in the first, the second, and third bands respectively independent of each other's motion. Furthermore no transition of electrons to the p-band, and no conversion from the slow holes to the fast ones will take place, and vice versa.

model (q = 2), was first introduced by Jones[32] in 1936. Later, developments by Sondheimer and Wilson,[33] by Chambers,[34] and many others[35] followed. These studies are restricted as follows.

Restriction 4: The energy is no more general than a quadratic function in reciprocal space.

Restriction 5: The parameters used are (magnetic) field dependent, rendering it impossible to study the effect of crystal symmetry in general.

Another drawback of the two-band model in the hands of Wilson et al. is that, because of the restrictions used, it always gives zero longitudinal magneto resistance contrary to all known experiments.

The "many-valley" model is equivalent to a multiband model with ellipsoidal energy surfaces for each one of the noninteracting bands, arranged to conform with the crystal symmetry of the substance.* The model was used by Blochinzev and Nordheim[36] in 1933 and was recently elaborated by many authors.[37-40]

2. THE SINGLE-BAND MODEL

a. The Definition of the Brackets.—If we write

$$f(k,t) = f_0(E) - \Phi \frac{\partial f_0}{\partial E}$$

and substitute into (3.4), omitting the superscript $\lambda = 1$ and neglecting terms in F^2 or higher; we have

$$\frac{1}{\tau(\underline{k})} \Phi + \frac{e}{\hbar} \underline{F} \cdot \nabla_k \underline{E} - \frac{e}{\hbar^2 c} \underline{B} \cdot \underline{\Omega} \Phi = 0 , \tag{3.5}$$

where $\underline{\Omega}$ is an operator defined by

$$\underline{\Omega} \equiv - \nabla_k E \times \nabla_k = (\Omega_1, \Omega_2, \Omega_3) . \tag{3.6}$$

The solution Φ from (3.5) is well known.** It can be expressed in an ascending

*If this model is interpreted as containing many valleys in a single band, one must justify the assumption that only intravalley transitions can take place and that overlapping ellipsoids contribute independently and additively.

**See reference 19, p. 225, or reference 29. Note that a sign difference in the odd powers of Φ is introduced according to the definition (16). (Equation numbers without a prefixing digit refer to equations of Chapter I.)

power series of $\underline{B}$, as follows:

$$\Phi = -\sum_{n=0}^{\infty}\left(\frac{e}{\hbar^2 c}\,\underline{B}\cdot\tau\underline{\Omega}\right)^n\left(\frac{e}{\hbar}\,\tau\nabla_k E\cdot\underline{F}\right). \tag{3.7}$$

Consequently, the magneto-electric current density $\underline{J}$ can be written as:

$$\underline{J} = (-e/4\pi^3)\iiint \underline{V}\, f(\underline{k},t)\,d\underline{k}$$

$$= (e/4\pi^3\hbar)\iiint \nabla_k E\;\Phi\,\frac{\partial f_o}{\partial E}\,d\underline{k}\ , \tag{3.8}$$

or in component form,

$$J_i = \sum_{n=0}^{\infty} B^n \sum_{m=0}^{n}\sum_{p=0}^{m}[m-p,p,n-m]_{ij}\;\gamma_1^{\,m-p}\,\gamma_2^{\,p}\,\gamma_3^{\,n-m}\,F_j\ , \tag{3.9}$$

where $i,j = 1,2,3$, and

$$[m-p,p,n-m]_{ij} = ab^n\iiint\left(-\frac{\partial f_o}{\partial E}\right)\frac{\partial E}{\partial k_i}\,P\left\{(\tau\Omega_1)^{m-p}(\tau\Omega_2)^{p}(\tau\Omega_3)^{n-m}\right\}\left(\tau\frac{\partial E}{\partial k_j}\right)d\underline{k}\ , \tag{3.10}$$

with

$$a = e^2/4\pi^3\hbar^2\ ; \qquad b = e/\hbar^2 c\ . \tag{3.11}$$

$P\{\}$ means the sum of all permutations of $(m-p)$ operators $\tau\Omega_1$, p operators $\tau\Omega_2$, and $(n-m)$ operators $\tau\Omega_3$, in different order. This sum consists of $n!/(m-p)!p!(n-m)!$ terms. Φ has the dimension of energy, $\Omega/\hbar^2$ that of mass^{-1}, and $b\tau\Omega$ that of gauss^{-1}; hence a bracket of order n has the dimension of Ohm^{-1}cm^{-1} gauss^{-n}. By comparing equations (3.9) and (3.1) with (10a) it is obvious that the brackets defined by (3.10) are identical to those introduced in the phenomenological theory.

It is interesting to observe that the assumptions II(Onsager's relation) and III [power series expansion of $\sigma_{ij}(\underline{B})$] of the phenomenological theory come out automatically as consequences of equations (3.5) to (3.9). Assumption II is a consequence of the integration by parts of (3.10), leading to (11), while assumption III is a consequence of the solution of the Boltzmann equation. This bears

out the fact that the microscopic model is consistent with the well established thermodynamical relations (7). Note that (3.10) is obtained without any restriction on the form of $\tau(\underline{k})$ and $E(\underline{k})$, except that $\tau(\underline{k})$ exists and that $\tau(\underline{k})$ and $E(\underline{k})$ must have the same symmetry as the crystal plus an inversion center. The addition of the inversion center, which is a necessary consequence of the principle of time reversal, was arrived at in the phenomenological theory from the fact that the vector $\underline{B}$ is an axial vector (antisymmetric second-rank tensor). Thus every bracket behaves like a tensor of even rank, in the sense that they transform identically into themselves under the operation of an inversion.

Since all isothermal galvanomagnetic effects can be expressed in terms of the brackets according to (26) for arbitrary orientations of $\underline{J}$, $\underline{B}$, and the crystal axes, equations (26) and (3.10) form the basis for a general microscopic theory of the isothermal galvanomagnetic effects according to the single-band model, without any of the restrictions mentioned in the previous section. Therefore, this theory contains all previous works as special cases: For crystal classes D_{2h}, D_{4h}, D_{6h}, T_h, O_h, equations (27), (32), and (28) become equations (8), (9), and (7) of Davis, respectively, except that all higher power terms are written out explicitly, without introducing anything new in principle. If one considers terms up to B^2 only, equations (34) and (35) and Table XVII for O_h give equation (4) of Pearson and Suhl, which was essentially obtained by Seitz.

Further development of the theory starting from this point depends on what information is available about $\tau(k)$ and $E(k)$. Unfortunately, at the present, no reliable information about these quantities is available. A summary of various representative, simple assumptions about $\tau(k)$ and $E(k)$ is given in Table XX. In an effort to obtain further insight into the theory the following three mathematical lemmas are useful.

TABLE XX

TYPICAL ASSUMPTIONS FOR $\tau(\underline{k})$ and $E(\underline{k})$

$\tau(\underline{k})$	$E(\underline{k})$	Authors	Applications
Constant		Kohler[41]	Kohler Diagram
$\tau(E)$	$E = ak^2 + \epsilon$	Jones and Zener[29]	Li
$\tau(E)$	$E = \sum a_i k_i^2$	Jones[32]	Bi
$\tau(E)$	E even in k_1, k_2, k_3	Davis[30]	--
$\tau = a_1k^2 + a_2y_4$*	$E = b_1k^2 + b_2y_4$*		
$\tau = a_1k^2 + a_2y_4$*	$E = ak^2$	Seitz[14]	Cubic Crystals
	$E = \sum_{ij} \alpha_{ij}k_ik_j$	Shoenberg[42]	Bi
$\tau = \tau(E)$	warped surface	Lax and Mavroides[43]	Ge and Si

*y_4 is the cubic harmonics of 4th order.

b. Three Mathematical Lemmas.—

Lemma I. A Variation of the Schwartz Inequality.

