ANISOTROPIC RELAXATION TIME FOR
SOLIDS WITH ELLIPSOIDAL
FERMI SURFACES

DISSERTATION

Presented to the Graduate Council of the
North Texas State University in Partial
Fulfillment of the Requirements

For the Degree of

DOCTOR OF PHILOSOPHY

By

Troy D. Fuchser, B. S., M. S.
Denton, Texas
May, 1971

Many solids have Fermi surfaces which are approximated as ellipsoids. A comprehensive solution for the magnetoconductivity of an ellipsoid is obtained which proves the existence of a relaxation time tensor which can be anisotropic and which is a function of energy only. (It is not a function of magnetic field or of position on the Fermi surface.) By expanding each term of the Boltzmann transport equation in spherical harmonics within a deformed coordinate system, a solution is found for only the conductivity portion of the electron distribution function which is much simpler than the solution for the total distribution function. The resulting conductivity is \( \sigma = n e c (c/e) \tau^{-1} H^{-1} \), where \( \tau \) is the relaxation time tensor and \( H \) is a tensor describing the magnetic field. The Jones-Zener series is readily obtained to arbitrary order by expanding \( \sigma \) in a matrix series in powers of \( H \), and its exact limits of convergence are given. Onsager reciprocity requires \( \tau^{-1} \) to be symmetric and power density surfaces to be ellipsoidal. Crystal symmetry further restricts \( \sigma \) and thus the relaxation time tensor \( \tau \).

A theoretical solution of \( \tau \) is obtained for fixed scatterers with screened coulomb potentials. The collision term is evaluated by expanding in powers of the screening
length, or alternately in powers of the anisotropy of the mass. The relaxation time tensor for the total distribution function has elements which depend on position on the Fermi surface, in contrast to the $\hat{\tau}$ for the conductivity. The conductivity $\hat{\tau}$ is an analytic expression in terms of the screening length, the Fermi energy, and the mass tensor. The anisotropic mass is the causitive factor in making the relaxation time anisotropic.
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I. 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.\(^3,4\) A previous paper by Mackey and Sybert,\(^5\) 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,\(^6\) in theories for bismuth by Hartman\(^2\) and by Samoylovich and Pinchuk,\(^7\) and in theories for bismuth telluride by Korenblit\(^8\) and by Hubner.\(^3\)

The theories for bismuth and bismuth telluride are applicable to the whole group of solids which have ellipsoidal Fermi surfaces (e.g. indium antimonide under uniaxial stress), and it is unfortunate that exposure has been restricted to researchers working with these two materials. It was also found that in many cases the results could be written in a simpler form which greatly facilitates further calculations. Thus, it seemed worthwhile to extend the results of these papers and to provide a more comprehensive treatment for anisotropic relaxation time tensors.

This treatment consists of three primary sections. The first is Section II, which starts with the Boltzmann transport
equation and shows that a relaxation time tensor always exists in the electrical conductivity of an ellipsoidal Fermi surface. It also concludes that in a general distribution function for electrons, only a special part contributes to the electrical conductivity. This part only is solved for in Section III, and the electrical conductivity is solved for the case where the relaxation time tensor is to be found experimentally or by a separate theoretical calculation. When the relaxation time tensor is independent of the magnetic field, the conductivity is readily expanded in a Jones-Zener series to arbitrary order in the magnetic field. A critical field value for which the series is no longer valid is given exactly. The conductivity is also investigated under the restrictions imposed by the Onsager reciprocity relation and by crystal symmetry requirements. These considerations restrict the possible form of the relaxation time tensor, as well as pointing out the existence of ellipsoidal power density surfaces. Finally, Section IV calculates the relaxation time tensor from first principles assuming fixed scattering centers. This calculation results in an analytical expression showing the dependence of the relaxation time tensor upon the mass tensor.

These three sections present derivations in sufficient detail for one to observe the methods used, the assumptions made, and the conclusions drawn. The appendixes supply additional information and the more involved calculations for those who wish to follow a derivation in greater detail.
II. IDENTIFICATION OF INVERSE RELAXATION TIME TENSOR $\tau^{-1}$

The Boltzmann transport equation is

$$\nabla_x f \cdot \frac{\partial f}{\partial x} - \nabla_y f \cdot \left[ eE + (e/c) \frac{\partial \mathbf{H}}{\partial y} \right] = \left( \frac{\partial f}{\partial t} \right)_c,$$

(1)

where $e = |e|$ is the electron charge and $f$ is the distribution function for the electrons. Here $f$ is calculated as though the electron has no spin. The spin degeneracy then appears as a factor of two in all calculations involving the number of electrons, such as the electrical current density. This convention is discussed further in Section IV and in Appendix F on electron spin degeneracy. For ellipsoidal energy surfaces the energy is

$$2e = \mathbf{p} \cdot \mathbf{p}^{-1} \mathbf{p} = \mathbf{p} \cdot \mathbf{a} \mathbf{p},$$

(2)

and the velocity is given by

$$\dot{v} = \nabla_p e = \mathbf{a} \mathbf{p}.$$

(3)

Now define $f_1(k)$, abbreviated as $f_1$, as a small perturbation of the distribution function from the equilibrium distribution function $f_0$, or $f_1 = f - f_0$. Assuming isothermal conditions and $\nabla_x f = 0$ in Eq. (1), using Eq. (3), and keeping only first order terms yields

$$e \left( \frac{\partial f_0}{\partial e} \right) \ddot{v} \cdot \mathbf{E} + (e/c) \dddot{v} \cdot \mathbf{H} \cdot \nabla_p f_1 = - \left( \frac{\partial f}{\partial t} \right)_c.$$

(4)

If the collision term $\left( \frac{\partial f}{\partial t} \right)_c$ is known, then the solution of Eq. (4) will yield $f_1$. However, it is shown in Appendix A
that if $f_1$ is expanded in a spherical harmonic series and then used to calculate the electrical conductivity or current density, only part of $f_1$ designated as $f_1^{(c)}$, is actually needed. From expanding the collision term $(\partial f/\partial t)_c$ in Eq. (4) as a spherical harmonic series, it is also shown that only part of the collision term, designated $(\partial f/\partial t)^{(c)}_c$, is needed to solve for $f_1^{(c)}$. These conductivity portions can always be written in the form

$$f_1^{(c)} = -(\partial f_\circ/\partial \varepsilon)^c \cdot p,$$  

(5)

$$(\partial f/\partial t)^{(c)}_c = (\partial f_\circ/\partial \varepsilon)^c \cdot p^{-1} m \cdot \tau^{-1} m \cdot p,$$  

(6)

where $\tau^{-1}$ depends on $p$ only through the energy.

To obtain the significance of $\tau^{-1}$, consider the standard scalar relaxation time approximation used in calculating the conductivity of spherical energy surfaces,

$$(\partial f/\partial t)_c = -\tau^{-1} f_1.$$  

(7)

Comparing Eqs. (5) and (6) with Eq. (7), one notes that for spherical energy surfaces, $\tau^{-1}$ must reduce to the scalar $\tau^{-1}$. Therefore, the total terms $f_1$ and $(\partial f/\partial t)_c$ may or may not reduce to Eq. (7), but the conductivity portions $f_1^{(c)}$ and $(\partial f/\partial t)^{(c)}_c$ always do. Thus, $\tau^{-1}$ is called the inverse relaxation time tensor for the conductivity, and it always exists for ellipsoidal energy surfaces, as pointed out by Korenblit. This fact is also apparent in the conductivity
III. CONDUCTIVITY SOLUTION FOR INDEPENDENTLY DETERMINED $\hat{\tau}$

If one calculates $\hat{\tau}$ from first principles and the scattering integral, then usually more than the $f_{1}^{(c)}$ portion of $f_{1}$ is needed in order to calculate $(\partial f/\partial t)^{(c)}$. This will be the case in the next section where such a calculation is carried out. On the other hand, if one is interested in determining the magnitude of the elements of $\hat{\tau}$ experimentally or in a separate calculation, a much simpler solution of $f_{1}^{(c)}$ is possible. Then $\hat{\tau}^{-1}$ in Eq. (6) is treated as an unknown function of energy, and according to Appendix A, a new transport equation is obtained by replacing $f_{1}$ by $f_{1}^{(c)}$ and $(\partial f/\partial t)^{(c)}$ by $(\partial f/\partial t)^{(c)}$ in Eq. (4). This gives

$$
(\partial f^{(c)}/\partial t)[ev \cdot \hat{E} - (e/c)v \times \hat{H} \cdot \nabla p(C \cdot \hat{p}) + m^{-1} \cdot \nabla \cdot mC \cdot \hat{p}] = 0. \quad (8)
$$

Solving this equation for $\hat{C}$ gives $f_{1}^{(c)}$ in terms of $\hat{\tau}^{-1}$ and the applied electric and magnetic fields.

