used for the calculations. Instead, it may be because the calculations of Seeger *et al.* (Refs. 17 and 18) allowed for the anisotropy of the dilatation field around the interstitials, whereas the calculations of Johnson assumed an (unrealistic) isotropic displacement field at large distances.

[22]G. Lück and R. Sizmann, Phys. Status Solidi 14, 507 (1966).
[23]J. R. Beeler, Phys. Rev. 150, 470 (1966).
[24]U. Himmler, H. Peisl, A. Sepp, W. Waidelich, and H. Wenzl, Z. Angew. Phys. 28, 175 (1969); Phys. Rev. Letters 19, 956 (1967).

PHYSICAL REVIEW B VOLUME 2, NUMBER 10 15 NOVEMBER 1970

Anisotropic Relaxation Times and Magnetoconductivity for Ellipsoidal Energy Surfaces: Onsager Reciprocity Restrictions and Jones-Zener Expansions

T. D. Fuchser, H. J. Mackey, and J. R. Sybert
Department of Physics, North Texas State University, Denton, Texas 76203
(Received 15 June 1970)

The magnetoconductivity is obtained using anisotropic relaxation-time tensors for materials having Fermi surfaces consisting of a group of ellipsoids. Each ellipsoid is described in terms of a number of carriers and a saturation field tensor. From crystal symmetry and Onsager reciprocity, it is proven in some cases and inferred for all other cases that all saturation field tensors must be symmetric. The anisotropic relaxation-time tensor is thereby restricted, but need not be symmetric itself. The saturation-field-tensor symmetry also requires the existence of ellipsoids of constant power density upon application of an electric field and no magnetic field. The Jones-Zener expansion of the conductivity in terms of magnetic field is simply derived, including anisotropic relaxation-time tensors. The Jones-Zener series diverges to infinity if a critical magnetic field H_c is reached. An expression for H_c is obtained and compared with past criteria for convergence.

INTRODUCTION

Magnetoconductivity theories are common in the literature for semiconductors and semimetals whose constant-energy surfaces are approximated by a group of ellipsoids. Most of these theories have assumed isotropic relaxation times, but lately there has been evidence for anisotropic relaxation times in copper,[1] bismuth,[2] and bismuth telluride.[3] A previous paper by Mackey and Sybert,[4] hereafter called Paper I, used anisotropic relaxation times in the calculation of the conductivity for a group of ellipsoids. Anisotropic relaxation times have also been used in theories for many-valley semiconductors by Herring and Vogt,[5] in theories for bismuth by Hartman[2] and by Samoylovich and Pinchuk,[6] and in theories for bismuth telluride by Korenblit[7] and by Hübner.[3]

The theories for bismuth and bismuth telluride are applicable to the whole group of solids which have ellipsoidal Fermi surfaces, and it is unfortunate that exposure has been restricted to researchers working with these two materials. Thus, it seemed worthwhile to make an extension of Paper I, providing a more comprehensive treatment for the use of anisotropic relaxation-time tensors. At the same time the simplicity of the results is stressed.

Some confusion seems to exist on whether or not to assume the principal-axis system of the relaxation-time tensor coincides with that of the effective-mass tensor. In either case, the principal-axis system of the relaxation-time tensor is restricted by the Onsager reciprocity relation and by crystal symmetry requirements. These restrictions are developed here, and one finds a rather simple physical interpretation of the results.

The theory of Paper I is generalized in this paper by inserting anisotropic scattering into the original Boltzmann transport equation, and by including formulas applicable to semiconductor calculations as well as for the degenerate case. The Jones-Zener series is then derived in matrix form to arbitrary order. From this, the Jones-Zener coefficients which properly include anisotropic relaxation are readily identified. The regions of convergence and divergence of the Jones-Zener series are separated by a "critical" magnetic field strength which is derived and found to be a function of the magnetic field direction.

BOLTZMANN TRANSPORT EQUATION WITH ANISOTROPIC RELAXATION TIME

The Boltzmann transport equation for electrons is

$$\nabla_x f \cdot \vec{v} - \nabla_p f\left(e\vec{E} + \frac{e}{c}\vec{v}\times\vec{H}\right) = \left(\frac{\partial f}{\partial t}\right)_c , \qquad (1)$$

where $e = |e|$ is the electron charge and f is the

distribution function for the electrons. After Wilson[8] (also see Paper I), let f_1, the perturbation of the distribution function from equilibrium defined as $f - f_0(\epsilon)$, be of the form

$$f_1 = -(\vec{C}\cdot\vec{p})\frac{\partial f_0}{\partial \epsilon} \quad . \tag{2}$$