Let $\underline{f}$, $\underline{g}$, $\underline{F}$, $\underline{G}$ be four vector functions of $\underline{k}$, then

(1) $$I \equiv \int \underline{f} \cdot \underline{f}d\underline{k} \int \underline{g} \cdot \underline{g}d\underline{k} + \int \underline{F} \cdot \underline{F}d\underline{k} \int \underline{G} \cdot \underline{G}d\underline{k} - 2\int \underline{f} \cdot \underline{G}d\underline{k} \int \underline{F} \cdot \underline{g}d\underline{k} \geq 0, \tag{3.12}$$

where each integtal sign represents a three-fold integration and

$$d\underline{k} \equiv dk_1\, dk_2\, dk_3 .$$

(2) The equality of equation (3.12) holds if and only if

$$\begin{aligned} \underline{f} &= c\underline{G} \\ \underline{F} &= c\underline{g} , \end{aligned} \tag{3.13}$$

where c is an arbitrary constant.

If the four vector functions span an n-dimensional space, then equations (3.12) and (3.13) become respectively

$$\int\left(\sum_{i=1}^{n} f_i^2\right) d\underline{k} \int \left(\sum_{i=1}^{n} g_i^2\right) d\underline{k} + \int\left(\sum_{i=1}^{n} F_i^2\right) d\underline{k} \int\left(\sum_{i=1}^{n} G_i^2\right) d\underline{k} -$$

$$- 2\int\left(\sum_{i=1}^{n} f_i\, G_i\right) d\underline{k} \int\left(\sum_{i=1}^{n} F_i\, g_i\right) d\underline{k} \geq 0 \qquad (3.14)$$

and

$$\begin{aligned} f_i &= c\, G_i \\ F_i &= c\, g_i \end{aligned} \qquad i = 1,2,3\ldots,n\ . \qquad (3.15)$$

Proof Schwartz's inequality is:

$$\int \underline{f} \cdot \underline{f}\, d\underline{k} \int g \cdot g\, d\underline{k} - \left(\int f \cdot g\, d\underline{k}\right)^2 \geq 0\ . \qquad (3.16)$$

The equality of equation (3.16) holds if and only if

$$\underline{f} = c\, \underline{g}\ . \qquad (3.17)$$

One can now rewrite the left hand side of equation (3.12) as

$$I \equiv \left\{\left(\int \underline{f} \cdot \underline{f}\, d\underline{k} \int \underline{g} \cdot \underline{g}\, d\underline{k}\right)^{1/2} - \left(\int \underline{F} \cdot \underline{F}\, d\underline{k} \int \underline{G} \cdot \underline{G}\, d\underline{k}\right)^{1/2}\right\}^2 +$$

$$+ 2\left\{\left[\left(\int \underline{f} \cdot \underline{f}\, d\underline{k} \int \underline{g} \cdot \underline{g}\, d\underline{k}\right)\left(\int \underline{F} \cdot \underline{F}\, d\underline{k} \int \underline{G} \cdot \underline{G}\, d\underline{k}\right)\right]^{1/2} - \int \underline{f} \cdot \underline{G}\, d\underline{k} \int \underline{F} \cdot \underline{g}\, d\underline{k}\right\}.$$

The first term of I is nonnegative. We can rewrite the second term as

$$2\left\{\left[\int \underline{f} \cdot \underline{G}\, d\underline{k} + \alpha_1\right]^{1/2}\left[\int \underline{F} \cdot \underline{g}\, d\underline{k} + \alpha_2\right]^{1/2} - \int \underline{f} \cdot \underline{G}\, d\underline{k} \int \underline{F} \cdot \underline{g}\, d\underline{k}\right\}$$

which is also nonnegative, because both α_1 and α_2 are nonnegative constants according to equation (3.16). This proves the first part of the lemma.

It is obvious that equation (3.13) is sufficient for the equality of (3.12) to hold. Now we prove the necessity: If the equality of equation (3.12) holds, then one has both terms of I vanishing separately. Since the second term of I vanishes, it is required by equation (3.17) that

$$f = C_1 G$$

$$F = C_2 g ,$$

where C_1, C_2 are two arbitrary constants. Since the first term of I vanishes, it is necessary to have

$$C_1 = C_2 = C .$$

q.e.d.

Lemma II. The necessary and sufficient condition that

$$U_{2\eta} = 0 \tag{3.18}$$

for all η, is

$$\Omega_3(\tau E_1) = cE_2 \tag{3.19}$$

where c is an arbitrary constant, $E_i = \partial E/\partial k_i$ $(i = 1,2,3)$, and

$$U_{2\eta} \equiv \sum_{q=0}^{\eta-1} \left\{ [2(\eta - q)]_{11} [2q]_{22} + [2q + 1]_{12} [2\eta - 2q - 1]_{12} \right\} \tag{3.20}$$

with the abbreviation $[\eta]_{ij} = [0,0,n]_{ij}$.

Proof Sufficiency.

If (3.19) holds, then

$$[2q + 2]_{11} = - c^2 [2q]_{22}$$

and

$$[2q + 1]_{12} = - c[2q]_{22} .$$

Substituting these into (3.20), it can be seen that the terms within $\{\ \}$ vanish for all values of η and q.

Necessity.

If (3.18) is true in general, then

$$U_2 = [2]_{11}[0]_{22} + [1]_{12}^2 = 0 . \tag{3.21}$$

If the explicit form of the brackets is written out according to equation (3.10), the last expression is a Schwartz equality. According to (3.17) the necessary and sufficient condition for this to vanish is that the square root of the in-

tegrands of $[2]_{11}$ and $[0]_{22}$ be linearly dependent. This is just equation (3.19).

q.e.d.

An interesting corollary of this lemma is as follows. If $U_{2\eta} = 0$ for any value of η, then it is zero for all values of η. The first step for proving the corollary is to rewrite equation (3.20) as:

$$U_{2\eta} = \sum_{\mu=0}^{\lambda-1}\left\{[4\lambda+2-2\mu]_{11}[2\mu]_{22} + [2\mu+2]_{11}[4\lambda-2\mu]_{22} + 2[2\mu+1]_{12}[4\lambda-2\mu+1]_{12}\right\} +$$

$$+ [2\lambda+2]_{11}[2\lambda]_{22} + [2\lambda+1]_{12}^{2} \quad \text{for} \quad \eta = 2\lambda + 1 \tag{3.22}$$

$$U_{2\eta} = \sum_{\mu=0}^{\lambda-1}\left\{[4\lambda-2\mu]_{11}[2\mu]_{22} + [2\mu+2]_{11}[4\lambda-2\mu-2]_{22} + 2[2\mu+1]_{12}[4\lambda-2\mu-1]_{12}\right\}$$

$$\text{for} \quad \eta = 2\lambda\,. \tag{3.23}$$

The last term of (3.22) is of the form of (3.16). The terms within curly brackets of (3.22) and (3.23) are of the form of (3.14). Thus by applying Lemma I the proof of the corollary follows immediately.

Lemma III. The necessary and sufficient condition that

$$[oo2\eta]_{33} = 0 \tag{3.24}$$

for all η is

$$\Omega_3(\tau E_3) = 0 \tag{3.25}$$

provided that τ is finite and positive, which is plausible on account of its physical meaning.

Proof Since the proof for sufficiency is obvious, one only needs to prove the the necessity. If equation (3.24) holds, then

$$[oo2]_{33} = ab^2 \iiint -\frac{\partial f_o}{\partial E} E_3\,(\Omega_3\tau)^2(\tau E_3)\,d\underline{k}$$

$$= +ab^2 \iiint \left(\frac{\partial f_o}{\partial E}\,\tau\right)\left\{\Omega_3(\tau E_3)\right\}^2 d\underline{k} = 0\,.$$

Since $-(\partial f_0/\partial E)\tau$ is nonnegative, (3.25) is true.

q.e.d.

A consequence of this lemma is that if $[oo2\eta]_{33} = 0$ then $[oo2\eta']_{33} = 0$ for all $\eta' \geq \eta$.

Note that similar lemmas also hold if both the inner and outer indices 1,2,3 in equations (18) through (25) are permuted cyclically. Therefore it is expedient to combine Lemmas II and III into one lemma as follows.