Solution of Transport Equation

The cross product term of Eq. (8) yields $-(e/c)v \cdot \hat{H} \times \hat{C}$. But $\hat{H} \times \hat{C}$ can be written in matrix form as

$$
\hat{H} \times \hat{C} = \hat{H} \hat{C}, \quad (9)
$$

where

$$
\hat{H} = \begin{bmatrix}
0 & -H_3 & H_2 \\
H_3 & 0 & -H_1 \\
-H_2 & H_1 & 0
\end{bmatrix}. \quad (10)
$$
Using Eqs. (3) and (9) in Eq. (8), and noting that Eq. (8) must be satisfied for arbitrary \( \hat{v} \), one finds

\[
\frac{\partial \hat{\eta}}{\partial v} - \hat{\eta} + \left( \frac{c}{e} \right) \hat{m} \hat{\eta} = 0,
\]

(11)

Equation (11) has the solution

\[
\hat{\eta} = -c \hat{G} \hat{E},
\]

(12)

where

\[
\hat{G} = (\hat{F} - \hat{H})^{-1},
\]

(13)

\[
\hat{F} = \left( \frac{c}{e} \right) \hat{m}. \tag{14}
\]

Equations (12) and (5) yield

\[
f^{(c)}_1 = c \left( \frac{\partial f}{\partial \varepsilon} \right) \hat{P} \hat{G} \hat{E} \tag{15}
\]

This is a closed form solution of the conductivity portion of the distribution function for ellipsoidal energy surfaces. To find the Jones-Zener expansion\(^{10}\) of \( f^{(c)}_1 \) (and thus of the conductivity calculated from \( f^{(c)}_1 \)), one first expands \((\hat{F} - \hat{H})^{-1}\) in a matrix series\(^{11}\) about the matrix \( \hat{H} \), giving

\[
(\hat{F} - \hat{H})^{-1} = \hat{F} + \hat{F} \hat{H} \hat{F}^{-1} \hat{H} + \hat{F} \hat{H} \hat{F}^{-1} \hat{H} \hat{F}^{-1} + \cdots \tag{16}
\]

This expansion in Eq. (15) gives the Jones-Zener series for \( f^{(c)}_1 \) as

\[
f^{(c)}_1 = c \left( \frac{\partial f}{\partial \varepsilon} \right) \left( \hat{P} \hat{F}^{-1} \hat{H} + \hat{P} \hat{F}^{-1} \hat{H} \hat{F}^{-1} \hat{H} + \cdots \right). \tag{17}
\]
Note that Eq. (17) is a power series in the magnitude of the magnetic field $\hat{H}$,\(^{12}\) for one can define a unit vector $\hat{U}$ in the direction of the magnetic field such that

$$\hat{H} = \hat{H}\hat{U},$$

(18)

and

$$\hat{H} = \hat{H}\hat{U}.$$  \(19\)

($\hat{U}$ is an orientation matrix containing the same information as the vector $\hat{U}$.) 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.\(^{12,13}\) The critical field of the Jones-Zener series is derived in Appendix C to be

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

where $\hat{F}$ is a symmetric matrix (to be 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

$$eH_c\tau/mc = 1.$$  \(21\)

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 $\mathbf{F}^{-1}\mathbf{H}$ 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 $H < H_c$, where $H_c$ is given by Eq. (20). However, for electron ellipsoids in bismuth with the magnetic field along the 3-fold axis Hartman's condition gives $H < 0.96 H_c$.

Conductivity

The current density is calculated as

$$\mathbf{J} = -2e\hbar^{-3} \int \mathbf{v} \mathbf{f} \, d^3\mathbf{p}, \quad (22)$$

which from Eq. (15) becomes

$$\mathbf{J} = -2e\hbar^{-3} \mathbf{v} \left( G^* \mathbf{E} \right) (\partial f_0 / \partial c) \, d^3\mathbf{p}. \quad (23)$$

Note that $\mathbf{G}$ or $\mathbf{G}$ perform operations which differ according to the direction of $\mathbf{p}$, 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 $w$-space such that constant energy surfaces are expressed as

$$2\epsilon = \alpha \mathbf{w} \cdot \mathbf{w}, \quad (24)$$

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

\[
\hat{\sigma} = -(16/3)\sqrt{2}\varepsilon_e h^{-3} |\hat{\sigma}|^{-1/2} \int \varepsilon^{3/2} \left( \frac{\partial f_0}{\partial \varepsilon} \right) (\hat{F} - \hat{H})^{-1} d\varepsilon.
\]  

(25)

This expression is applicable to either semiconductors or semimetals where Eqs. (2) and (3) hold. The energy dependence for the elements of the relaxation time tensor 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

\[
(\frac{\partial f_0}{\partial \varepsilon}) = -\delta(\varepsilon - \varepsilon_f),
\]

(26)

where \(\varepsilon_f\) is the Fermi energy. The conductivity tensor is then

\[
\hat{\sigma} = \text{ne}c(\hat{F} - \hat{H})^{-1},
\]

(27)

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

\[
n = \frac{(16/3)\sqrt{2}\pi h^{-3}}{|\hat{\sigma}|^{-1/2}} \varepsilon_f^{3/2}
\]

(28)

is the number of electrons per unit crystal volume in the energy ellipsoid \(2\varepsilon_f = \hat{p} \cdot \hat{\sigma} \hat{p}\). 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 C.
Equation (16) can also be combined with Eq. (27) to yield 
the Jones-Zener series for the conductivity. These coef-
ficients are given in Appendix D.

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

\[
\hat{\sigma}_t = ec \sum_k n_k (\hat{F}_k - \hat{H})^{-1}.
\]  \hspace{1cm} (29)

If \( \hat{r} \) and \( \hat{m} \) are given in an ellipsoid's principle axis system, 
they must be transformed to the laboratory reference system 
by a similarity transformation. Let \( \hat{R}_k \) be a rotation tensor 
relating the \( k \)-th ellipsoidal principle 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

\[
\hat{\sigma}_t = ec \sum_k n (\hat{R}_k \hat{F}_k \hat{R}_k^{-1} - \hat{H})^{-1}.
\]  \hspace{1cm} (30)
Onsager Reciprocity

The Onsager reciprocity relation\textsuperscript{1,2} requires the conductivity tensor to satisfy

\[ \hat{\sigma}(\hat{H}) = \tilde{\sigma}(-\hat{H}). \]  

(31)

This puts restrictions on the tensor \( \hat{F} \) and thus on the relaxation time tensor \( \hat{\tau} \). 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

\[ \hat{F} = \tilde{F}, \]  

(32)

since

\[ \tilde{H} = -\hat{H}. \]  

(33)

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

\[ \int \varepsilon^{3/2} \left( \frac{\partial f_o}{\partial \varepsilon} \right) (\hat{F} - \hat{H})^{-1} \, d\varepsilon = \int \varepsilon^{3/2} \left( \frac{\partial f_o}{\partial \varepsilon} \right) (\tilde{F} - \tilde{H})^{-1} \, d\varepsilon \]  

(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 proposes that for bismuth a predominant form of 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

\[ \hat{\sigma}_t(\hat{H}) = \hat{\sigma}_t(-\hat{H}). \]  

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 E shows that Onsager reciprocity requires the \( \hat{F} \) tensor of each ellipsoidal surface to be symmetric. The \( \hat{F} \) (or \( \hat{H}^S \)) of Paper I was thought to satisfy Onsager reciprocity, but it is not symmetric and therefore does not. This error resulted from checking Eq. (35) for a magnetic field in the Z direction only.

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

\[ n_k \text{ec}(\hat{F}_k^e-\hat{H})^{-1}. \] 

(36a)
where

\[ \hat{F}_l = \hat{F}_k, \]  

(36b)

and

\[ n_l = n_k. \]  

(36c)

But finding a physical situation in which ellipsoids could pair off according to Eqs. (36a) through (36c) 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. (14) one has

\[ \hat{\tau}^{-1} \hat{m} = \hat{m}^{-1}. \]  

(37)

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

\[ \hat{\tau}^{-1} \hat{m} = \hat{m}^{-1}. \]  

(38)

which in the ellipsoidal principal axis system gives

\[ \tau_{ij} = (m_i/m_j) \tau_{ji}, \]  

(39)

in agreement with Korenblit\(^8\) and others.\(^3,7\) \( \hat{\tau} \) must be symmetric if it is to have an orthogonal principal axis system in p-space. With Eq. (38) this gives
\[ \hat{m} \hat{m} = \hat{m} \hat{m}. \] (40)

Since for this case \( \hat{r} \) 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,\(^6\) and by Hartman.\(^2\) However, when the crystal symmetry does not completely specify the ellipsoidal energy surface orientation, Onsager reciprocity does not require \( \hat{r} \) to be completely symmetric.

For nonsymmetric \( \hat{r} \) it is instructive to consider bismuth telluride where the energy ellipsoids are symmetrically placed about a three-fold axis. These ellipsoids may be tilted an angle \( \theta \) from the three-fold axis. (Crystal symmetry specifies the orientation of the energy ellipsoids about symmetry axes in p-space except for the angle \( \theta \).)