ϵ is the energy and $\vec{C}$ is a function of energy to be determined. For ellipsoidal energy surfaces the energy is

$$2\epsilon = \vec{p}\cdot(\hat{m})^{-1}\vec{p} = \vec{p}\cdot\hat{\alpha}\vec{p}\,, \tag{3}$$

and the velocity is defined as

$$\vec{v} = \nabla_p \epsilon = (\hat{m})^{-1}\vec{p}\,. \tag{4}$$

Assuming isothermal conditions, $\nabla_x f = 0$, and keeping only first-order terms, gives

$$\frac{\partial f_0}{\partial \epsilon}\,\vec{v}\cdot\left(e\vec{E} - \frac{e}{c}\,\vec{H}\times\vec{C}\right) = -\left(\frac{\partial f}{\partial t}\right)_c \quad . \tag{5}$$

For the most general relaxation-time approximation, the right-hand side of Eq. (5) is written in the form

$$\left(\frac{\partial f}{\partial t}\right)_c = \frac{-f_1}{\tau(\vec{p})}\,, \tag{6}$$

where τ is a function of $\vec{p}$. (When τ is isotropic, it is a function of energy only.) Because only ellipsoidal energy surfaces are considered, it will be assumed that the relaxation time can be written as a tensor whose elements are functions of energy only. Using Eq. (2), it is then possible to write the collision term in the following forms:

$$\left(\frac{\partial f}{\partial t}\right)_c = \frac{\partial f_0}{\partial \epsilon}\,\vec{C}\cdot\hat{m}\,(\hat{\tau})^{-1}(\hat{m})^{-1}\vec{p}\,, \tag{7a}$$

$$\left(\frac{\partial f}{\partial t}\right)_c = \frac{\partial f_0}{\partial \epsilon}\,\vec{C}\cdot(\hat{\tau}')^{-1}\vec{p}\,. \tag{7b}$$

The matrices $\hat{\tau}^{-1}$ and $(\hat{\tau}')^{-1}$ are not equivalent, in general, but a solution for one yields the other by the equation

$$(\hat{\tau}')^{-1} = \hat{m}(\hat{\tau})^{-1}(\hat{m})^{-1}\,. \tag{8}$$

Equation (7a) is the most convenient form to substitute into Eq. (5), and yields

$$\frac{\partial f_0}{\partial \epsilon}\left[\vec{v}\cdot\left(e\vec{E} - \frac{e}{c}\,\vec{H}\times\vec{C}\right) + \vec{p}\cdot(\hat{m})^{-1}(\hat{\tau})^{-1}\hat{m}\vec{C}\right] = 0, \tag{9}$$

where use has been made of the identity $\vec{A}\cdot\hat{M}\vec{B} = \tilde{M}\vec{A}\cdot\vec{B}$ and the symmetry of the mass tensor. $\tilde{M}$ is the transpose of $\hat{M}$. Replacing the vector cross product by its matrix equivalent gives

$$\vec{H}\times\vec{C} = \hat{H}\vec{C}, \tag{10}$$

where

$$\hat{H} = \begin{bmatrix} 0 & -H_3 & H_2 \\ H_3 & 0 & -H_1 \\ -H_2 & H_1 & 0 \end{bmatrix} \quad . \tag{11}$$

Using Eqs. (4) and (10) in Eq. (9), and noting that Eq. (9) must be satisfied for arbitrary $\vec{v}$, one finds

$$c\vec{E} - \hat{H}\vec{C} + (c/e)(\hat{\tau})^{-1}\hat{m}\vec{C} = 0\,. \tag{12}$$

Equation (12) has the solution

$$\vec{C} = -c\hat{G}\vec{E}\,, \tag{13}$$

where

$$\hat{G} = (\hat{F} - \hat{H})^{-1}, \tag{14a}$$

$$\hat{F} = (c/e)(\hat{\tau})^{-1}\hat{m}\,. \tag{14b}$$

Equations (13) and (2) yield

$$f_1 = c\,\frac{\partial f_0}{\partial \epsilon}\,\vec{p}\cdot\hat{G}\vec{E}\,. \tag{15}$$

This is a closed-form solution of the distribution function for ellipsoidal energy surfaces. To find the Jones-Zener expansion[9] of f_1 (and thus of the conductivity calculated from f_1), one first expands $[\hat{F} - \hat{H}]^{-1}$ in a matrix series[10] about the matrix $\hat{H}$, giving

$$(\hat{F} - \hat{H})^{-1} = \hat{F}^{-1} + \hat{F}^{-1}\hat{H}\hat{F}^{-1} + \hat{F}^{-1}\hat{H}\hat{F}^{-1}\hat{H}\hat{F}^{-1} + \cdots\,. \tag{16}$$

This expansion in Eq. (15) gives the Jones-Zener series for f_1 as

$$f_1 = c\,\frac{\partial f_0}{\partial \epsilon}\,(\vec{p}\cdot\hat{F}^{-1}\vec{E} + \vec{p}\cdot\hat{F}^{-1}\hat{H}\hat{F}^{-1}\vec{E} + \cdots)\,. \tag{17}$$