Lemma. The necessary and sufficient condition that

$$U_{2\eta}^{ij} = 0 \quad \text{and} \quad [2\eta]_{ii} = 0 \tag{3.26}$$

is

$$\Omega_i(\tau E_j) = E_k C_{ijk} \qquad i,j,k = 1,2,3\ , \tag{3.27}$$

where

$$C_{ijk} = \begin{cases} C_j & \text{if ijk is an even permutation of 123.} \\ -C_j' & \text{if ijk is an odd permutation of 123.} \\ 0 & \text{if any two indices of ijk are equal.} \end{cases} \tag{3.28}$$

C_j and C'_j are arbitrary constants. $U_{2\eta}^{ij}$ is defined such that equation (3.20) stands for $U_{2\eta}^{31}$. $[2\eta]_{ii}$ stands for a bracket in which all the inner indices are zero except the i-th one, i.e., $[2\eta,0,0]_{11}$, $[0,2\eta,0]_{22}$, and $[0,0,2\eta]_{33}$.

c. Special Conditions Satisfying Equation (3.27).—By inspection one can find various special conditions under which either equation (3.19) or equation (3.25) or both, i.e., (3.27), are satisfied. These conditions are listed in Table XXI. In using this table, one follows each row and reads: If I and II are given, then III is satisfied.

For example, the second row states: If $\tau(\underline{k})$ is a function of the energy $E(\underline{k})$, which is given by $E = \sum_{i=1,2,3} a_i k_i^2$, and if the temperature is at absolute zero, the equation (3.27) is satisfied [of course (3.25) is also satis-

fied]. However, if one reads the 4th or 5th row, then only equation (3.25) is satisfied.

TABLE XXI

SPECIAL CONDITIONS SATISFYING EQUATION (3.27)

<table>
<tr><th>I
Relaxation Time $\tau(k)$</th><th>II
Energy $E(k)$</th><th colspan="2">III
Equations Satisfied</th></tr>
<tr><td>$\tau(\underline{k})$ = constant</td><td rowspan="2">$E(\underline{k}) = \sum_{i=1,2,3} a_i k_i^2$</td><td rowspan="2">$\Omega_i(\tau E_j) = C_{ijk} E_k$</td><td rowspan="3">$\Omega_i(\tau E_i) = 0$</td></tr>
<tr><td>$\tau(\underline{k}) = \tau(E)$, T = 0°K</td></tr>
<tr><td>$\tau(\underline{k}) = Ck/\frac{dE}{dk}$</td><td>$E(\underline{k}) = E(k)$</td></tr>
<tr><td>$\tau(\underline{k})$ = constant</td><td>$E(\underline{k}) = E(\sum_n a_n k^n)$</td><td rowspan="2"></td><td rowspan="2"></td></tr>
<tr><td>$\tau(\underline{k}) = \tau(E)$</td><td>$E(\underline{k}) = E\left(\sum_n \sum_i a_{n,i} k_i^n\right)$</td></tr>
</table>

The verification of Table XXI is straightforward. As a help one might employ an operator $\underline{O}(O_1, O_2, O_3)$:

$$O_k = k_i \frac{\partial}{\partial k_j} - k_j \frac{\partial}{\partial k_i} \quad . \tag{3.29}$$

It is readily shown that

$$O_k k_i = - k_j \epsilon_{ijk} \, , \tag{3.30}$$

where ϵ_{ijk} is the Levi Civita symbol. Two illustrative examples will be proved as follows.

Example I. If $E = ak^2$, then the necessary and sufficient condition that

$\tau(\underline{k}) = f(|k|)$ or $f(E)$ satisfies equation (3.27) is that

$\tau(\underline{k})$ is a constant.

Proof Sufficiency. Obvious from Table XXI.

Necessity.

Since

$$E_j = 2ak_j$$

$$\Omega_i = 2aO_i ,$$

$$O_i f(|k|) = 0$$

and

$$O_i f(E) = 0 .$$

Thus

$$O_i(\tau E_j) = -2\tau(\underline{k})k_k .$$

Now if

$$\Omega_i(\tau E_j) = C_{ijk}E_k = C'_{ijk}k_k ,$$

then $\tau(k)$ must be a constant.

Example II. If $\tau(k)$ is a constant, then the necessary and sufficient condition that $E = \sum a_n k^n$ satisfies equation (3.27) is that $n = 2$ (or 0).

Proof Sufficiency. Obvious from Table XXI.

Necessity.

Since

$$E_i = E'k_i$$

$$\Omega_i E_j = (E'O_i)E'k_j = -(E')^2 k_k = \text{const } k_k$$

with

$$E' \equiv \sum n a_n k^{n-2} .$$

Therefore, $E' = \text{const.}$

This is so only if $n = 2$ (or 0).

d. Discussion.—A number of interesting consequences are deduced directly from the three mathematical lemmas. These will be stated and proved for the single-band model whereas their validity for the multiband model is clear. These consequences clarify some ideas previously held without a rigorously valid basis; e.g.,

a) The transverse magneto resistance change is always positive because of the Schwartz inequality.*

b) The longitudinal magneto resistance change is always smaller than the transverse one.**

(i) Zero magneto resistance and odd Hall effect. In Table XXI we have listed various simple conditions on $\tau(\underline{k})$ and $E(\underline{k})$ under which (3.27) holds. The physical significance of the mathematical lemma given by equations (3.26) and (3.27) is revealed by the vanishing of the even part of the galvanomagnetic tensor $\rho^{\alpha 1}(\underline{B})$. The results are stated in terms of three corollaries. Corresponding statements about the Corbino effect can be easily deduced from these corollaries and equations (2.11) and 2.12).

Corollary I. A Condition for Zero Magneto Resistance Change.

If: (1) for all crystal symmetries except S_2 and C_{2h}, the 3-axis is taken either along a rotational axis of three-, or four-, or six-fold symmetry, or along a two-fold axis if it is accompanied by another two-fold axis if it is accompanied by another two-fold axis normal to it;

(2) laboratory coordinates coincide with symmetry coordinates, i.e.,

$$\ell_1^1 = \ell_2^2 = \ell_3^3 = 1 ,$$

(3) the magnetic field is along k_3, i.e., $\gamma_3 = 1$; then the necessary and sufficient condition for vanishing isothermal magneto resistance change $\rho^{11}(\underline{B}) - \rho^{11}(B=0) = 0$, is equation (3.27).

Proof The proof is trivial if the mathematical Lemmas II and III are applied to equations (27) and (32) of Chapter I.

Corollary II. A Condition for Odd Hall Effect.

If: (1) for crystal symmetries T_h and O_h, the coordinates are taken

*See, for example, Davis (reference 30); Brooks (reference 28).

**See, for example, Wilson (reference 19), p. 227.

as described in Section 2.a of Chapter I;

(2) the magnetic field is along the k_i axis;

then the necessary and sufficient condition for $\rho^{\alpha\beta}(\underline{B})$ being an odd function of $\underline{B}$ is equation (3.27).

Proof It is sufficient to prove the corollary for the case i = 3; i.e. $\gamma_3 = 1$.

Sufficiency. Using the conditions (1) and (2) with i = 3, it follows that:

$$P_{2\eta}^{\alpha\beta} = \sum_{q=0}^{\eta}\left\{\ell_1^\alpha\ell_1^\beta[2q]_{22}[2(\eta-q)]_{33} + \ell_2^\alpha\ell_2^\beta[2q]_{11}[2(\eta-q)]_{33} + \ell_3^\alpha\ell_3^\beta[2(\eta-q)]_{11}[2q]_{22}\right\} +$$

$$+ \sum_{q=0}^{\eta-1} \ell_3^\alpha\ell_3^\beta[2q+1]_{12}[2\eta-2q-1]_{12}$$

$$= \ell_1^\alpha\ell_1^\beta\ [2\eta]_{22}[0]_{33} + \ell_2^\alpha\ell_2^\beta[2\eta]_{11}[0]_{33} + \ell_3^\alpha\ell_3^\beta[0]_{11}[2\eta]_{22} +$$

$$+ \sum_{q=0}^{\eta-1}\left(\ell_1^\alpha\ell_1^\beta[2q]_{22} + \ell_2^\alpha\ell_2^\beta[2q]_{11}\right)\ [2(\eta-q)]_{33} + U_{2\eta}^{31}\ , \qquad (3.31)$$

where $$U_{2\eta}^{31} = \sum_{q=0}^{\eta-1}\left([2(\eta-q)]_{11}[2q]_{22} + [2q+1]_{12}[2\eta-2q-1]_{12}\right)\ .$$

Because of condition (1) we have

$$[0]_{11} = [0]_{22} = [0]_{33}$$

and

$$[2\eta]_{22} = [2\eta]_{11}\ .$$

The first term on the right side of equation (3.31) is zero because of the orthogonality condition, and the last two terms are zero because of the lemma.