First consider the conductivity of a single energy ellipsoid with no magnetic field, which is

\[ \hat{\sigma} = O c \hat{F}^{-1}. \] (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. (2), a symmetric conductivity tensor yields ellipsoidal power density surfaces from the equation

\[ P = \hat{E} \cdot \hat{J} = \hat{E} \cdot \hat{\sigma} \hat{E}, \] (42)
where $P$ is the power density resulting from the application of an electric field $\mathbf{E}$. Both $\hat{m}$ and $\hat{e}|_{H=0}$ 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 $\theta_1$ and a power density ellipsoid of tilt angle $\theta_2$ from the three-fold axis. If $\hat{r}$ is symmetric, then $\theta_1$ equals $\theta_2$. However, if $\hat{r}$ is not symmetric, then $\theta_1$ and $\theta_2$ are not equal. According to Mallinson, Rayne, and Ure, bismuth telluride has a $\theta_1$ of $25.4^\circ$ while $\theta_2$ is either plus or minus $14^\circ$. 
IV. THEORETICAL DERIVATION OF $\hat{\tau}$

In the previous section, the inverse relaxation time tensor $\tau^{-1}$, and thus the collision term $(\partial f/\partial t)_c$, was treated as an unknown to be found either by fitting the conductivity expression to experimental data, or by a separate theoretical calculation. Such a separate theoretical calculation is obtained in this section by evaluating the collision term from first principles. This term is then used in the Boltzmann transport equation, Eq. (4), to solve for $f_1$ with an electric field only. Equation (22) then yields the conductivity. This calculation is of particular interest because it yields theoretical expressions for $\hat{\tau}$, and thus gives insight into the origin of anisotropic relaxation times.

Collision Term Calculation

The transition rate of the distribution function due to collisions is

$$
(\partial f/\partial t)_c = \sum_{\vec{k}' \to \vec{k}} \left( \frac{p}{\hbar} f(\vec{k}') [1-f(\vec{k})] - f(\vec{k}) [1-f(\vec{k}')]) \right),
$$

where $\hbar = (\hbar/2\pi)\vec{k}'$, $S_{\vec{k}' \to \vec{k}}$ is the transition probability per unit time that an electron in state $\vec{k}'$ will go to an empty state $\vec{k}$, $f(\vec{k}')$ is the probability of state $\vec{k}'$ being occupied by an electron, and $[1-f(\vec{k})]$ is the probability that state $\vec{k}$ is empty. The $[1-f(\vec{k})]$ factor is an expression of the Pauli exclusion principle for fermions and prevents scattering into already filled states. Thus, $\sum_{\vec{k}' \to \vec{k}} S_{\vec{k}' \to \vec{k}} f(\vec{k}') [1-f(\vec{k})]$ gives the
scattering into state \( \vec{k}_k \), and \( \sum_{k' \rightarrow k} S_{k' \rightarrow k} f(\vec{k}) [1 - f(\vec{k})] \) gives the scattering out of state \( \vec{k}_k \). If \( S_{k' \rightarrow k} = S_{k \rightarrow k'} \) as will be evident later, then Eq. (43) can be simplified. From the definition of equilibrium, \( (\partial f / \partial t) = 0 \). With \( f_1(\vec{k}) = f(\vec{k}) - f_0(\vec{k}) \), this allows Eq. (43) to be written as

\[
(\partial f / \partial t) = \sum_{k' \rightarrow k} S_{k' \rightarrow k} [f_1(\vec{k}') - f_1(\vec{k})].
\] (44)

In accounting for the spin of electrons, the usual convention is taken that two electrons can exist in a particular state \( \vec{k} \), and the number of electrons per unit crystal volume is

\[
n = \left( \frac{2}{L^3} \right) \sum_{\vec{k}} f(\vec{k}),
\] (45)

where the factor of two is due to the spin degeneracy and \( L^3 \) is the volume of the sample. In this convention, \( \sum_{\vec{k}} f(\vec{k}') \) and \( (\partial f / \partial t)_c \) are calculated without regard to spin. Appendix F gives an expanded explanation of how spin enters into the calculations and the derivation of the equivalent integral equations

\[
n = 2 \int d^3 k \rho(\vec{k}') f(\vec{k}'),
\] (46)

\[
(\partial f / \partial t)_c = \int d^3 k \rho(\vec{k}') S_{k' \rightarrow k} [f_1(\vec{k}') - f_1(\vec{k})],
\] (47)

where

\[
\rho(\vec{k}') = \frac{1}{8\pi^3}.
\] (48)

\( \rho(\vec{k}) \) is the density of states in the space \( d^3 k \). \( \rho(\vec{k}') \) and
f(\hat{k}) are also calculated as if the electron has no spin (or equivalently as if it has only one possible spin state). The spin degeneracy then shows up when the f calculated using Eq. (47) in the Boltzmann equation is substituted into Eqs. (22) or (46) involving the number of electrons.

The effective mass theorem, which is assumed valid for the solid under consideration, allows the Schroedinger equation to be written as

$$[\varepsilon(-i\nabla)+V-e(\hat{k})]\psi = \left[-\left(\frac{\hbar^2}{8\pi^2}\right)\nabla\cdot\hat{\nabla}+V-e(\hat{k})\right]\psi = 0, \quad (49)$$

where \(V\) is the potential for fields externally applied to the sample. When \(V = 0\), one has the "free electron" state (the electron with an effective mass due to the lattice) which is a plane wave \(L^{-3/2} e^{i\hat{k} \cdot \hat{x}}\). This is the state of an electron between collisions. A collision then scatters the electron into other plane wave states. Let \(V(\hat{r})\) be the potential of a single scattering center. From standard time perturbation theory the probability of this center scattering a normalized plane wave state \(\hat{k}\) into the normalized plane wave state \(\hat{k}'\) per unit time is (in the first Born approximation)

$$\frac{4\pi^2}{\hbar^2} |V_{kk'}|^2 \delta[\varepsilon(k)-\varepsilon(k')] \quad (50)$$

where

$$V_{kk'} = L^{-3} \int e^{i\hat{r} \cdot (\hat{k}'-\hat{k})} V(\hat{r}) d^3\hat{r}. \quad (51)$$

Appendix H investigates the validity of the Born approximation.
If there are $N_s$ scattering centers in the sample then one has

$$S_{kk'} = \left(4\pi^2 N_s / h\right) |V_{kk'}|^2 \delta[\varepsilon(k) - \varepsilon(k')] .$$ \quad (52)

This is the quantity needed in Eq. (47).

For simplicity, let the scattering center be at a fixed location in the lattice such as an ionic impurity. Hartman\(^2\) has indicated that electron-electron scattering may be the primary scattering mechanism in bismuth. The above analysis could be extended by treating this scattering in the center of momentum system,\(^16\) and then transforming back to the laboratory coordinate system. Let the potential due to the impurity be the screened coulomb potential

$$V(r) = v_o r^{-1} e^{-r/\lambda_s} ,$$ \quad (53)

which yields

$$|V_{kk'}|^2 = 16\pi^2 v_o L^{-6} \left[ |k-k'|^2 + \lambda_s^2 \right]^{-2} .$$ \quad (54)

$\lambda_s$ is the Debye screening length. Equations (54) and (52) are substituted into Eq. (47) to obtain $\partial f / \partial t_c$. It is then convenient to transform to $w$-space where constant energy surfaces are spheres. This transformation is

$$\alpha_o^{1/2} \w = \hat{\alpha}^{1/2} \hat{\w} = (\hbar / 2\pi) \hat{\alpha}^{1/2} \hat{k} ,$$ \quad (55)

and gives Eq. (24) for the energy. In Eq. (47), this transformation yields

$$d^3 k' \rho(k') = \hbar^{-3} |\hat{\alpha}|^{-1/2} (2\pi)^{1/2} d\varepsilon d\hat{k}' .$$ \quad (56)
where \(|a|^{-1/2}\) is the determinant of \(\hat{a}^{-1/2}\), and \(d\Omega^\prime\) is the solid angle in \(w\)-space. Equation (47) then becomes

\[
(\partial f/\partial t)_c = v_0^2 |a|^{-1/2} (4N_s/L^3 h^2) \int (2\epsilon^\prime)^{1/2} (f^\prime - f_1) \\
\times [\alpha_o^{1/2} |a^{-1/2}(\hat{w} - \hat{w}^\prime)|^2 + (h^2/4\pi^2 \lambda_s^2)]^{-2} d\epsilon^\prime d\Omega^\prime.
\] (57)

From Eq. (57) on, the arguments of \(\epsilon\) and \(f\) are dropped as it will be evident from the formula or the variables of integration whether they should be considered as functions of \(\hat{k}, \hat{p},\) or \(\hat{w}\). Thus, \(f_1(\hat{k}^\prime), f_1(\hat{p}^\prime),\) and \(f_1(\hat{w}^\prime)\) are written as \(f_1^\prime\). Using Eq. (24), and defining \(\hat{\xi}\) as a unit vector in the direction of \(\hat{w}\), the energy integration yields

\[
(\partial f/\partial t)_c = B [f_1^\prime - f_1] [1 + (\hat{\xi} - \hat{\xi}^\prime) \cdot (2\gamma a)^{-1}(\hat{\xi} - \hat{\xi}^\prime)]^{-2} d\Omega^\prime,
\] (58)

where

\[
\gamma = (h^2/16\pi^2 \lambda_s^2 \epsilon),
\] (59)

and

\[
B = 16\pi^2 v_0^2 N_s (2\epsilon)^{1/2} \lambda_s^4 |a|^{-1/2} h^{-4} L^{-3}.
\] (60)

If the form of \(f_1^\prime\) is known, the integral of Eq. (58) may be evaluated in a straightforward way, at least numerically. However, to keep the mathematical solution simple, the assumption will now be made that each element of \((2\gamma a)^{-1}\) is much less than one. The denominator (the bracket to the
minus two power) of Eq. (58) may now be expanded, and keeping only first order terms in \((\gamma a_i)^{-1}\) gives

\[
\frac{\partial f}{\partial t} = \frac{B}{(f_1^2 - f_1)} \left[ 1 - (\xi - \xi') \cdot (\gamma a)^{-1}(\xi - \xi') \right] d\Omega'.
\]  

(61)

Appendix G gives an alternate, more complicated expansion of the denominator which converges faster than the expansion of Eq. (61), particularly for a nearly isotropic mass tensor.