Note that this is a power series in the magnitude of the magnetic field H, since one can define a unit vector $\vec{U}$ in the direction of the magnetic field such that

$$\vec{H} = H\vec{U} \tag{18}$$

and

$$\hat{H} = H\hat{U}\,. \tag{19}$$

($\hat{U}$ is an orientation matrix containing the same information as the vector $\vec{U}$.) If the magnetic field strength is equal to or greater than a critical value, the Jones-Zener series diverges and is no longer equivalent to the closed-form expression of Eq. (15). However, Eq. (15) is finite and is valid above the critical field value unless the effective-mass theorem fails, or the splitting of electron states by the magnetic field becomes important.[11] The critical field of the Jones-Zener series is derived in Appendix B to be

$$H_c^4 = (|\hat{F}|/\vec{U}\cdot\hat{F}\vec{U})^2\,, \tag{20}$$

where $\hat{F}$ is a symmetric matrix (as is shown below)

and $|\hat{F}|$ is the determinant of the matrix $\hat{F}$.

For the case of spherical energy surfaces and an isotropic relaxation time, Eq. (20) reduces to

$$eH_c\tau/mc = 1 . \tag{21}$$

Hartman[2] indicates a matrix expansion similar to the above for his electrical conductivity matrix. His convergence condition is for the magnitude of each element of $(\hat{F}^{-1}\hat{H})$ to be less than one, which always gives a magnetic field strength less than the critical field. For the spherical isotropic case, Hartman's criterion reduces to $H < H_c$ whereby H_c is given by Eq. (20). However, for electron ellipsoids in bismuth with the magnetic field along the threefold axis, Hartman's condition gives $H < 0.096 H_c$.

CONDUCTIVITY

The current density is calculated as

$$\vec{J} = -2eh^{-3}\int \vec{v} f_1 \, d^3p , \tag{22}$$

which from Eq. (15) becomes

$$\vec{J} = -2eh^{-3}c\int \vec{v}(\tilde{G}\vec{p}\cdot\vec{E})\frac{\partial f_0}{\partial \epsilon}\, d^3p. \tag{23}$$

Note that $\hat{G}$ or $\tilde{G}$ perform operations which differ according to the direction of $\vec{p}$, but their elements are assumed to be functions of energy only. Consequently, all but the energy integration can be carried out immediately. To do this, one uses a deformed coordinate system or $\vec{w}$ space such that constant-energy surfaces are expressed as

$$2\epsilon = \alpha_0 \vec{w}\cdot\vec{w} , \tag{24}$$

where α_0 is an arbitrary constant with the dimensions of $\hat{\alpha}$. The resulting transformations and integrations are carried out in Appendix A. From the expression for current density, one then identifies the conductivity tensor as

$$\hat{\sigma} = \tfrac{16}{3}\sqrt{2}\; eh^{-3}\pi c(\alpha_1\alpha_2\alpha_3)^{-1/2}\int \epsilon^{3/2}\frac{\partial f_0}{\partial \epsilon}(\hat{F}-\hat{H})^{-1} d\epsilon . \tag{25}$$

This expression is applicable to either semiconductors or semimetals where Eqs. (3) and (4) hold. The energy dependence of the relaxation-time elements must be known to proceed further, except for the degenerate electron case (such as semimetals at low temperatures). Results are then simplified by the relation

$$\frac{\partial f_0}{\partial \epsilon} = -\delta(\epsilon - \epsilon_F) , \tag{26}$$

where ϵ_f is the Fermi energy. The conductivity tensor is then

$$\hat{\sigma} = nec(\hat{F}-\hat{H})^{-1}, \tag{27}$$

where the elements of $\hat{\tau}$ are evaluated at the Fermi energy and

$$n = \tfrac{16}{3}\sqrt{2}\,\pi h^{-3}(\alpha_1\alpha_2\alpha_3)^{-1/2}\epsilon_F^{3/2} \tag{28}$$

is the number of electrons per unit crystal volume in the energy ellipsoid $2\epsilon_F = \vec{p}\circ\hat{\alpha}\vec{p}$. Equation (27) was derived in Paper I, where $\hat{H}^s$ in that paper is designated as $\hat{F}$ here to avoid superscripts. $\hat{H}^s$ or $\hat{F}$ is referred to as the saturation field tensor.

Equation (27) gives all the components of $\hat{\sigma}$ in a straightforward manner. However, if only a few components are to be calculated, and if one wishes to capitalize on $\hat{H}$ being antisymmetric, alternate expressions using Levi-Cevita symbols may be used. These are given in Appendix B. Equation (16) can also be combined with Eq. (27) to yield the Jones-Zener series for the conductivity. These coefficients are given in Appendix C.