Necessity.

If $P_{2\eta}^{\alpha\beta} = 0$ for arbitrary ℓ_i^α and ℓ_j^β, then the second and third terms of (3.31) must vanish separately, that is $U_{2\eta}^{31} = 0$. Thus the proof is established by using the lemma.

Corollary III. A Condition for the Vanishing of Quadratic Terms.

If: (1) $E(\underline{k})$ and $\tau(\underline{k})$ are even functions in k_1, in k_2, and in k_3;

(2) only terms up to B^2 are considered;

then equation (3.27) is the necessary and sufficient condition for:

$$\rho^{\alpha 1}(\underline{B}) - \rho^{\alpha 1}(\underline{B}=0) = \begin{cases} 0 & \text{if } \alpha = 1 \\ \text{Odd function of } \underline{B}, & \text{if } \alpha \neq 1 \end{cases} .$$

Condition (1) limits the validity of the corollary to crystal symmetries of D_{2h}, D_{4h}, D_{6h}, T_h, and O_h. These are general enough to include all elements except Po, Hg, As, Sb, Bi, and the transition metals. Note that for T_h and O_h, $\rho^{\alpha B}(\underline{B}=0)$ is zero because of the orthogonality and symmetry conditions.

Proof It suffices to prove the corollary for D_{2h} only, because all the other symmetries contain D_{2h} as subgroup. When $\alpha \neq 1$ the conclusion deals with the Hall potential; when $\alpha = 1$ it deals with the magneto resistance change. The proof for both cases is established by showing $R_{ij}^{\alpha 1} = 0$ if and only if equation (3.27) holds. [See equation (38) of Chapter I for the definition of $R_{ij}^{\alpha 1}$.]

Sufficiency.

$$\underline{i = j} .$$

$R_{ii}^{\alpha 1}$ for D_{2h}, given by Table XV of Chapter I, consists of terms either of the form of (3.19) or (3.25). These are all zero, according to the lemma, if equation (3.27) is true for all values of i and j.

$$\underline{i \neq j} .$$

The proof will be established by showing that a typical coefficient, for example,

$$R_{23}^{\alpha 1} = [o11]_{23}[ooo]_{11} - [o10]_{31}[oo1]_{12}$$

is zero if equation (3.27) holds. Then the proofs for the coefficients of $R_{31}^{\alpha 1}$ and $R_{12}^{\alpha 1}$ follow identically if one permutes the indices 1,2,3 cyclically. Now if (27) holds one has

$$[011]_{23} = C_2C_1[000]_{22}$$
$$[010]_{31} = -C_1[000]_{11}$$
$$[001]_{12} = -C_2[000]_{22} \quad .$$

Consequently

$$[011]_{23}[000]_{11} - [010]_{31}[001]_{12} = 0 \quad .$$

Necessity.

If $R_2^{\alpha 1} = 0$ for arbitrary values of γ's, then $R_{ii}^{\alpha 1}$ = and $R_{i<j}^{\alpha 1}$ are zero separately. Since $R_{ii}^{\alpha 1} = 0$ also for arbitrary values of ℓ's, then each coefficient of $\ell_i^{\alpha}\ \ell_i^{\beta}$ in $R_{ii}^{\alpha 1}$ is zero separately. Therefore, equation (3.27) is true according to the lemma.

The proof is completed by recalling the second part ($i < j$) of the sufficiency proof.

Corollaries I to III, supplemented by Table XXI, might be considered as the microscopic counterparts to the parity statements of Chapters I and II. However, the phenomenological statements are perfectly general while the validity of the corollaries is limited to the microscopic models.

(ii) Remarks about the longitudinal magneto resistance change. Many microscopic models lead to zero longitudinal magneto resistance change. This was not always supported by experiments. Thus a question arises: What conditions made these calculated values zero? An answer is provided immediately by Lemma III and Table XXI of Section c of this chapter. For example, if can be shown that for $\eta \geq 1$, $[00_{2\eta}]_{33}$ and its cyclic equivalents are identically zero if

(a) $\tau(\underline{k}) = \tau(E)$ only (or $\tau(\underline{k})$ is a constant),

(b) $E(\underline{k})$ is a function of $\sum_n a_n k^n$ or of $\sum_n \sum_i a_{n,i} k_i^{\,n}$.

Now $[00_{2\eta}]_{33}$ is directly proportional to the longitudinal magneto resistance change (see equation (32)) when both the current and the magnetic field are

along the 3-axis. This axis is also taken as the principal axis of a crystal class of order higher than C_{2h}. Consequently, zero longitudinal magneto resistance change resulted in the works of Jones for Bi[32] and of Abeles and Meiboom for p-type Ge[37]. Similar results under wider classes of conditions can be predicted from Table XXI.

It is often claimed that condition (a) can be used for interpreting experiments.* Assumptions (a) and (b) probably constitute good approximations for certain materials under suitable conditions, e.g., Cu and Ag at high temperature and under small magnetic field. Since there are more functions satisfying equation (3.25) than equation (3.19) (see Table XXI), this may imply that equation (3.24) is approximately true more often than equation (3.18). Thus one could speculate that one more often finds the longitudinal magneto resistance change smaller than the transverse one. However, this should not be used to rule out cases where the situation is otherwise.**

(iii) About the nonnegative magneto resistance change. It has been found experimentally that, as a rule, $\rho^{\alpha\beta}(\underline{B}) - \rho^{\alpha\beta}(\underline{B}=0)$ is a positive quantity,*** for substances involving no transition elements. Davis[30] in 1939 and others,**** using equation (27) of Chapter I for $\eta = 1$, stated that the Schwartz inequality

$$U_2^{31} = [001]_{12}^2 + [002]_{11}[000]_{22} \geq 0 \qquad (3.32)$$

provides the explanation. However, one has to use equation (26) of Chapter I to claim a general proof. Unfortunately, even for the cases of equations (27) and (32) of Chapter I, no general proof of the positive definite nature is established as yet. Nevertheless, one can make some statements as follows.

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*See, for example, references 37, 41.

**See, for example, Figure 4 of Pearson and Suhl (reference 11).

***There are exceptions to this statement; for example, see reference 46.

****See, for example, Brooks (reference 28).

In the case of equation (32) of Chapter I, if η is an odd integer, then by integrating by parts η times it is clear that*

$$- [oo2\eta]_{33} \geq 0 . \tag{3.33}$$

If also in the power-series expansion

$$\sum_{\eta=1} B^{2\eta} [oo2\eta]_{33} \tag{3.34}$$

the magnitude of a term is always greater than that of the subsequent term, then (3.34) is always nonnegative. We do not know of any convincing evidence that this monotonic condition holds.** However, if it does, it means that the longitudinal magneto resistance change is nonnegative for isotropic substances and for crystals except C_{2h} and S_2 when the measuring current is along the principal axis.

By use of equations (3.22) and (3.23) and Lemma I, it can be shown in general that

$$-U_{2\eta}^{ij} \geq 0 \quad \text{if} \quad \eta = 2\lambda + 1 \tag{3.35}$$

$$-U_{2\eta}^{ij} \leq 0 \quad \text{if} \quad \eta = 2\lambda . \tag{3.36}$$

Thus a similar statement can be made about the transverse magneto resistance change. That is, if in equation (3.34) and in

$$\sum_{\eta=1} B^{2\eta} U_{2\eta} \tag{3.37}$$

the magnitude of each term is larger than that of the subsequent one, then, from equations (27), (30), and (31) of Chapter I, the transverse magneto resistance change is always nonnegative, for cases where the laboratory coordinates coincide with the symmetry coordinates or where an isotropic sample is used. However, even if the monotonic nature of the expression (3.34) and (3.37) were granted,

*This statement is true for any of the brackets $[oo2\eta]_{ii}$, i = 1,2,3, and those obtained from $[oo2\eta]_{ii}$ by cyclically permuting the indices 1,2, and 3.

**However, Blom stated (reference 9, p. 94): "Experimentally we find as a rule that the higher (power) terms are smaller than the lower (power) ones."

one still has to study the most general equation (26) of Chapter I for the magneto resistance.

Therefore, it should be emphasized that at present no theory predicts the positive magneto resistance change in general.