Solution of Transport Equation

Combining Eqs. (61) and (4) with \(\dot{H} = 0\) gives

\[
-e(\partial f_0 / \partial \varepsilon) \hat{v} \cdot \hat{E}
\]

\[
= \frac{B}{(f_1^2 - f_1)} \left[ 1 - (\xi - \xi') \cdot (\gamma a)^{-1}(\xi - \xi') \right] d\Omega',
\]  

where the relation \(\nabla \varepsilon = \hat{v}\) has been used.

The collision term of Eq. (62) includes \(f_1^2\) in the integrand, which is unknown at this point. One method of finding \(f_1\) is to correctly guess the dependence of \(f_1^2\) on the direction of the solid angle \(d\Omega'\), so that the integration can be carried out. Writing \(f_1\) in such a form and integrating, one has an equation for the unknown parameters of \(f_1\), thereby giving \(f_1\). If the proper form is not apparent, Eq. (62) may be solved by iteration. This iterative method of solution is used in Appendix I. Assume the form of \(f_1\) to be

\[
f_1 = -\left(\partial f_0 / \partial \varepsilon\right)(\dot{C}_1 + \gamma^{-1} C_2 + \gamma^{-1} \beta \gamma C_3) \cdot \hat{p},
\]  

(63)
where $\hat{C}_1, \hat{C}_2$, and $\hat{C}_3$ are functions of energy only. Substituting Eq. (63) into Eq. (62), recognizing that integrand terms which are odd with respect to reversal of direction in $w$-space do not contribute, and neglecting terms of the order $\gamma^{-2}$ or higher, one obtains

$$(4\pi B)^{-1} (2\varepsilon)^{-1/2} e^{\nu} \cdot \hat{E} = -\hat{C}_1 \cdot \hat{a}^{1/2} \xi$$

$$+ \gamma^{-1} [-\hat{C}_2 \cdot \hat{a}^{1/2} \xi + p \hat{C}_3 \cdot \hat{a}^{1/2} \xi + (\hat{C}_1 \cdot \hat{a}^{1/2} \xi) (\xi \cdot \hat{a}^{-1} \xi)]$$

$$+(4\pi\gamma)^{-1} \left[ \hat{a}^{1/2} \xi \hat{C}_1 \cdot \xi (\xi \cdot \hat{a}^{-1} \xi) + 2 \hat{a}^{1/2} \xi \hat{C}_1 \cdot \xi (\xi \cdot \hat{a}^{-1} \xi) \right] d\Omega.$$  

Using spherical coordinates in $w$-space, the integral term gives

$$(4\pi/3\gamma) (\hat{C}_1 \cdot \hat{a}^{1/2} \xi) [1 + \text{Tr}(\hat{a}^{-1})],$$

where $\text{Tr}(\hat{a}^{-1})$ is the trace of the tensor $\hat{a}^{-1}$. Transforming back to $p$-space in all the terms gives

$$(4\pi B)^{-1} e\hat{p} \cdot \hat{a} \hat{E} = \hat{p} \cdot [-\hat{C}_1 + (p^2/2\varepsilon \gamma) \hat{C}_1 + (1/3\gamma) \text{Tr}(\hat{a}^{-1}) \hat{C}_1$$

$$+(2/3\gamma) \hat{a}^{-1} \hat{C}_1 \hat{a}^{-1} \hat{C}_2 \hat{a}^{-1} \hat{C}_3] .$$

$\hat{p}$ and $\gamma$ are independent parameters, so the unknown parameters in $f_1$ are obtained as

$$\hat{C}_1 = -(e/4\pi B) \hat{a} \hat{E},$$

$$\hat{C}_2 = (1/3) \text{Tr}(\hat{a}^{-1}) \hat{C}_1 + (2/3) \hat{a}^{-1} \hat{C}_1,$$

$$\hat{C}_3 = (1/2\varepsilon) \hat{C}_1.$$
Finally, one has

\[
f_1 = \frac{e}{4\pi B}(\partial f_o / \partial \varepsilon)
\]

\[\times \hat{p} \cdot \hat{\alpha} \left[ 1 + \frac{1}{3\gamma} \text{Tr} (\hat{\alpha}^{-1}) + \frac{2}{3\gamma} \hat{\alpha}^{-1} + \frac{p^2}{2\varepsilon\gamma} \right] \hat{E}. \tag{70}\]

Equation (70) is a solution of Eq. (4) giving the total \( f_1 \) and is not just the conductivity part \( f_1^{(c)} \) discussed in Section II. Note, however, that it is in real vector form and would be equivalent to \( f_1^{(c)} \) except for the term proportional to \( \frac{p^2}{2\varepsilon\gamma} \). This term is a function of the direction of \( \hat{p} \) for ellipsoidal energy surfaces, and thus is not a function of energy only as is the vector \( \hat{C} \) in Eq. (5). The \( f_1^{(c)} \) part of this term could be obtained by finding its expansion for the \( \ell = 1 \) spherical harmonics as discussed in Appendix A. But here the total \( f_1 \) will be used in Eq. (22) for the current density, which has the same effect.

Since \( f_1 \) and \( f_1^{(c)} \) are not the same, one might expect the relaxation times for \( f_1 \) and \( f_1^{(c)} \) to be different. The relaxation time for \( f_1 \) can be found by comparison to Eq. (7) for the scalar relaxation time. The collision term \( (\partial f / \partial t)^{c} \) is identified from Eq. (4) as \(-e(\partial f_o / \partial \varepsilon) \hat{p} \cdot \hat{\alpha} \hat{E}\), and Eq. (70) can be written as

\[
f_1 = e(\partial f_o / \partial \varepsilon) \hat{p} \cdot \hat{\alpha} \hat{E}, \tag{71}\]

where

\[
\hat{\tau} = \frac{1}{4\pi B} \left\{ \left[ 1 + \frac{1}{3\gamma} \text{Tr} (\hat{\alpha}^{-1}) + \frac{2}{2\varepsilon\gamma} \right] + \frac{2}{2\varepsilon\gamma} \hat{\alpha}^{-1} \right\}. \tag{72}\]
For spherical energy surfaces \( \hat{\tau} \) becomes a scalar, which from Eq. (7) is the relaxation time for \( f_1 \). Therefore, \( f_1 \) can be written in the same form as Eqs. (13) to (15) for \( f_1^{(c)} \), but the diagonal elements of \( \hat{\tau} \) in Eq. (72) are functions of direction in \( p \)-space rather than functions of energy only. On the other hand, Section II and Appendix A proved that the elements of \( \hat{\tau} \) for the conductivity must be functions of energy only.

**Conductivity**

Write Eq. (70) as

\[
f_\perp = \epsilon (\partial f_0 / \partial \epsilon) \mathbf{v} \cdot [(\hat{T} + (P^2 / 8 \pi B \gamma)) \mathbf{E}],
\]

where

\[
\hat{T} = (1/4 \pi B) \left\{ \left[ 1 + (1/3 \gamma) \text{Tr}(\hat{\alpha}^{-1}) \right] \hat{\mathbf{r}} + (2/3 \gamma) \hat{\alpha}^{-1} \right\},
\]

contains all the terms which are functions of energy only. Then the conductivity for the first term (terms belonging to \( \hat{T} \)) in Eq. (73) is given by Eq. (27). The result is

\[
\sigma(1) = n e^2 \alpha \hat{T}.
\]

The current density due to the last term of Eq. (73) is

\[
\mathbf{j}^{(2)} = -\left( e^2 / 4 \pi h^3 \right) \int (\partial f_0 / \partial \epsilon) (P^2 / 8 \pi B \gamma) \mathbf{v} \cdot (\mathbf{v} \cdot \mathbf{E}) \, d^3 p^*.
\]

\( \gamma \) and \( B \) are left in the integral because they are functions of energy. Following the assumptions used in the derivation of Eq. (27), one transforms to \( w \)-space, and uses the
highly degenerate approximation of Eq. (26). Equation (76) yields for the conductivity elements

\[ \sigma^{(2)}_{ij} = (2\pi B \gamma)^{-1} h^{-3} e^{-2(2\varepsilon_{\xi})^{3/2} |\tilde{\alpha}|^{-1/2}} \]

\[ \times \int (\xi_i^{-1} \tilde{\alpha}^{-1} \xi_j) (\tilde{\alpha}^{1/2} \xi_i) (\tilde{\alpha}^{1/2} \xi_j) d\Omega. \] (77)

(The energy which appears in $\gamma$ and $B$ is now the Fermi energy.) Since $(\tilde{\alpha}^{1/2} \xi_i)_i = \alpha^{1/2} \xi_i$, the integrand has odd symmetry over the energy surface if $i \neq j$, giving zero.