To calculate the conductivity for a group of ellipsoids, one may assume that the conductivity of each ellipsoid can be calculated separately. The total conductivity is then given by summing the conductivities of the individual ellipsoids in a common reference system. In Eq. (27), the only quantities dependent on the individual ellipsoids are the elements of the saturation field matrix $\hat{F}$ and the number of carriers n. Then in the laboratory reference system, the total conductivity takes the form

$$\hat{\sigma}_t = ec\sum_k n_k(\hat{F}_k - \hat{H})^{-1} . \tag{29}$$

If $\hat{\tau}$ and $\hat{m}$ are given in the ellipsoid principal-axis system, they must be transformed to the laboratory reference system by a similarity transformation. Let $\hat{R}_k$ be a rotation matrix relating the kth ellipsoidal principal-axis system with the laboratory system. If all ellipsoids belong to the same $\hat{F}$ and are identical (except for rotation), then Eq. (29) can be written as

$$\hat{\sigma}_t = ec\sum_k n(\hat{R}_k\hat{F}\hat{R}_k^{-1} - \hat{H})^{-1} . \tag{30}$$

ONSAGER RECIPROCITY

The Onsager reciprocity relation[11] requires the conductivity tensor to satisfy

$$\hat{\sigma}(\vec{H}) = \tilde{\sigma}(-\vec{H}) . \tag{31}$$

This puts restrictions on the matrix $\hat{F}$ and thus on the relaxation-time matrix $\hat{\tau}$. If one treats each individual ellipsoidal energy surface as independent, then Eq. (31) must be satisfied by Eq. (27) for the degenerate case, and one obtains

$$\hat{F} = \tilde{F} , \tag{32}$$

since

$$\tilde{H} = -\hat{H} . \tag{33}$$

For the nondegenerate case, Eq. (31) applied to Eq. (25) gives

$$\int \epsilon^{3/2} \frac{\partial f_0}{\partial \epsilon} (\hat{F} - \hat{H})^{-1} d\epsilon = \int \epsilon^{3/2} \frac{\partial f_0}{\partial \epsilon} (\tilde{F} - \hat{H})^{-1} d\epsilon \tag{34}$$

for all $\hat{H}$. Equation (32) is obviously a solution again. Other solutions are mathematically feasible, but the solution must converge to Eq. (32) for the low-temperature degenerate case, and thus Eq. (32) seems the most plausible solution at higher temperatures.

The independence assumption above is consistent with the assumption of no interellipsoidal scattering. However, Hartman[2] proposes that for bismuth a predominant scattering is between carriers from different ellipsoids. Thus one is led to ask what happens if the conductivity can still be accurately approximated by adding individual ellipsoid conductivities according to Eq. (29), perhaps by the use of an "averaged" interellipsoid scattering contribution to the relaxation-time tensor, but the Onsager reciprocity can be only applied to the total conductivity as

$$\hat{\sigma}_t(\vec{H}) = \tilde{\sigma}_t(-\vec{H}) . \tag{35}$$

In order to consider a simple example and to correct an error in Paper I, consider three identical ellipsoids symmetrically placed around the Z axis, such as the electron ellipsoids for bismuth. For this example, Appendix D shows that Onsager reciprocity requires the $\hat{F}$ matrix of each ellipsoidal surface to be symmetric. The $\hat{F}$ (or $\hat{H}^s$) of Paper I is not symmetric and, therefore, does not satisfy Onsager reciprocity. It was originally thought to satisfy Onsager reciprocity because it was only checked for the magnetic field in the Z direction. However, for the magnetic field in the X or Y directions, the example of Paper I no longer satisfies Onsager reciprocity, in agreement with the results of Appendix D.

For larger groups of ellipsoids, solutions of Eq. (35) other than each matrix $\hat{F}$ being symmetric are mathematically feasible. For example, in Eq. (29), one might add to every term $n_k ec(\hat{F}_k - \hat{H})^{-1}$, a term

$$n_l ec(\hat{F}_l - \hat{H})^{-1} , \tag{36a}$$

where

$$\hat{F}_l = \tilde{F}_k \tag{36b}$$

and

$$n_l = n_k . \tag{36c}$$

But finding a physical situation in which ellipsoids could pair off according to Eq. (36a), when referred to the same coordinate system, seems extremely unlikely. Since crystal symmetry seriously restricts the ellipsoid arrangement, one is inclined, after working through a few examples, to consider Eq. (32) as the only practical solution to Onsager reciprocity.

Using the symmetry of $\hat{F}$ and Eq. (14b), one has

$$(\tilde{\tau})^{-1} \hat{m} = \hat{m} \hat{\tau}^{-1} , \tag{37}$$

since $\hat{m}$ is symmetric from its definition. The $\hat{\tau}$ tensor can be inverted to give

$$\hat{\tau} \hat{m} = \hat{m} \tilde{\tau} , \tag{38}$$

which in the ellipsoidal principal-axis system gives

$$\tau_{ij} = (m_j / m_i) \tau_{ji} , \tag{39}$$

in agreement[12] with Korenblit[7] and others.[3,6] $\hat{\tau}(\hat{\tau}')$ must be symmetric if it is to have an orthogonal principal-axis system in velocity space ($\vec{p}$ space). With Eq. (38), this gives

$$\hat{\tau} \hat{m} = \hat{m} \hat{\tau} . \tag{40}$$

Since for this case $\hat{\tau}$ and $\hat{m}$ commute, they share the same principal-axis system which is that of the energy ellipsoid. This is the case considered by Herring and Vogt[5] and by Hartman.[2] Equation (40) also implies that $\hat{\tau} = \hat{\tau}'$. Whether $\hat{\tau}$ is symmetric or not is not determined by Onsager reciprocity and crystal symmetry.