3. THE MULTIBAND MODEL

The multiband model, as described in Section 1.b of this chapter, is so postulated that all formal derivations of the single-band model can be taken over directly simply by writing

$$[m\text{-}p,p,n\text{-}m]_{ij} = \sum_{\lambda=1,2,..,q} [m\text{-}p,p,n\text{-}m]_{ij}^{(\lambda)} \tag{3.38}$$

with

$$[m\text{-}p,p,n\text{-}m]_{ij}^{(\lambda)} = ab^n \iiint \left(-\frac{\partial f_o^{(\lambda)}}{\partial E^{(\lambda)}}\right) \frac{\partial E^{(\lambda)}}{\partial k_i} \times$$

$$\times P\left\{(\tau^{(\lambda)}\Omega_1^{(\lambda)})^{m-p}(\tau^{(\lambda)}\Omega_2^{(\lambda)})^{p}(\tau^{(\lambda)}\Omega_3^{(\lambda)})^{n-m}\right\} (\tau^{(\lambda)} \frac{\partial E^{(\lambda)}}{\partial k_j}) \, d\underline{k} \, . \tag{3.39}$$

If $\lambda = 1$, then, by dropping the superindex 1, equation (3.39) becomes (3.10). Therefore all the formal developments of Chapters I and II can now be interpreted according to the multiband model, without any of the restrictions mentioned in Section 1.c of this chapter.

As an example, we can reformulate the often used two-band formula as follows. If one limits oneself to terms up to B^2 and to special geometries and symmetries as specified for equations (27) through (32) of Chapter I, and interprets the brackets according to two noninteracting bands, then equations (27) and (28) of Chapter I are comparable to equations (8.523.4) and (8.521.9), respectively, of Wilson's book.[19] The additional formula of (32) would be zero if more restrictions such as used by Wilson et al. on E's and τ's were made. The

equations (27) through (32) contain no field-dependent variables, such as the carrier densities n_1 and n_2, so that the effect of the crystal symmetry can be studied. Furthermore, they can be extended to cases, say by using Tables XV to XVII, where both geometry and symmetry are arbitrary, and to cases where more noninteracting bands and higher powers of B are desired.

The mathematical lemmas, given by equations (3.18)through (3.28) in terms of the single-band model, can all be re-established for the multiband model. To see this one only needs to read all the brackets contained in equations (3.22) through (3.24) as defined by (3.38) and (3.39). Therefore, the mathematical lemma given by equations (3.26) through (3.28) can be repeated, replacing equation (3.27) by

$$\Omega_i^{(\lambda)}(\tau^{(\lambda)}E_j^{(\lambda)}) = C_{ijk}E_k^{(\lambda)}, \quad \lambda = 1,2,\ldots q . \tag{3.40}$$

Note that equation (3.40) is more stringent than (3.27) in the sense that the same constant C_{ijk} is required for all values of λ. Consequently, all three corollaries, for the single-band model, will hold also for the multiband model if and only if condition (3.40) is read instead of condition (3.27). Then one can repeat all the remarks about the zero, the nonnegative, and the relative magnitudes of the longitudinal and transverse magneto resistance.

All these formal results followed from the assumption that transitions between bands do not occur. However, experiments have shown that recombination of electrons and holes does occur. Studies* allowing transitions between bands based on the present work may prove to be very fruitful.

*One example of such studies was given recently by Rittner (reference 47).

APPENDIX I

PROOF OF THE THEOREM CONCERNING AN N-FOLD ROTATION AXIS ALONG k_3

Let $k_1'k_2'k_3'$ be a set of symmetry coordinates of a point and let $k_1''k_2''k_3''$ be the transformed set of the same point after rotation of the coordinate axes through an angle $\phi = 2\pi/N$ about k_3. With respect to these two systems of axes the components of a tensor T of arbitrary rank are related by

$$T''_{ij\ldots\ell} = \sum_{\lambda\mu\ldots\tau} a_{i\lambda}\, a_{j\mu} \cdots a_{\ell\tau}\, T'_{\lambda\mu\ldots\tau} \quad , \tag{A.1}$$

where

$$a_{i\lambda} = \begin{pmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} . \tag{A.2}$$

This is true in particular for the components of the position vector $\underline{k}$ of a point, of the components of the magnetic field vector B, and of the components σ_{ij} of the second-rank conductivity tensor. Thus by such a rotation of coordinate axes any equation between singly primed tensor components is transformed into one with doubly primed tensor components. If the rotation is a "covering" operation of the crystal, then the equation must be invariant, i.e., its form in terms of singly primed quantities must be identical to that in terms of doubly primed quantities. This principle can be applied to equation (10). Thus, for a covering operation the coefficients (brackets) in the singly primed and doubly primed forms of (10) must be identical, hence can be written without any primes.

Now the doubly primed forms of equations (10) can be transformed by applying the equations A.1 and A.2 to the doubly primed components of σ and B. The transformed equations so obtained in terms of singly primed components

must be equivalent to equations (10) in their direct singly primed form. This equivalence requirement yields certain identities between the brackets. It will be shown that these identities are just described by equations (13) and (14). In order to simplify the proof we shall not apply the above reasoning to the Cartesian components of the tensors involved but rather refer to a pair of coordinate systems of a different type (complex, nonorthogonal) defined by

$$\left.\begin{aligned} \overline{k_1'} &= k_1' + i\,k_2' \\ \overline{k_2'} &= k_1' - i\,k_2' \\ \overline{k_3'} &= k_3' \end{aligned}\right\} \qquad (A.3)$$

and likewise for double primes. Quantities referring to the complex coordinates will be marked by a bar throughout. We define the complex components of $\underline{B}$ by

$$\left.\begin{aligned} \overline{B_1'} &= B_1' + i\,B_2' \\ \overline{B_2'} &= B_1' - i\,B_2' \\ \overline{B_3'} &= B_3' \end{aligned}\right\} \qquad (A.4)$$

and likewise for double primes. The complex components of the second-rank conductivity tensor are defined by*

*For a tensor of arbitrary rank n the complex component $\overline{T}_{ij\ldots\ell}$ is defined as follows.

a. Replace every index in the given order by a symbol according to this scheme: the index one by (l_1+i_2), the index two by (l_1-i_2), the index three by (l_3).
b. Multiply the n-fold product of symbols so obtained according to the associative and distributive law, but do not use the commutative law.
c. Replace each "term" of the symbolic polynomial so obtained by T with the indices of that term in the given order and with a coefficient equal to the product of the coefficient parts (upper parts) of the "factors" of that term. The resulting polynomial in T is the desired expression.

For example, one wants to find the appropriate definition of $\overline{T}_{123}$. According to (a) he writes the symbol $(l_1+i_2)(l_1-i_2)(l_3)$. According to (b) he obtains the symbolic polynomial $(l_1)(l_1)(l_3) - (l_1)(i_2)(l_3) + (i_2)(l_1)(l_3) - (i_2)(i_2)(l_3)$. According to (c) the definition is now $\overline{T}_{123} = T_{113} - i\,T_{123} + i\,T_{213} + T_{223}$.

$$\overline{\sigma_{ij}} = \begin{pmatrix} \sigma_{11} - \sigma_{22} + i(\sigma_{12} + \sigma_{21}) & \sigma_{11} + \sigma_{22} - i(\sigma_{12} - \sigma_{21}) & \sigma_{13} + i\sigma_{23} \\ \sigma_{11} + \sigma_{22} + i(\sigma_{12} - \sigma_{21}) & \sigma_{11} - \sigma_{22} - i(\sigma_{12} + \sigma_{21}) & \sigma_{13} - i\sigma_{23} \\ \sigma_{31} + i\sigma_{32} & \sigma_{31} - i\sigma_{32} & \sigma_{33} \end{pmatrix} \quad (A.5)$$

According to Onsager's relation

$$\overline{\sigma_{ij}}(\underline{B}) = \overline{\sigma_{ji}}(-\underline{B}) \quad , \quad (A.6)$$

hence terms below the diagonal of A.5 are dependent and it suffices to consider those above the diagonal.