Using Eq. (28) for $n$, Eq. (77) becomes

\[ \sigma^{(2)}_{ij} = \delta_{ij} (3n e^2 \alpha_i / 16\pi^2 B) \int (\xi_i^{-1} \tilde{\alpha}^{-1} \xi_i) (\xi_i^{2/3}) d\Omega. \] (78)

The remaining integral is readily evaluated, and one obtains

\[ \sigma^{(2)} = n e^2 \tilde{\alpha} / (1/20\pi B) [2 \tilde{\alpha}^{-1} + \text{Tr}(\tilde{\alpha}^{-1}) \hat{1}] . \] (79)

The total conductivity is obtained by adding Eqs. (75) and (79), which yields

\[ \hat{\sigma} = n e^2 \tilde{\alpha} / (1/4\pi B) \{ [1 + (8/15\gamma) \text{Tr}(\tilde{\alpha}^{-1})] \hat{1} + (16/15\gamma) \tilde{\alpha}^{-1} \}. \] (80)

Comparing Eq. (80) to Eqs. (27) and (14), the relaxation time for the conductivity is found to be

\[ \hat{\tau} = \tilde{\tau} = (1/4\pi B) \{ [1 + (8/15\gamma) \text{Tr}(\tilde{\alpha}^{-1})] \hat{1} + (16/15\gamma) \tilde{\alpha}^{-1} \}. \] (81)

Note that this $\hat{\tau}$ has elements which are functions of energy only, in agreement with Section II. Because it is the relaxation time tensor for the conductivity, it is the same
tensor $\hat{\tau}$ as in Eq. (6). Therefore it follows the complete derivation of Section III yielding Eq. (27), which gives the solution in a magnetic field.
V. CONCLUSIONS

Several features are significant about relaxation times in the electrical conductivity of ellipsoidal Fermi surfaces. First is the result that a relaxation time tensor exists in the conductivity and its elements are functions of energy only regardless of the form of the electron distribution function or the type of electron scattering. If one wishes to obtain the electrical current and not the total distribution function, this considerably simplifies the solution of the Boltzmann transport equation. Also note that thermal currents can be written in analogy to Eq. (A5), except with a different energy dependence. Thus Eq. (5) is sufficient for finding these currents, and a tensor relaxation time with elements that are functions of energy only exists for the thermal conductivity.

The electrical conductivity can always be written in the very simple form of Eq. (27) for degenerate electrons and in the form of Eq. (25) otherwise. This conductivity expression is valid for all magnitudes of magnetic field for which Eqs. (3) and (4) hold, which is whenever the effective mass theorem is valid and quantization by the magnetic field can be neglected. This simple form is readily expanded in a matrix series in $\hat{H}$ which yields the Jones-Zener expansion to arbitrary order in the magnetic field. Since it is a series expansion about zero magnetic field, there exists a magnetic field amplitude at which the series diverges. This value is given exactly by Eq. (20) which is a function of the
direction of the applied field. In fitting experimental
data to conductivity expressions, one could avoid the diffi-
culty of divergence by fitting directly to Eq. (27) rather
than the series expansion.

The Onsager reciprocity relation and Eq. (27) require
the surfaces of constant power density (upon application of
an electric field but zero magnetic field) to be ellipsoidal.
These ellipsoidal surfaces must satisfy the same crystal
symmetry requirements as the energy ellipsoids. If the
crystal symmetry completely specifies the ellipsoid orien-
tation (i.e. both ellipsoids share the same principle axes),
then the relaxation time tensor is symmetric and commutes
with the mass tensor. Otherwise the relaxation time tensor
may be asymmetric, and from Eq. (39) has at most six inde-
dependent components. However, the theoretically derived
relaxation time tensor in Eq. (81) is symmetric regardless
of crystal symmetry.

A significant feature of the theoretical solution for \( \gamma \)
in Section IV is that an anisotropic mass causes an anisotropic
relaxation time even though the scattering centers are spher-
ically symmetric potentials. The relation is given by Eq. (81)
if the assumption is made that all the elements of \((2\gamma a)^{-1}\)
are small compared to one. Note that the relaxation time is
isotropic only if the screening length goes to zero or the
mass tensor is isotropic. A knowledge of the screening length,
the Fermi energy, and the effective masses then gives one an
estimate of the magnitude of the higher order terms which were dropped in Eq. (61). This is in contrast to previous theoretical solutions\(^6,\)\(^9\) which use spherical harmonic expansions that converge somewhat faster, but give little indication of how the magnitudes of the neglected terms are affected by the fundamental physical conditions. However, Eq. (81) will not yield relaxation times with large anisotropies. The largest ratio of the elements of the relaxation time tensor consistent with the above assumption is approximately 1.1. Thus several more terms are needed to fit data for bismuth\(^2\) or bismuth telluride.\(^{18}\)

The assumption on (2\(\gamma\delta\)) was made in this analysis to produce simple analytic results. The analysis could be made more inclusive in several ways. For example, the expansion of Appendix G converges faster (or conversely can use less restrictive assumptions) and still yields terms similar to Eq. (81). With nearly isotropic masses, it converges quickly for any value of screening constant. For a theoretical calculation of highly anisotropic relaxation time tensors, one can evaluate Eq. (58) directly by numerical techniques or by the method of Korenblit.\(^9\)

Another significant feature in the theoretical solution of the relaxation time for the conductivity is that Eq. (27) allows one to use only an electric field. The magnetic field dependence of the conductivity is correctly given by Eq. (27). If one desires the total \(f_1\) distribution
instead of the conductivity portion of \( f_1 \), several difficulties arise. First, the relaxation times which correspond to the total \( f_1 \) distributions are not functions of energy only. Likewise the magnetic field dependence of the total \( f_1 \) will be more complex than the simple form of Eq. (15) appropriate for the conductivity portion of \( f_1 \). Consequently, conductivity calculations (and thus relaxation time tensor calculations) for an ellipsoidal Fermi surface are simplified considerably by solving for only that portion of the distribution function which contributes to the conductivity.
VI. APPENDIX A: DEFINITIONS OF $f_1^{(c)}$ AND $(3f/3t)_c^{(c)}$

Equation (22) gives the calculation of the electrical current density as

$$\mathbf{J} = -2e\hbar^{-3}\mathbf{v}f_1 d^3p.$$  (A1)

To evaluate this integral (and all integrals over p-space), define a w-space such that constant energy surfaces are spherical. The transformation equation between these spaces is

$$\hat{a}_{1/2}^p = a_{1/2}^w.$$  (A2)

The energy equation is then

$$2\varepsilon = a_o^2 w^2.$$  (A3)

In Eq. (A1)

$$d^3p = a_o^{3/2}|\hat{a}|^{-1/2} d^3w = |\hat{a}|^{-1/2}(2\varepsilon)^{1/2}d\varepsilon d\Omega_w,$$  (A4)

where $|\hat{a}|^{-1/2}$ is the determinant of $\hat{a}^{-1/2}$, and $d\Omega_w$ is a differential solid angle in w-space. Thus, the current density in the X direction is

$$J_x = -2e\hbar^{-3}|\hat{a}|^{-1/2}2\varepsilon d\varepsilon \int (\hat{e}_x \cdot \hat{\alpha}^{1/2}\xi) f_1 d\Omega_w,$$  (A5)

where $\xi$ is a unit vector in w-space, and $\hat{e}_x$ a unit vector in the X direction of coordinate space. Now let $f_1$ be expanded in w-space as a spherical harmonic series,
\[ f_1(\hat{\omega}, \hat{\xi}) = \sum_{l,m} A_{l,m}(\varepsilon, \hat{\xi}) Y_{l,m}(\Omega). \]  

(A6)

In Eq. (A5), the product \( \hat{\varepsilon}_x \hat{a}^{1/2} \hat{\xi} \) can also be expanded in spherical harmonics. Any real vector product \( \hat{\nu} \cdot \hat{\xi} \), where \( \hat{\nu} \) is not a function of the direction of \( \Omega \), is expanded as

\[ \hat{\nu} \cdot \hat{\xi} = \sum_m B_{l,m} Y_{l,m}(\Omega), \]  

(A7)

where

\begin{align*}
B_{1,0} & = (4\pi/3)^{1/2} V_3, \\
B_{1,1} & = -B_{1,-1} = -(8\pi/3)^{1/2}(V_1-iV_2).
\end{align*}

(A8)

(A9)

Expanding \( \hat{\varepsilon}_x \hat{a}^{1/2} \hat{\xi} \) according to Eq. (A7) and using Eq. (A6) for \( f_1 \) in Eq. (A5), the integration over the solid angle \( \Omega \) can be done. Due to the orthogonality of the spherical harmonics, only the \( l=1 \) terms in the \( f_1 \) expansion contribute to \( \mathbf{j} \).