For nonsymmetric $\hat{\tau}$, it is instructive to consider bismuth telluride where three ellipsoids are symmetrically placed about a threefold axis. The energy ellipsoids may be tilted an angle θ from the threefold axis. (Crystal symmetry specifies the orientation of the energy ellipsoids about symmetry axis in p space except for the angle θ.) The conductivity of a single energy ellipsoid with no magnetic field is

$$\hat{\sigma} = nec(\hat{F})^{-1} . \tag{41}$$

Since $\hat{F}^{-1}$ is symmetric, the conductivity tensor is also symmetric and can be diagonalized by a rotation.

Just as a symmetric mass tensor yields ellipsoidal energy surfaces through Eq. (3), a symmetric conductivity matrix yields ellipsoidal power-density surfaces from the equation

$$P = \vec{E} \cdot \vec{J} = \vec{E} \cdot \hat{\sigma} \vec{E} , \tag{42}$$

where P is the power density resulting from the application of an electric field $\vec{E}$. Both $\hat{m}$ and $\hat{\sigma}|_{H=0}$ must satisfy crystal symmetry, which means that the ellipsoidal energy surfaces and the power-density surfaces in zero magnetic field also satisfy crystal symmetry.

So for bismuth telluride, one may have an energy ellipsoid of tilt angle θ_1 and a power-density ellipsoid of tilt angle θ_2 from the threefold axis. If $\hat{\tau}$ is symmetric, then θ_1 equals θ_2. However, if $\hat{\tau}$ is not symmetric, then θ_1 and θ_2 are not equal. Using the data table of Hübner[3] for bismuth telluride, one finds θ_2 of about 35° while θ_1 is unknown.

CONCLUSIONS

The use of an anisotropic relaxation time in magnetoconductivity calculations for a group of ellipsoids is straightforward. It can be included in the original Boltzmann equation as a collision term, which permits extending the calculations to transport coefficients other than the electrical conductivity. The Jones-Zener series is readily obtained from a matrix expansion. The proper insertion of anisotropic relaxation times in each coefficient is obtained by this approach. The closed-form solution for the magnetoconductivity of ellipsoidal energy surfaces is good for all values of magnetic field for which Eq. (1) is valid. The Jones-Zener expansion of this solution, on the other hand, is valid only up to the critical field value given in Eq. (20). The Onsager reciprocity relation indicates the existence of ellipsoidal surfaces of constant power density in zero magnetic field, and thereby puts restrictions on the relaxation-time matrix $\hat{\tau}$.

APPENDIX A: CONDUCTIVITY IN DEFORMED COORDINATES

Using Eq. (24), the quantities in Eq. (23) transform as

$$\vec{p} = \alpha_0^{1/2}\hat{\alpha}^{-1/2}\vec{w}\ , \tag{A1}$$

$$\vec{v} = \alpha_0^{1/2}\hat{\alpha}^{1/2}\vec{w}\ , \tag{A2}$$

and

$$d^3p = \alpha_0^{3/2}(\alpha_1\alpha_2\alpha_3)^{-1/2}d^3w\ . \tag{A3}$$

The current density then becomes

$$\vec{J} = 2eh^{-3}c\alpha_0^{5/2}(\alpha_1\alpha_2\alpha_3)^{-1/2} \times\int \hat{\alpha}^{1/2}\vec{w}\,(\vec{G}\,\hat{\alpha}^{-1/2}\vec{w}\cdot\vec{E})\,\frac{\partial f_0}{\partial\epsilon}\,d^3w\ .$$

Letting $dS(\epsilon)$ be an element of area on the constant-energy sphere in w space gives

$$d^3w = dS(\epsilon)d\epsilon/(\alpha_0 w)\ . \tag{A4}$$

Writing all matrix products in the form

$$(\hat{A}\hat{B})_{ij} = \textstyle\sum_k A_{ik}B_{kj}\ , \tag{A5}$$

and using the relations

$$\int w_k w_m dS(\epsilon) = \tfrac{4}{3}\pi w^4\delta_{mk}\ , \tag{A6}$$

$$w^3 = (2\epsilon/\alpha_0)^{3/2}\ , \tag{A7}$$

$$\textstyle\sum_k (\hat{\alpha}^{1/2})_{ik}(\hat{\alpha}^{-1/2})_{lk} = \delta_{il}\ , \tag{A8}$$

yields the result

$$\vec{J} = (\tfrac{16}{3}\sqrt{2})\,eh^{-3}\pi c(\alpha_1\alpha_2\alpha_3)^{-1/2}\int \epsilon^{3/2}\,\frac{\partial f_0}{\partial\epsilon}\,\hat{G}\vec{E}d\epsilon\ . \tag{A9}$$

The conductivity matrix is then identified as the right-hand side of Eq. (A9) except for $\vec{E}$, the electric field, which is Eq. (25) of the paper.