For convenience we shall now introduce another notation. Let s denote the number of ones and twos together, and z the number of twos, among the indices of a $\overline{\sigma_{ij}}$. This definition of z is consistent with that given in Section 3b. The numbers s,z define uniquely one of the six independent pairs of indices ij and vice versa. We write (note the indices between parentheses):

$$\overline{\sigma_{(s,z)}} \equiv \overline{\sigma_{ij}} \quad . \quad (A.7)$$

Thus, for example, $\overline{\sigma_{(11)}}$ is another notation for $\overline{\sigma_{23}}$. It can be verified by direct substitution of these definitions and comparison with A.1 and A.2 that the complex tensor components as defined transform under a rotation of coordinates about k_3 according to

$$\overline{T'_{ij\ldots l}} = \sum_{\lambda\mu\ldots\tau} \overline{a_{i\lambda}}\ \overline{a_{j\mu}} \cdots \overline{a_{l\tau}}\ \overline{T^{\tau}_{\lambda\mu\ldots\tau}} \quad (A.8)$$

with the diagonalized matrix

$$\overline{a_{i\lambda}} = \begin{pmatrix} e^{-i\phi} & 0 & 0 \\ 0 & e^{i\phi} & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (A.9)$$

In particular,

$$\left.\begin{aligned} \overline{B_1''} &= \overline{B_1'}\, e^{-i\phi} \\ \overline{B_2''} &= \overline{B_2'}\, e^{i\phi} \\ \overline{B_3''} &= \overline{B_3'} \\ \sigma''_{(s,z)}(\underline{B}) &= \sigma'_{(s,z)}(\underline{B})\, e^{-i\phi(s-2z)} \quad . \end{aligned}\right\} \qquad (A.10)$$

We are now ready to apply the invariance principle. The equations to which it will be applied are the expansions of $\overline{\sigma'}_{(s,z)}$ and $\overline{\sigma''}_{(s,z)}$ in powers of $\overline{B_k'}$ and $\overline{B_k''}$, respectively, analogous to equation (10):

$$\overline{\sigma'}_{(s,z)}(\underline{B}) = \sum_{n=0}^{\infty} \sum_{m=0}^{n} \sum_{w=0}^{m} C'_{(s,z)}(n,m,w)\, \overline{B_1'}^{w}\, \overline{B_2'}^{m-w}\, \overline{B_3'}^{n-m} \quad . \qquad (A.11)$$

Comparison of A.11 with equations (10) and (11) yields

$$C'_{(s,z)}(n,m,w) \equiv (1/2)^m\, (-)^w \sum_{p=0}^{m} \sum_{\Theta} g(m,p,w)\, \epsilon(s,\Theta,z)\, [m-p,p,n-m]_{(s,\Theta)} \quad , \qquad (A.12)$$

where g and ϵ are the functions defined in the text by equation (15) and Table III. Equations of identical form, but with double primes, hold for the components with respect to the doubly primed coordinate system.

From the equality of singly and doubly primed brackets for a covering operation of the crystal, arrived at earlier, it follows now that

$$\overline{C''}_{(s,z)}(n,m,w) = \overline{C'}_{(s,z)}(n,m,w) \quad . \qquad (A.13)$$

According to the plan outlined at the beginning of this section, one must now express the doubly primed components of $\overline{\sigma''}_{(s,z)}$ and $\overline{B_k''}$ in the doubly primed analog of A.11 in terms of the singly primed ones by means of A.10.

We obtain

$$\overline{\sigma'}_{(s,z)} = \sum_{n=0}^{\infty} \sum_{m=0}^{n} \sum_{w=0}^{m} \overline{C''}_{(s,z)}(n,m,w)\, e^{i\phi h}\, \overline{B_1'}^{w}\, \overline{B_2'}^{m-w}\, \overline{B_3'}^{n-m} \qquad (A.14)$$

with $h = m + s - 2(w + z)$. Comparing A.14 with A.11 it is seen in view of A.13 that the two results are only compatible if

$$\left.\begin{array}{ll} \text{either} & \overline{C''}_{(s,z)}\,(n,m,w) = 0 \\ \text{or} & e^{i\phi h} = 1 \ . \end{array}\right\} \quad \text{(A.15)}$$

In connection with A.12, the equations A.15 are identical with (13) and (14) in the text, and the theorem is proved.

APPENDIX II

COMPLETENESS OF THE EQUATIONS (13)

Consider the complete set of equations (13) for given n,m,s, that is, the equations (13) for all values of $0 \leq w \leq m$ and $0 \leq z \leq s$, regardless of the value of h.

Theorem

The only solution of the complete set of equations (13) for given n,m,s is that all the brackets with the given n,m,s vanish.

Proof

In the power-series expansion (10) the brackets for given n,m,s, with the six independent pairs of outer indices are independent constants as long as no symmetry restrictions are introduced

The moduli of the transformations from B_i to $\overline{B_i}$ and from σ_{ij} to $\overline{\sigma_{ij}}$ or $\overline{\sigma}_{(s,z)}$ are nonvanishing, according to A.4 and A.5. Consequently, in the power-series expansion A.11 the constants $C_{(s,z)}$ for given n,m,s, are independent constants and the equations A.12 for given n,m,s can be inverted, leading to homogeneous expressions of the brackets in terms of the C's.

The complete set of equations (13) for given n,m,s, states that all C's vanish; consequently, all brackets with these n,m,s values vanish.

q.e.d.

In this proof use has been made of the fact that for given n,m,s, the number of brackets $[m\text{-}p,p,n\text{-}m]_{(s,\theta)}$ is equal to the number of constants $C_{(s,z)}(n,m,w)$, hence equal to the number of equations (13) [without (14)]. This equality is easily verified. Indeed, the number of equations for given n,m,s, is determined by the ranges of the integers w and z, given by $0 \leq w \leq m$ and $0 \leq z \leq s$, while the number of brackets is determined by the ranges of the in-

tegers p and $1/2(s - \theta)$, given by $0 \leq p \leq m$ and $0 \leq 1/2(s - \theta) \leq s$.

The theorem of this appendix is useful in spotting vanishing brackets and in counting nonvanishing ones. It also follows from this theorem and Appendix I that the symmetry properties of the brackets are completely described by the equations (13) with the condition (14).

APPENDIX III

PROOF OF TABLE VIII - ZERO BRACKETS FOR A THREEFOLD AXIS OF SYMMETRY

Consider the set of equations (13) for given values of n,m,s and different w,z. According to Corollary IV and the remarks made immediately thereafter, it is expedient to select from the original complex equations those satisfying the selection rule

$$s - 2z \geq 0 \qquad \text{(C.1)}$$

and equating their real and imaginary parts to zero. The number of real equations so obtained is equal to the number of the original complex equations with s - 2z unrestricted by C.1. It is also equal to the number of brackets having the given values n,m,s that occur in these equations (see Appendix II).

A first type of zero bracket arises through the application of the theorem of Appendix II. If no equation of the set is invalidated by h = kN, then all the brackets of the set vanish. The h values of the equations, for any particular value of s - 2z, range from m + s - 2z downward in steps of two for the various values of $0 \leq w \leq m$. In order to avoid h = 0, this type of analysis is restricted to m + s = odd. In order to avoid $h = \pm 3$ as well, it is necessary that

$$m + s - 2z = 1 \qquad \text{(C.2)}$$

for all values of z, compatible with the given n,m,s values and C.1. This condition can only be realized in three ways. First, m = 1, s - 2z = 0, and s = 0; consequently, z = 0 and n must be even. Second, m = 1, s - 2z = 0, and s = 2; consequently, z = 1 must be the only compatible z value, necessitating n = odd (see Table III). Third, m = 0, s - 2z = 1; consequently, s = 1, and the only z value compatible with C.1 is z = 0. The corresponding zero brackets are,

respectively,

$$\left.\begin{array}{l} [1\omega]_{33}\ [0\omega]_{33} \\ [1e]_{12}\ [0e]_{12} \\ [oon]_{23}\ [oon]_{31}\ . \end{array}\right\} \quad (C.3)$$

A second type of zero brackets can arise for m + s = even. According to the definitions of g and ϵ, the coefficients $g\epsilon$ of any bracket in the complex equations are $i^{p+1/2(s-\theta)}.i^{s}$ times a real number. Thus, all the real parts of the equations with given n,m,s, contain only brackets of one parity of p', defined by

$$p' = p + 1/2(s - \theta) \ , \qquad (C.4)$$

and all the imaginary parts of these equations contain only brackets of the other parity of p'. The brackets with given n,m,s thus fall into two subgroups according to the parity of p'. In each subgroup there are as many real independent equations as there are brackets. There is one way in which the condition h = kN can affect one of these two subgroups without affecting the other. The brackets in the unaffected subgroup must then vanish on the same grounds, as before the condition h = kN was applied. In order that h = kN shall affect only one subgroup, it is necessary and sufficient that it affect only self-conjugate complex equations. According to Corollary IV, these occur only for h = 0; namely, if both

$$\left.\begin{array}{l} (s - 2z) = 0 \\ (m - 2w) = 0 \ , \end{array}\right\} \quad (C.5)$$

hence m,s, and m + s are all even. Since h = 6 is inadmissible, the possible values of m are 0,2,4. These can be realized in three ways, compatible with C.5. First, s = 0; consequently, z = 0 and n = even. The case m = 0 must here be excluded since the remaining subgroup is empty. Second, s = 2, n = odd; consequently, z = 1. On the same grounds as in the first case, m = 0 is excluded.