Since \( f_1 \) is real, \( A_{l,m} \) and \( A_{l,-m} \) are related through

\[ f_1 = \sum_{l,m} A_{l,m} Y_{l,m} = \sum_{l,m} A^*_{l,m} Y^*_{l,m} = \sum_{l,m} (-1)^m A^*_{l,m} Y_{l,-m} \]

\[ = \sum_{l,m} A_{l,-m} Y_{l,-m}. \]  

(A10)

This yields

\[ A_{l,m} = (-1)^m A^*_{l,-m}, \]  

(A11)

and thus the \( l=1 \) terms of \( f_1 \) contributing to the current density can always be written as a vector product \( \hat{\nu}(\varepsilon) \cdot \hat{\xi}, \)
where

\[ V_1 = (3/4\pi)^{1/2} A_{11,0}, \]

\[ V_2 = -i(3/8\pi)^{1/2}(A_{11}^{*} - A_{11}), \]

\[ V_3 = -(3/8\pi)^{1/2}(A_{11}^{*} + A_{11}). \]  \hspace{1cm} (A12)

Defining the vector

\[ \hat{C}(\epsilon) = -(2\epsilon)^{-1/2} (\partial f_0 / \partial \epsilon)^{-1/2} \hat{a} \cdot \hat{\nu}, \]  \hspace{1cm} (A13)

this portion of \( f_1 \), designated as \( f_1^{(c)} \), is written in p-space as

\[ f_1^{(c)} = -(\partial f_0 / \partial \epsilon) \hat{C} \cdot \hat{p}, \]  \hspace{1cm} (A14)

which is Eq. (5).

Thus far it has been shown that for an arbitrary function \( f_1 \), the portion of \( f_1 \) contributing to the electrical current density can always be written as a vector product in \( \omega \)-space or p-space. Furthermore, the vectors \( \hat{V} \) and \( \hat{C} \) are functions of energy only, and not functions of the direction of the solid angle \( \Omega \). The next step is to show how Eq. (4) can be solved directly for \( f_1^{(c)} \) if an inverse relaxation time tensor \( \hat{\tau}^{-1} \), to be defined later, is independently determined either from experimental data or by a separate calculation.

Considering Eq. (4), the first term is a driving term proportional to the electric field \( \hat{E} \) and can be written in
the form of Eq. (A7). Thus it can be expressed (in \( \nu \)-space) in terms of the \( l = 1 \) spherical harmonics. Due to the orthogonality of the spherical harmonics, each term of Eq. (4) can be expanded as a harmonic series, and Eq. (4) must then be satisfied for each value of \( l \) and \( m \). Thus Eq. (4) becomes an infinite set of independent equations.
Consider now only those equations containing \( \hat{E} \), or the \( l = 1 \) set. It will be convenient, since each term of Eq. (4) is real (no imaginary components), to add the \( l = 1 \) set of equations together. Then each term of the added set will be a real vector product and the first term of Eq. (4) is unchanged.

In the second term of Eq. (4), the operation \( \hat{\nu} \times \hat{H} \cdot \hat{r} \) becomes \( \hat{\alpha}^{1/2} \hat{w} \times \hat{H} \cdot \hat{r} \) in \( \nu \)-space and can be expanded in terms of the angular momentum operators.\(^9\) This means the operation changes the value of \( m \) but not the value of \( l \) of a spherical harmonic. Thus, the \( l = 1 \) set for the magnetic term of Eq. (4) is obtained by operating on the \( l = 1 \) set of spherical harmonics contained in \( f_1 \), or \( f_1^{(c)} \). When considering the \( l = 1 \) set as a single equation, this says the vector product part of the second term of Eq. (4) is obtained by \( \hat{\nu} \times \hat{H} \cdot \hat{r} \) operating on \( f_1^{(c)} \), the vector product part of \( f_1 \).

The collision term or right hand side of Eq. (4) is real, and so its \( l = 1 \) set, written as \((\partial f/\partial t)^{(c)}_c\), can also be written as a general vector product \( \hat{w} \cdot \hat{\xi} \), or in \( p \)-space as \((\partial f_\alpha/\partial \alpha) \hat{\beta} \cdot \hat{p} \), where \( \hat{\beta} \) is an unknown which is a function of
energy only. Since \( \hat{C} \) of Eq. (A14) and \( \hat{D} \) are vectors which are functions of energy only, an energy dependent tensor transformation can always be defined so that

\[
\hat{C} = \hat{m}^{-1} \hat{m} D.
\]  

(A15)

where \( \hat{m} \) is the effective mass tensor, which is a function of energy only. Nothing is known about \( \hat{\tau} \) at this point other than it is a function of energy only. The collision term is now

\[
\frac{\partial f}{\partial t}^c = \left( \frac{\partial f_o}{\partial \epsilon} \right) \hat{m}^{-1} \hat{m} \hat{C}_p \cdot \hat{p},
\]  

(A16)

which is Eq. (6).

Collecting the terms of the \( l = 1 \) set of Eq. (4) and adding them together to give vector products as in Eqs. (A14) and (A16) gives

\[
e \left( \frac{\partial f_o}{\partial \epsilon} \right) \hat{v} \cdot \hat{E} - \left( \frac{\epsilon}{c} \right) \hat{v} \times \hat{A} \cdot \hat{v}_p \left( \frac{\partial f_o}{\partial \epsilon} \right) \hat{C}_p \cdot \hat{p} + \left( \frac{\partial f_o}{\partial \epsilon} \right) \hat{m}^{-1} \hat{m} \hat{C}_p \cdot \hat{p}.
\]  

(A17)

Since the operator \( \hat{v} \times \hat{A} \cdot \hat{v}_p \) commutes with a function of energy only, this yields Eq. (8).
VII. APPENDIX B: CONDUCTIVITY IN DEFORMED COORDINATES

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

\[
\begin{align*}
\mathbf{p} &= \alpha_o \frac{1}{2} \mathbf{a} - \frac{1}{2} \mathbf{w}, \\
\mathbf{v} &= \alpha_o \frac{1}{2} \mathbf{a} + \frac{1}{2} \mathbf{w}, \\
\mathbf{d}^3 p &= \alpha_o \frac{3}{2} |\alpha|^{-1/2} d^3 w.
\end{align*}
\] (B1)

The current density then becomes

\[
\mathbf{j} = 2e\hbar c \alpha_0 \frac{5}{2} |\alpha|^{-1/2} \mathbf{w} (\mathbf{a}^\dagger \mathbf{w}^\dagger \mathbf{E}) (\partial f / \partial \epsilon) d^3 w.
\] (B2)

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

\[
d^3 w = dS(\epsilon) d\epsilon / (\alpha_w).
\] (B3)

Writing all matrix products in the form

\[
(AB)_{ij} = \sum_k A_{ik} B_{kj},
\] (B4)

and using the relations

\[
\int w^3 \, w dS(\epsilon) = \frac{4}{3} \pi w^4 \delta_{mk},
\] (B5)

\[
w^3 = (2\epsilon / \alpha_o)^{3/2},
\] (B6)

\[
\sum_k (\alpha^{1/2})_{ik} (\alpha^{-1/2})_{pk} = \delta_{ip},
\] (B7)

yields the result

\[
\mathbf{j} = (16/3) \sqrt{2} \hbar c \mathbf{a}^\dagger (\alpha)^{-1/2} \int \epsilon \frac{3}{2} (\partial f / \partial \epsilon) \mathbf{E} d\epsilon.
\] (B8)
The conductivity matrix is then identified as the right hand side of Eq. (B8) except for $\mathbf{E}$, the electric field, which is Eq. (25).
VIII. APPENDIX C: ALTERNATE CONDUCTIVITY EXPRESSIONS AND CONVERGENCE OF JONES-ZENER SERIES

The $[\hat{F} - \hat{H}]^{-1}$ term of Eq. (27) can be expanded by tensor analysis\(^{19}\) using the Levi-Cevita symbol defined as

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

(C1)

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

$$
(\hat{M}^{-1})_{ij} = \sum_{a, b, c, d} (1/2) \delta_{abc} \delta_{cdj} M_{ia} M_{db}.
$$

(C2)

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

$$
\sigma_{ij} = \text{neg} \left[ |\hat{F}| + \hat{H} \cdot \hat{F} + \sum_{a, b, c, d} \delta_{abc} H F_{ia} F_{jd} \right]^{-1}
$$

$$
\times \sum_{\ell, m, r, s, p} (1/2) \delta_{\ell mj} \delta_{r \ell s} \delta_{m ij} F_{rp} + \delta_{mpj} H_{i} + \delta_{imj} H_{p} F_{mp}.
$$

(C3)

Using the result of Eq. (32) that $\hat{F}$ is symmetric, Eq. (C3) simplifies to give

$$
\sigma_{ij} = \text{neg} \left[ |\hat{F}| + \hat{H} \cdot \hat{F} \right]^{-1} \left[ |\hat{F}| (\hat{F}^{-1})_{ij} + H_{i} H_{j} + \sum_{m, p} \delta_{imj} H_{p} F_{mp} \right].
$$

(C4)
Convergence of the Jones-Zener Series

When the conductivity is expressed in the form of Eq. (C4) the denominator can be expanded as an infinite series in the magnetic field magnitude \( H \) as

\[
\left( |\hat{F}| + \hat{U} \cdot \hat{F} \hat{U} \right)^{-1} = \left( |\hat{F}| + H^2 \hat{U} \cdot \hat{F} \hat{U} \right)^{-1}
\]

\[
= |\hat{F}|^{-1} \left[ 1 - \hat{U} \cdot \hat{F} \hat{U} + (\hat{U} \cdot \hat{F} \hat{U}) H - \cdots \right], \quad (C5)
\]

where \( \hat{U} \) is a unit vector in the direction of the magnetic field. When this series is multiplied into the numerator of Eq. (C4) the Jones-Zener series for \( \sigma_{ij} \) is obtained. Because this numerator is always finite, the convergence of the series of Eq. (C5) coincides with the convergence of the Jones-Zener series. Equation (C5) 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

\[ H^4 < (a/b)^2. \quad (C6) \]