APPENDIX B: ALTERNATE CONDUCTIVITY EXPRESSIONS AND CONVERGENCE OF JONES-ZENER SERIES

The $[\hat{F}-\hat{H}]^{-1}$ of Eq. (27) can be expanded by tensor analysis[13] using the Levi-Civita symbol defined as

$$\delta_{abc} = \begin{cases} 0 & \text{if any two indices are equal} \\ 1 & \text{if } a,\ b,\ c \text{ is an even permutation of } 1,\ 2,\ 3 \\ -1 & \text{if } a,\ b,\ c \text{ is an odd permutation of } 1,\ 2,\ 3. \end{cases} \tag{B1}$$

Using this symbol, the inverse of a matrix can be written as

$$(\hat{M}^{-1})_{ij} = \sum_{a,b,c,d}\frac{1}{2}\,\frac{\delta_{abi}\delta_{cdj}M_{ca}M_{db}}{|\hat{M}|}\ . \tag{B2}$$

The determinant $|\hat{M}|$ can also be expanded using Levi-Cevita symbols. Applying this technique to Eq. (27) yields the result

$$\sigma_{ij} = nec\sum_{l,m,r,s,p}[\tfrac{1}{2}\delta_{lmj}\delta_{rsi}F_{lr}F_{ms} + (\delta_{mpj}H_i + \delta_{imj}H_p)F_{mp} + H_iH_j]/ [|\hat{F}| + \vec{H}\circ\hat{F}\vec{H} + \sum_{a,b,c,d}\delta_{abc}H_dF_{ad}F_{bc}]\ . \tag{B3}$$

Using the result of Eq. (32) that $\hat{F}$ is symmetric, Eq. (B3) simplifies to give

$$\sigma_{ij} = nec[|\hat{F}|(\hat{F}^{-1})_{ij} + H_iH_j + \sum_{m,p}\delta_{imj}H_pF_{mp}]/[|\hat{F}| + H\cdot\hat{F}H]\ . \tag{B4}$$

Convergence of Jones-Zener Series

When the conductivity is expressed in the form of Eq. (B4), the denominator can be expanded as an infinite series in the magnetic field magnitude H as

$$[|\hat{F}| + \vec{H}\cdot\hat{F}\vec{H}]^{-1} = [|\hat{F}| + H^2\vec{U}\circ\hat{F}\vec{U}]^{-1} = [1 - \vec{U}\circ\hat{F}\vec{U}H^2 + (\vec{U}\circ\hat{F}\vec{U}H^2)^2 - \cdots]/|\hat{F}|\ , \tag{B5}$$

where $\vec{U}$ is a unit vector in the direction of the magnetic field. When this series is multiplied into the numerator of Eq. (B4), the Jones-Zener series for σ_{ij} is obtained. Because this numerator is always finite, the convergence of the series of Eq. (B5) coincides with the convergence of the Jones-Zener series. The denominator of Eq. (B5) is of the form $(a+bH^2)^{-1}$, where a and b are constants independent of the magnitude of the magnetic field. (Of course,

b depends on the direction of the magnetic field.) The convergence of this series expansion is determined by the ratio test of adjacent terms of the series. Convergence requires that

$$H^4 < (a/b)^2. \tag{B6}$$

An equality sign in Eq. (B6) makes the series diverge, and, therefore, gives the "critical" magnitude of the magnetic field. Using Eq. (B5) for the values of the constants a and b gives the critical field value

$$H_c^4 = (|\hat{F}|/\vec{U}\cdot\hat{F}\vec{U})^2 , \tag{B7}$$

which is Eq. (20) of the paper. One observes that this value is a function of the direction of the magnetic field through the unit vector $\vec{U}$.

APPENDIX C: JONES-ZENER COEFFICIENTS FOR CONDUCTIVITY

Experimental papers[2,3] normally determine coefficients of the Jones-Zener expansion of the conductivity, which is written as

$$\sigma_{ij} = \sigma_{ij}^{(0)} + \sigma_{ijk}^{(1)} H_k + \sigma_{ijk_1k_2}^{(2)} H_{k_1} H_{k_2} + \cdots . \tag{C1}$$

This amounts to a Taylor series with the coefficients given by

$$\sigma_{ijk_1k_2\cdots k_N}^{(N)} = \frac{1}{N!}\left(\frac{\partial^N \sigma_{ij}}{\partial H_{k_1}\cdots\partial H_{k_N}}\right)\Bigg|_{H=0} . \tag{C2}$$