Third, s = 2, n = even; consequently, z = 1 according to C.5. But the equations with s = 2, z = 0 must now also be admitted, while no equation that is not self-conjugate complex should be ruled out by h = k.3. This configuration allows only m = 0. The corresponding zero brackets are:

$$\left.\begin{array}{l} [11e]_{33}\ [31e]_{33}\ [13e]_{33} \\ [11\omega]_{12}\ [31\omega]_{12}\ [13\omega]_{12} \\ [ooe]_{12}\ . \end{array}\right\} \text{(C.6)}$$

It can be shown that a threefold axis produces no other zero brackets than those listed in C.3 and C.6.

APPENDIX IV

AN ALTERNATE METHOD OF OBTAINING TABLE XI

Let $I(n)$ be the number of nonvanishing independent brackets for any given value of n. Then one has

$$I(n) = \sum_{m=0}^{n} I(m)$$

with

$$I(m) = P(m) - E^*(m)$$

where $P(m)$ is the number of possible brackets for given $m \leq n$ and is given by Table XXII. $E^*(m)$ is the number of valid equations between $P(m)$ possible brackets for given m; it is given by the number of possible combinations of w, s, and z such that

$$h \equiv (m + s) - 2(w + z) \neq kN .$$

If Corollary IV is used, one only needs to count the equations pertaining to $h > 0$, thus one obtains equations (23) and (24) for I_{C_N}, from which I_{D_N} and I_{T_h} (which is just one third of that for D_{2h}) can be obtained. $E^*(n)$ is then summarized in Table XXIII. Note that one of the counting methods for O_h is here presented.

TABLE XXII

POSSIBLE NUMBER OF BRACKETS P(m) FOR GIVEN m

	n	m	s = 0	s = 1	s = 2
C_N	e		(m + 1)	2(m + 1)	3(m + 1)
	ω		0	2(m + 1)	(m + 1)
O_h [1]	e	2λ	λ + 1	0	λ
	ω	2λ+1	0	0	λ + 1

(1) Applying Corollary I twice, once to index 1 once to index 2.

(2) Because the brackets for O_h are invariant under cyclic permutation of the inner and outer indices, it is sufficient to count the brackets only with outer index pairs 33 and 12.

TABLE XXIII

NUMBER OF VALID EQUATIONS FOR GIVEN m†

$E^*_{C_N}(m) = 2E^*_{D_N}(m)$

	n = even		n = odd	
	m = 2λ	m = 2λ - 1	m = 2λ	m = 2λ + 1
C_{2h}	$2(2\lambda+1)$	8λ	$2(2\lambda+1)$	$2(\lambda+1)$
C_{3i}	$4(2\lambda+1)$	8λ	$2(2\lambda+1)$	$4(\lambda+1)$
C_{4h}	$4(2\lambda+1)$	10λ	$2(2\lambda+1+\delta_4)$	$4(\lambda+1)$
C_{6h}	$2(4\lambda+2+\delta_1)$	$2(4\lambda+\delta_1+\delta_2)$	$2(2\lambda+1+\delta_1)$	$2(\lambda+1+\delta_1+\delta_3)$
O_h††	$\frac{1}{2}\delta_4+(\frac{1}{2}\delta_4-\delta_{\lambda,2q-1}) = \lambda$		$\frac{1}{2}\delta_4$	

† $\delta_1 = 2q\delta_{\lambda,3q} + (2q+1)\delta_{\lambda,3q+1} + 2(q+1)\delta_{\lambda,3q+2}$

$\delta_2 = 2q\delta_{\lambda,3q} + 2q\delta_{\lambda,3q+1} + (2q+1)\delta_{\lambda,3q+2}$

$\delta_3 = (2q+1)\delta_{\lambda,3q} + 2(q+1)\delta_{\lambda,3q+1} + 2(q+1)\delta_{\lambda,3q+2}$

$\delta_4 = 2q(\delta_{\lambda,2q} + \delta_{\lambda,2q-1})$

$\delta_{\lambda,q} = \begin{cases} 1 & \text{if } \lambda = q \\ 0 & \text{otherwise} \end{cases}$

††Here E*(m) means the number of adjoining relations between the brackets given in Table XXII.

APPENDIX V

A LIST OF PROBLEMS FOR FURTHER STUDY

We shall list a number of problems closely related to the present work. Further study is needed in order to achieve:

I. A simple rule to tabulate all the brackets for three- and six-fold axes.

II. A general analysis of the relations between the measurements and the brackets.

Solutions of these two problems are considered the most desired but unfinished aspects of the phenomenological theory. The first one is important theoretically, the second experimentally.

III. A formally identical treatment of the thermo-galvanomagnetic effects.

IV. A generalized application of the theorem given by equations (13) and (14) to an arbitrary tensor, such as the dielectric, the elastic constants, the magnetic susceptibility, piezoelectric constant, etc.

V. A physical picture of condition (3.27). Since the quantity $\Omega/\hbar^2$ has the dimension of a reciprocal mass, it might be investigated via the effective-mass theory. The effect of slight deviations from equation (3.27) on the brackets might be traced.

VI. Analysis of the temperature dependence of the galvanomagnetic effects according to the approach suggested by the last problem, i.e., sight deviations from equation (3.27), might be fruitful.

VII. A study of the case if some kind of transition between bands is allowed. The formal simplicity of the multiband is attractive, but such a model is no doubt a zero-th approximation.

APPENDIX VI

HOW TO USE THE TABLES V TO XVII

In order that Tables V to XVII* can be used by a reader who does not have the time to read the whole dissertation, a few illustrative examples will be given in this appendix.

Remember that the explicit expressions of the galvanomagnetic tensor $\rho^{\alpha_1}(\underline{B})$ for any crystal classes can be obtained from equations (25) and (26) if, for these crystal classes, one knows the explicit expression of equation (10), i.e.,

$$\sigma_{ij}(\underline{B}) = \sum_{n=0}^{\infty} B^n \sum_{m=0}^{n} \sum_{p=0}^{m} [m-p,p,n-m]_{ij} \gamma_1^{m-p} \gamma_2^{p} \gamma_3^{n-m}$$

$$ij = 11,22,33,12,23,31 .$$

Example I. What is the coefficient of B^3 in $\sigma_{12}(\underline{B})$?

The coefficient of B^3 in $\sigma_{12}(\underline{B})$ in general is:

$$\left.\begin{aligned} & [003]_{12}\, \gamma_3^3 + \\ & + [012]_{12}\, \gamma_2\, \gamma_3^2 + [102]_{12}\, \gamma_3^2\, \gamma_1 + \\ & + [021]_{12}\, \gamma_2^2\, \gamma_3 + [201]_{12}\, \gamma_1^2\, \gamma_3 + [111]_{12}\, \gamma_1\, \gamma_2\, \gamma_3 + \\ & + [300]_{12}\, \gamma_1^3 + [030]_{12}\, \gamma_2^3 \quad , \end{aligned}\right\} \qquad (F.1)$$

where the lines correspond to m = 0, 1, 2, 3, respectively.

Example II. What is the coefficient of B^3 in σ_{ij} $(i \neq j)$ for D_{2h}?