An equality sign in Eq. (C6) would make the series diverge and therefore gives the "critical" magnitude of the magnetic field. Using Eq. (C5) for the values of the constants \( a \) and \( b \) gives the critical field value

\[ H_C^4 = \left( |\hat{F}|/\hat{U} \cdot \hat{F} \hat{U} \right)^2, \quad (C7) \]
which is Eq. (20). One observes that this value is a function of the direction of the magnetic field through the unit vector $\mathbf{U}$. 
IX. APPENDIX D: JONES-ZENER COEFFICIENTS
FOR THE CONDUCTIVITY

Experimental papers\textsuperscript{2,3} normally determine coefficients of the Jones-Zener expansion of the conductivity, which is written as

\[
\sigma_{ij} = \sigma_{ij}^{(0)} + \sigma_{ijk}^{(1)} H_k + \sigma_{ijk_1k_2}^{(2)} H_{k_1} H_{k_2} + \cdots. \tag{D1}
\]

This amounts to a Taylor series with the coefficients given by

\[
\sigma_{ijk_1k_2\cdots k_N}^{(N)} = \frac{1}{N!} \partial^N \sigma_{ij} \partial H_{k_1} \cdots \partial H_{k_N} \bigg|_{H=0}. \tag{D2}
\]

Expanding Eq. (27) in a matrix series as given by Eq. (16) yields the Jones-Zener coefficients when Eq. (D2) is applied. (This development can be made for all equations containing \([\hat{F} - \hat{H}]^{-1}\).) The results are

\[
\sigma_{ij}^{(0)} = \text{nc}(\hat{F}^{-1})_{ij}, \tag{D3}
\]

\[
\sigma_{ijk}^{(1)} = \text{nc} \sum_{ab} (\hat{F}^{-1})_{ia} \delta_{abk} (\hat{F}^{-1})_{bj}, \tag{D4}
\]

\[
\sigma_{ijk_1k_2\cdots k_N}^{(N)} = \text{nc} / N! \sum_{k_1\cdots k_N} \delta_{a_1\cdots a_N} (\hat{F}^{-1})_{i a_1} \delta_{b_1\cdots b_N} \delta_{a_1b_1\cdots a_Nb_N} \delta_{a_2b_2\cdots a_Nb_N} \cdots \delta_{a_Nb_N} \tag{D5}
\]

where \(F_{k_1\cdots k_N}\) is a permutation operator which sums all possible permutations of the variables \(k_1, \cdots, k_N\). From
Eq. (14) one obtains

\[ \hat{F}^{-1} = \left( \frac{e}{c} \right) \hat{\tau}. \]  \hspace{1cm} (D6)

From this it is clear how the anisotropic relaxation time tensor fits into the Jones-Zener expansion. Equation (20) yields the region of magnetic field strength for which the expansion converges.
X. APPENDIX E: GROUP OF THREE ELLIPSOIDS

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

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

\[
(\hat{\sigma}_t)_{ij} \big|_{H=0} = (\hat{\sigma}_t)_{ji} \big|_{H=0},
\]

\[
(\hat{\sigma}_t)_{ijk} = -(\hat{\sigma}_t)_{jik},
\]

and more equations for the higher order coefficients. From Eq. (E2), consider the particular elements giving

\[
(\hat{\sigma}_t)_{333} = 0,
\]

\[
(\hat{\sigma}_t)_{231} + (\hat{\sigma}_t)_{321} = 0,
\]

\[
(\hat{\sigma}_t)_{111} = 0,
\]

\[
(\hat{\sigma}_t)_{112} = 0.
\]

From Eqs. (29) and (E1) one has

\[
(F^{-1})_{12} = (F^{-1})_{21},
\]

and

\[
(F^{-1})_{13} (F^{-1})_{32} (F^{-1})_{31} (F^{-1})_{23} = 0.
\]
Equation (E4) yields
\[
[(F^{-1})_{13}]^2 - [(F^{-1})_{31}]^2 = [(F^{-1})_{23}]^2 - [(F^{-1})_{32}]^2. \tag{E9}
\]
Equations (E8) and (E9) have the two nontrivial solutions
\[
(F^{-1})_{13} = (F^{-1})_{31} \tag{E10}
\]
and
\[
(F^{-1})_{23} = (F^{-1})_{32}, \tag{E11}
\]
or
\[
(F^{-1})_{13} = -(F^{-1})_{31} \tag{E12}
\]
and
\[
(F^{-1})_{23} = -(F^{-1})_{32}. \tag{E13}
\]
Equations (E5) and (E6) establish Eqs. (E10) and (E11) as the proper solution for the three ellipsoids. Equations (E7), (E10), and (E11) require \((\hat{F}_k)^{-1}\) and thus \(\hat{F}_k\), to be a symmetric tensor for all \(k\), which is identical to the single ellipsoid result.

The example of Paper I assumed a single tensor \(\hat{F}\) defined in the laboratory reference system. It should then not be transformed by the rotation tensor \(\hat{R}\). In this case the correct way to calculate the total conductivity is
\[
\hat{\sigma}_L = \text{nec}_L [c/e] \hat{\tau}^{-1} \hat{R}_k \hat{m} (\hat{R}_k)^{-1} \hat{R}^{-1}. \tag{E14}
\]
However, the $^\hat{t}$ 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

$$^\hat{R}_k ^\hat{t} -1 (^\hat{R}_k)^{-1} = ^\hat{t}^{-1}. \quad \text{(E15)}$$

Therefore, Eqs. (E14) and (30) are equivalent for that example, and one is left with the requirement that $^\hat{F}$ be symmetric.
XI. APPENDIX F: ELECTRON SPIN DEGENERACY

Let the spin states be explicitly shown. Denoting the two electron spin states \( \lambda \) by \( + \) and \( - \), one writes for the number of electrons per unit crystal volume

\[
N = \frac{L^{-3}N}{k_{\lambda} f(k, \lambda)} = \frac{L^{-3} \sum_{k} [f(k, +) + f(k, -)]}{k_{\lambda} f(k, \lambda)}.
\]

Here \( f(k, \lambda) \) is the probability that the state with wave vector \( k \) and spin \( \lambda \) is occupied by an electron. It has a value between zero and one. Likewise Eq. (44) in this notation is

\[
[\partial f(k, \lambda)/\partial t]_{C} = \sum_{k', \lambda'} S(k, \lambda; k', \lambda') \times [f_{\lambda}(k', \lambda') - f_{\lambda}(k, \lambda)],
\]

where \( S(k, \lambda; k', \lambda') \) is the transition probability per unit time that a filled state \((k, \lambda)\) will go to an empty state \((k', \lambda')\). \( f_{\lambda}(k, \lambda) \) is the perturbation of the distribution function from equilibrium evaluated at the state \((k, \lambda)\).

If the scattering processes considered do not flip the spin of the electron, and if processes exchanging electrons can be ignored, then

\[
S(k, \lambda; k', \lambda') = \delta_{\lambda, \lambda'} S(k, \lambda; k', \lambda'),
\]

and Eq. (F2) becomes

\[
[\partial f(k, \lambda)/\partial t]_{C} = \sum_{k', \lambda'} S(k, \lambda; k', \lambda') \times f_{\lambda}(k', \lambda') - f_{\lambda}(k, \lambda).
\]
If one also knows (or assumes) that the probability of occupation of spin up states is equal to the probability of occupation of spin down states, then define

\[ f_1(k,+) = f_1(k,+) \equiv f_1(k), \]  
\[ f_1(k',+) = f_1(k',+) \equiv f_1(k'), \]  
\[ S(k,+,k',+) = S(k,+,k',+) \equiv S(k,k') \equiv S_{k,k'} \]  

These definitions are chosen so that \( f_1(k) \) and \( f_1(k') \) have values from zero to one, and \( S(k,k') \) is the transition rate one arrives at by disregarding spin in the original scattering problem. Using these definitions, Eq. (F2) becomes

\[ \frac{\partial f}{\partial t} = \sum_{k,k'} S_{k,k'} [f_1(k') - f_1(k)], \]  

which is Eq. (44) and Eq. (F1) may be written as

\[ n = 2L^3 \sum_{k,k'} f(k'), \]  

which is Eq. (45).