Expanding Eq. (27) in a matrix series as given by Eq. (16) yields the Jones-Zener coefficients when Eq. (C2) is applied. [This development can be made for all equations containing $(F-H)^{-1}$.] The results are

$$\sigma_{ij}^{(0)} = nec(\hat{F})_{ij}^{-1} , \tag{C3}$$

$$\sigma_{ijk}^{(1)} = nec \sum_{ab} (\hat{F}^{-1})_{ia}\delta_{abk}(\hat{F}^{-1})_{bj} , \tag{C4}$$

$$\sigma_{ijk_1k_2\cdots k_N}^{(N)} = \frac{nec}{N!} P_{k_1\cdots k_N} \sum_{\substack{a_1\cdots a_N \\ b_1\cdots b_N}} (\hat{F}^{-1})_{ia_1} \times \delta_{a_1b_1k_1}(\hat{F}^{-1})_{b_1a_2}\delta_{a_2b_2k_2}\cdots(\hat{F}^{-1})_{b_{N-1}a_N} \times \delta_{a_Nb_Nk_N}(\hat{F}^{-1})_{b_Nj} , \tag{C5}$$

where $P_{k_1\cdots k_N}$ is a permutation operator which sums all possible permutations of the variables $k_1\cdots k_N$. Since

$$\hat{F}^{-1} = (e/c)\hat{\alpha}\hat{\tau} = (e/c)(\hat{\tau}')\hat{\alpha} , \tag{C6}$$

it is clear how the anisotropic relaxation-time matrix, whether it be in the form $\hat{\tau}$ or $\hat{\tau}'$, fits into the Jones-Zener expansion. Equation (20) yields the region for which the expansion converges.

APPENDIX D: GROUP OF THREE ELLIPSOIDS

Taking three identical ellipsoids symmetrically placed about the Z axis, one calculates the total conductivity by Eq. (30), where $\hat{R}_k$ is the rotation matrix which rotates the ellipsoid (and $\hat{F}$) about the Z axis by 120° increments.

Doing this, and expanding $\hat{\sigma}_t$ in a Jones-Zener expansion, Eq. (35) requires

$$(\hat{\sigma}_t)_{ij}\big|_{H=0} = (\hat{\sigma}_t)_{ji}\big|_{H=0} , \tag{D1}$$

$$(\hat{\sigma}_t)_{ijk} = -(\hat{\sigma}_t)_{jik} , \tag{D2}$$

and more equations for the higher-order coefficients. From Eq. (D2), consider the particular elements giving

$$(\hat{\sigma}_t)_{333} = 0, \tag{D3}$$

$$(\hat{\sigma}_t)_{231} + (\hat{\sigma}_t)_{321} = 0, \tag{D4}$$

$$(\hat{\sigma}_t)_{111} = 0, \tag{D5}$$

$$(\hat{\sigma}_t)_{112} = 0 . \tag{D6}$$

From Eqs. (30) and (D1) one has

$$(\hat{F}^{-1})_{12} = (\hat{F}^{-1})_{21} \tag{D7}$$

and

$$(\hat{F}^{-1})_{13}(\hat{F}^{-1})_{32} - (\hat{F}^{-1})_{31}(\hat{F}^{-1})_{23} = 0 , \tag{D8}$$

and from Eq. (D4)

$$(\hat{F}^{-1})_{13}^2 - (\hat{F}^{-1})_{31}^2 = (\hat{F}^{-1})_{23}^2 - (\hat{F}^{-1})_{32}^2 . \tag{D9}$$

Equations (D8) and (D9) have the two nontrivial solutions

$$(\hat{F}^{-1})_{13} = (\hat{F}^{-1})_{31} \tag{D10}$$

and

$$(\hat{F}^{-1})_{23} = (\hat{F}^{-1})_{32} , \tag{D11}$$

or

$$(\hat{F}^{-1})_{13} = -(\hat{F}^{-1})_{31} \tag{D12}$$

and

$$(\hat{F}^{-1})_{23} = -(\hat{F}^{-1})_{32} . \tag{D13}$$

Equations (D5) and (D6) establish Eqs. (D10) and (D11) as the proper solution for the three ellipsoids. Equations (D7), (D10), and (D11) require $(\hat{F}_k)^{-1}$ and thus $\hat{F}_k$ to be a symmetric matrix for all k, which is identical to the single ellipsoid result.

The example of Paper I assumed a single matrix $\hat{\tau}$ defined in the laboratory reference system. It should then not be transformed by the rotation matrix $\hat{R}$. In this case, the correct way to calculate the total conductivity is

$$\hat{\sigma}_t = nec \sum_k [(c/e)(\hat{\tau})^{-1}\hat{R}_k\hat{m}(\hat{R}_k)^{-1} - \hat{H}]^{-1} . \tag{D14}$$

However, the $\hat{\tau}$ for that example was chosen isotropic in the X-Y plane and the rotation $\hat{R}$ was about the Z axis, giving the special result

$$\hat{R}_k(\hat{\tau})^{-1}(\hat{R}_k)^{-1} = (\hat{\tau})^{-1} . \tag{D15}$$

Therefore, Eqs. (D14) and (D30) are equivalent for that example, and one is left with the requirement that $\hat{F}$ be symmetric.