For D_{2h} all brackets marked by 0 and $\oplus$ in Table V are zero, thus (F.1) becomes

$$[003]_{12}\, \gamma_3^3 + [021]_{12}\, \gamma_2^2\, \gamma_3 + [201]_{12}\, \gamma_1^2\, \gamma_3 \quad . \qquad (F.2)$$

This is the coefficient of B^3 in $\sigma_{12}(\underline{B})$ for D_{2h}.

Similarly, that of B^3 in $\sigma_{23}(\underline{B})$ and $\sigma_{31}(\underline{B})$ for D_{2h} are, respectively:

$$\left.\begin{aligned} & [300]_{23}\, \gamma^3 + [102]_{23}\, \gamma_1\, \gamma_3^2 + [120]_{23}\, \gamma_1\, \gamma_2^2 \\ & [030]_{31}\, \gamma_2^3 + [012]_{31}\, \gamma_2\, \gamma_3^2 + [210]_{31}\, \gamma_2\, \gamma_1^2 \quad . \end{aligned}\right\} \qquad (F.3)$$

*For illustrations of Table XVII see Pearson and Suhl (reference 11).

Example III. What is the coefficient of B^3 in $\sigma_{ij}(\underline{B})(i \neq j)$ for D_{4h}?

From Table VI one reads off the zero brackets for D_{4h} as marked by 0, $\not{0}$, and $\dot{\not{0}}$. Incidentally, these are the same zero brackets as those for D_{2h}. Thus one would have the remaining coefficients of B^3 in $\sigma_{ij}(\underline{B})$ as given by (F.2) and (F.3). However, there exist adjoint relations between the non-vanishing brackets as indicated by the dotted lines in Table VI. For example, $[\dot{2}01]_{12} = [021]_{12}$. When this is taken into account, the coefficients of B^3 in $\sigma_{ij}(\underline{B})(i \neq j)$ are:

$$\left.\begin{aligned} &[003]_{12}\,\gamma_3^3 + [201]_{12}\,(\gamma_1^2\,\gamma_3 + \gamma_2^2\,\gamma_3) && \text{(in } \sigma_{12}) \\ &[300]_{23}\,\gamma_1^3 + [102]_{23}\,\gamma_1\,\gamma_3^2 + [120]_{23}\,\gamma_1\,\gamma_2^2 && \text{(in } \sigma_{23}) \\ &[300]_{23}\,\gamma_2^3 + [102]_{23}\,\gamma_2\,\gamma_3^2 + [120]_{23}\,\gamma_1^2\,\gamma_2 && \text{(in } \sigma_{31})\,. \end{aligned}\right\} \qquad \text{(F.4)}$$

Example IV. What is the coefficient of B^3 in $\sigma_{12}(\underline{B})$ for C_{3i}?

Dropping the zero brackets according to Table VIII, (F.1) becomes

$$\left.\begin{aligned} &[003]_{12}\,\gamma_3^3 + \\ &+ [201]_{12}\,\gamma_1^2\,\gamma_3 + [021]_{12}\,\gamma_2^2\,\gamma_3 + \\ &+ [300]_{12}\,\gamma_1^3 + [030]_{12}\,\gamma_2^3\,. \end{aligned}\right\} \qquad \text{(F.5)}$$

Example V. What is the coefficient of B^4 in σ_{33} for D_{3i}?

This can be obtained directly from Table X(s = 0, n = even), remembering that $[e\omega\omega]_{33} = 0$ from Table IX. Thus the answer is:

$$\left.\begin{aligned} &[004]_{33}\,\gamma_3^4 + [202]_{33}\,(\gamma_1^2 + \gamma_2^2)\,\gamma_3^2 + \\ &[031]_{33}\,(\gamma_2^3\,\gamma_3 - 3\,\gamma_1^2\,\gamma_2\,\gamma_3) + [400]_{33}\,(\gamma_1^4 + 2\,\gamma_1^2\,\gamma_2^2 + \gamma_2^4)\,. \end{aligned}\right\} \qquad \text{(F.6)}$$

If at a given temperature the magnetic field is so weak that only terms up to B^2 are experimentally significant, then equations (26) and (27) together with Tables XI to XVII give us all the galvanomagnetic tensors for each of the 32 point groups. The following examples illustrate some special cases:

Example VI. For a crystal of D_{2h} symmetry (for example Ga), if the current flows along the 1-axis ($\ell_1^1 = 1$) and the magnetic field is along the 3-axis ($\gamma_3 = 1$). Note that any one of the two-fold axes can be taken as the 1-axis; then the 3-axis must be chosen according to the right-hand rule.

Case a. ($\ell_1^1 = \ell_2^2 = \gamma_3 = 1$; D_{2h}) For Hall measurements ($\alpha = 2$), one has

$$\rho^{21} = (P_0^{21} + Q_1^{21} B + R_2 B^2)/M_0 \quad , \tag{F.7}$$

where M_0 and P_0^{21} are given by the second lines of Table XII and XIII, respectively, i.e.,

$$M_0 = [ooo]_{11}[ooo]_{22}[ooo]_{33}$$

$$P_0^{21} = 0 \ ,$$

while Q_1^{21} and R_2 are given by the third line and the third section of Tables XIV and XV respectively:

$$Q_1^{21} = [oo1]_{12}[ooo]_{33}$$

$$R_2 = 0$$

Case b. ($\ell_1^1 = \gamma_3 = 1$; D_{2h}) For magneto resistance measurements ($\alpha = 1$), one has

$$\rho^{11} = (P_0^{11} + R_2 B^2)/M_0 \ , \tag{F.8}$$

where M_0 and P_0^{11} are given by Tables XII and XIII respectively:

$$M_0 = [ooo]_{33}[ooo]_{11}[ooo]_{22}$$

$$P_0^{11} = [ooo]_{22}[ooo]_{33}$$

and R_2 is given by R_{33}^{11} of Table XV, i.e.,

$$R_2 = R_{33}^{11} = -([oo2]_{11}[ooo]_{22} + [oo1]_{12}^2)[ooo]_{33}/[ooo]_{11}$$

Example VII. ($\ell_1^1 = \ell_2^2 = \ell_2^1 = -\ell_1^2 = 1/\sqrt{2}$; $\gamma_3 = 0$, D_{6h})

For a crystal of D_{6h} symmetry (for example Zn, Cd), if the magnetic field, the current leads, and the Hall probes lie in a plane normal to the six-fold axis. Particularly, if the current and the Hall probes lie along the bisectors of the 1- and 2-axes. This "planar Hall field" measurement is given by equation

(F.7) with (reading from Tables XII and XIII)*

$$M_o = [ooo]_{33}[ooo]_{11}^2$$

$$P_o^{21} = 0$$

and (from Table XVI)

$$R_2 = R_{11}^{21} + R_{22}^{21} + R_{12}^{21} + R_{21}^{21} = \frac{1}{2}\left\{([2oo]_{11} - [2oo]_{22})[ooo]_{33} - [1oo]_{23}^2\right\}(\gamma_1^2 - \gamma_2^2).$$

Example VIII. For a crystal of D_{3i} symmetry (for example Sb, Bi), if the directions of the current, the probes, and the magnetic field are arbitrary with respect to the crystal axes and to each other. What is the lowest odd term in the Hall measurement $\rho^{21}(\underline{B})$ $(\alpha \neq 1)$(where superindex 2 denotes the direction of the Hall probe in the laboratory coordinates)? The answer is provided by the last line of Tables XIV and XII

$$\rho^{21}(\underline{B}) - \rho^{2\bar{1}}(\underline{B}) = 2\, Q_1^{21}\, B$$

with $\rho^{21}(\underline{B})$ and $\rho^{2\bar{1}}(\underline{B})$ denoting the same measurement but with the current reversed and

$$M_o = [ooo]_{11}^2[ooo]_{33}$$

$$Q_1^{21} = (\gamma_1 \ell_1^3 + \gamma_2 \ell_2^3)[1oo]_{23}[ooo]_{11} + \gamma_3 \ell_3^3 [oo1]_{12}[ooo]_{33}$$

where superindices 1, 2, and 3 form a right-hand orthogonal laboratory coordinate system.

*From Table IV one finds that Q_1^{21} becomes zero in this special case. This does not contradict the parity statements of Section 2.e of Chapter I, because $Q_{2\eta+1}^{21} \neq 0$ in general.

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