[1]*The Fermi Surface*, edited by W. A. Harrison and M. R. Webb (Wiley, New York, 1961).
[2]R. Hartman, Phys. Rev. 181, 1070 (1969).
[3]U. Hübner, Z. Naturforsch. 22, 2086 (1967).
[4]H. J. Mackey and J. R. Sybert, Phys. Rev. 180, 678 (1969).
[5]C. Herring and E. Vogt, Phys. Rev. 101, 944 (1956).
[6]A. G. Samoylovich and I. I. Pinchuk, Phys. Metals Metallog. (USSR) (English transl.) 20, 23 (1965).
[7]I. Ya. Korenblit, Fiz. Tverd. Tela 2, 3083 (1960) [Soviet Phys. Solid State 2, 2738 (1961)].
[8]A. H. Wilson, *The Theory of Metals*, (Cambridge U. P., Cambridge, England, 1958), p. 208 ff.
[9]H. Jones and C. Zener, Proc. Royal Soc. (London) A145, 268 (1934).
[10]Various ways of expanding $[\hat{A}-\hat{B}]^{-1}$ are given in the Appendix of P. O. Löwdin, J. Math. Phys. 3, 969 (1962).
[11]A. C. Smith, J. F. Janak, and R. B. Adler, *Electronic Conduction in Solids* (McGraw-Hill, New York, (1967).
[12]The $\hat{\tau}$ of this paper is the transpose of the $\hat{\tau}$ of Ref. 7 and Paper I, because in those papers the collision term is approximated as $(\partial f_0/\partial\epsilon)\hat{\tau}^{-1}\hat{m}\vec{C}\cdot\hat{m}^{-1}\vec{p}$.
[13]A. J. McConnell, *Applications of Tensor Analysis* (Dover, New York, 1957).

PHYSICAL REVIEW B VOLUME 2, NUMBER 10 15 NOVEMBER 1970

New Method for Computing the Weak-Field Hall Coefficient. II. Some Extensions and Modifications*

R. S. Allgaier
U. S. Naval Ordnance Laboratory, White Oak, Silver Spring, Maryland 20910
(Received 27 January 1970)

An earlier paper described a simple method for computing the weak-field Hall coefficient through the use of a Fermi surface composed entirely of planar faces. That paper developed a set of rules which linked the general behavior of the Hall coefficient to two fundamental properties of transport models, Fermi-surface shape and scattering anisotropy. The present paper reformulates those rules by adding a third ingredient to the model description, shape evolution. Exceptions to the earlier rules are thereby eliminated. The present paper also extends the simple method to noncubic models. The results for "undulating cylinders" (a Fermi-surface approximation for some hexagonal metals) and toroidal Fermi surfaces (a possible model for the wurtzite lattice) are analyzed. Finally, the effect of rounding the sharp edges at which the planar Fermi-surface faces intersect is investigated. The results resolve an apparent paradox pointed out by Stern, and provide some insight into the general magnetic field dependence of the Hall coefficient.

I. INTRODUCTION

In an earlier paper, a new method was described for computing approximate values of the weak-field Hall coefficient R_0.[1] The essential feature of the procedure is to replace the actual Fermi surface by one composed entirely of planar faces. The advantage of the method is its simplicity; it is possible to obtain results for a wide variety of models, including those in which both Fermi-surface distortion and anisotropic scattering play an important role, without becoming involved in complicated mathematics.

The Hall coefficient ought to be one of the best understood transport coefficients; after all, it depends essentially on a single electronic parameter, charge density. But R_0 is also influenced, in a more subtle way, by dimensionless functions of carrier velocity and scattering time. These functions stem from specific details of the model under consideration, but their effect on R_0 has never been well understood in a broad sense.

Those few papers which do discuss the general behavior of R_0 generally relate it to two fundamental properties of a model, the shape of the Fermi surface and the scattering anisotropy. In I, we attempted to develop a set of rules for the behavior of R_0 which were related to these two fundamental properties, and which would apply to all known models for which a scattering time was defined.

In Sec. II of the present paper, we reformulate those rules in terms of three fundamental model properties, the additional one being *shape evolution*, i.e., the manner in which the Fermi-surface shape changes as a function of the Fermi energy. As a consequence, we develop a distinctly different viewpoint from which to describe and understand the links between the essential characteristics of a model and the general behavior of R_0.

In I, all of the models discussed had over-all cubic symmetry. Section III of the present paper treats two noncubic models. Mathematically speaking, the extension is trivial and uninteresting. But the simple form of the results makes it possible to present, for the first time, a clear cut and realistic