When the number of states is large, the summations are replaced by integrals. The transition to an integral (including spin) is

\[ \sum_{k,k',\lambda} g(k',\lambda') = L^3 \int_{\lambda} \int g(k',\lambda') \rho(k',\lambda') d^3k', \]  

where \( \rho(k',\lambda') d^3k' \), the number of states per unit crystal volume in the \( k \) volume \( d^3k' \) with spin \( \lambda' \), is called the density of states. Here \( g(k',\lambda') \) is an arbitrary function.
Since \( \rho \) is a measure of the states which exist regardless of whether they are occupied or not, and since each spin up state has a corresponding spin down state, then the density of spin up states is always the same as the density of spin down states. Therefore, define

\[
\rho(k^-) = \rho(k^-,+) = \rho(k^-,+).
\] (F11)

Using this definition and Eq. (F10), one obtains from Eq. (F1)

\[
n = \int \rho(k^-) f(k^-) = \int \rho(k^-) f(k^-) + \rho(k^+) f(k^+)] d^3k
\]

\[
= 2\int \rho(k) f(k) d^3k,
\] (F12)

which is Eq. (46). Likewise, Eqs. (F2) and (F10) yield

\[
(\partial f / \partial t)_c = \int s(k, \lambda; k', \lambda') \rho(k', \lambda')
\]

\[
\times [f_1(k', \lambda') - f_1(k, \lambda)] d^3k,
\] (F13)

which with Eq. (F3) gives Eq. (47).
XII. APPENDIX G: ALTERNATE EXPANSION OF COLLISION INTEGRAL

One can obtain a series approximation for Eq. (58) which converges faster than the series of Eq. (61) by separating as much isotropic mass out of the tensor \( \widehat{a}^{-1} \) as possible. This results in

\[
\left( \partial f / \partial t \right)_C = B \int \left( f_1^2 - f_1 \right) \times \left[ 1 + \frac{1}{\gamma} (1 - \xi \cdot \xi') + \frac{1}{2 \gamma} (\xi - \xi') \cdot \widehat{M} (\xi - \xi') \right]^{-2} d\Omega', \quad (G1)
\]

where

\[
\widehat{M} = \widehat{a}^{-1} - \hat{1}. \quad (G2)
\]

The elements of \( \widehat{M} \) with the largest magnitudes are minimized by choosing

\[
A = 2 (m_+ + m_-)^{-1} = m_a^{-1}, \quad (G3)
\]

where \( m_+ (m_-) \) is the greatest (least) mass element of the diagonalized mass tensor. Therefore

\[
\widehat{M} = m_a^{-1} \widehat{a}^{-1} - \hat{1}, \quad (G4)
\]

and has two elements with the same magnitude but opposite in sign when diagonalized. Also as the mass tensor (or \( \widehat{a}^{-1} \)) approaches an isotropic mass, \( \widehat{M} \) goes to zero. Expanding the denominator or the brackets in Eq. (G1), and keeping only first order terms in \( \widehat{M} \) gives
\[
(\partial f/\partial t)_c = A^2 \gamma^2 B \int (f_1' - f_0') (1 + A \gamma - \xi \cdot \xi')^{-2} \\
\times \{1 - [1 + A \gamma - \xi \cdot \xi']^{-1} \{ (\xi - \xi') \cdot \hat{N} (\xi - \xi') \} + \cdots \} d\Omega'.
\] (G5)

The first order term involving \( \hat{N} \) is small if either \( \gamma \) is large or if the mass is nearly isotropic. In any case it converges faster than Eq. (61). It is not expected to converge as fast as the analysis by Korenblit using spherical harmonic expansions. However, this expansion maintains the ability to give analytic expressions for \( \hat{N} \). In fact it gives terms identical to those of Eqs. (72) and (81) except that the magnitude of each term is given by a more complicated scalar function.
The calculation carried out in Section IV is first order time-dependent perturbation theory, which is essentially the Born approximation. The same results are derivable from a time-independent approach in which the scattering problem is described by the total wave function

$$\psi(r) = \psi_i(r) + \psi_s(r),$$

(H1)

where $\psi_i(r)$ is the incoming wave and $\psi_s(r)$ is the scattered wave. Although this approach is not used in Section IV, it is convenient to use it here to investigate the validity of the Born approximation. The Born approximation is generally valid if at the center of a scattering potential, which will be chosen at $r = 0$, the condition

$$\frac{|\psi_s(0)|^2}{|\psi_i(0)|^2} << 1,$$

(H2)

is satisfied. The incoming wave in free space is a solution to the Schrödinger equation and thus is a plane wave. Here the wave function $\psi_i(r)$ must satisfy the effective mass equivalent, or Eq. (49), with $V = 0$. The plane wave also satisfies Eq. (49). But applying Eq. (49) to the case of bismuth or bismuth telluride presents a dilemma. The difficulty is that the energy expressions $\varepsilon(-iV)$ and $\varepsilon(k)$ in Eq. (49) are for the total energy and the total wave vector $k$. In these materials the total energy expression is not known, only
of an electron ellipsoidal energy surface which is not at the center of the Brillouin zone. To resolve this situation, Eq. (49) will be expanded to find the appropriate wave equation, and a \( \psi_i \) and \( \psi_s \) satisfying this equation will be found. Then Eq. (H2) can be applied to obtain a condition for the validity of the first Born approximation.

Effective Mass Equation for Displaced Ellipsoid

Let \( \mathbf{k} \) be the total wave vector, with \( \mathbf{k}_0 \) at the center of the ellipsoid. The energy can be expanded in a Taylor series about \( \mathbf{k}_0 \) as

\[
\varepsilon(\mathbf{k}) = \varepsilon(\mathbf{k}_0) + \frac{\hbar}{2\pi} \mathbf{v}(\mathbf{k}_0) \cdot (\mathbf{k} - \mathbf{k}_0) + \frac{\hbar^2}{8\pi^2} \mathbf{v}(\mathbf{k}_0) \cdot \hat{a} (\mathbf{k} - \mathbf{k}_0) + \cdots, \tag{H3}
\]

where Eq. (3) and the relation

\[
a_{ij} = \left( \frac{4\pi^2}{\hbar^2} \right) \partial^2 \varepsilon(k) / \partial k_i \partial k_j, \tag{H4}
\]

have been used. At the center of the ellipsoid, the group velocity \( \mathbf{v}(\mathbf{k}_0) \) is zero, so to first order

\[
\varepsilon(\mathbf{k}) = \varepsilon(\mathbf{k}_0) + \frac{\hbar^2}{8\pi^2} (\mathbf{k} - \mathbf{k}_0) \cdot \hat{a} (\mathbf{k} - \mathbf{k}_0). \tag{H5}
\]

It is the last term of this equation which is known in bismuth. The Fermi energy is given as

\[
\varepsilon_f = \left( \frac{\hbar^2}{8\pi^2} \right) (\mathbf{k}_f - \mathbf{k}_0) \cdot \hat{a} (\mathbf{k}_f - \mathbf{k}_0), \tag{H6}
\]
where \( \mathbf{k}_f \) is the \( k \) vector from the center of the Brillouin zone to the Fermi surface. Since \( \varepsilon(-iV) \) is \( \varepsilon(\mathbf{k}) \) where \( \mathbf{k} \) is replaced by the operator \(-iV\), Eq. (H5) yields \( \varepsilon(-iV) \) to first order as

\[
\varepsilon(-iV) = \varepsilon(\mathbf{k}_0) + \left( \frac{\hbar^2}{8\pi^2} \right) (-iV - \mathbf{k}_0) \cdot \mathbf{a}(-iV - \mathbf{k}_0). \tag{H7}
\]

Equations (H5), (H7), and (49) yield for the effective mass equation

\[
[(\mathbf{k} - \mathbf{k}_0) \cdot \mathbf{a}(\mathbf{k} - \mathbf{k}_0) - (\mathbf{i}V - \mathbf{k}_0) \cdot \mathbf{a}(\mathbf{i}V - \mathbf{k}_0)]\psi = U\psi, \tag{H8}
\]

where

\[
U = \left( \frac{8\pi^2}{\hbar^2} \right) V. \tag{H9}
\]

The case of an ellipsoid centered in the Brillouin zone is obtained throughout by setting \( \mathbf{k}_0 = 0 \). This case was assumed in the ellipsoidal formulas of the other sections and appendixes.

**Born Criterion**

The \( U = 0 \) or incoming wave solution of Eq. (H8) is still the plane wave

\[
\psi_i(\mathbf{r}) = L^{-3/2} e^{i\mathbf{k} \cdot \mathbf{r}}, \tag{H10}
\]

where \( \mathbf{k} \) here is the total vector from the center of the Brillouin zone. Note that in bismuth \( |\mathbf{k}_f| = |\mathbf{k}_0| \), and \( |\mathbf{k} - \mathbf{k}_0| \ll |\mathbf{k}| \), so it is important to use the total vector \( \mathbf{k} \) and not the vector \( \mathbf{k} - \mathbf{k}_0 \) from the ellipsoid center. The
scattered wave is a solution to Eq. (H8) with a potential and is obtained by finding the Green's function for the equation

\[ [(\mathbf{k} - \mathbf{k}_0) \cdot \mathbf{a}(\mathbf{k} - \mathbf{k}_0) - (-i\mathbf{V} - \mathbf{k}_0) \cdot \mathbf{a}(-i\mathbf{V} - \mathbf{k}_0)] G(\mathbf{r}) + \delta(\mathbf{r}) = 0, \]

which then gives \( \psi_\pi(\mathbf{r}) \) as

\[ \psi_\pi(\mathbf{r}) = -\int G(\mathbf{r} - \mathbf{r}') U(\mathbf{r}') \psi(\mathbf{r}') d^3 r'. \]  

The total wave function \( \psi(\mathbf{r}') \) in Eq. (H12) is replaced by \( \psi_\pi(\mathbf{r}') \) of Eq. (H10) in the first Born approximation. The Fourier transforms

\[ G(\mathbf{r}) = (1/2\pi)^3 \int g(\mathbf{n}) e^{i \mathbf{n} \cdot \mathbf{r}} d^3 \mathbf{n}, \]  
\[ \delta(\mathbf{r}) = (1/2\pi)^3 \int e^{i \mathbf{n} \cdot \mathbf{r}} d^3 \mathbf{n}, \]

are used in Eq. (H11) to solve for \( g(\mathbf{n}) \). Equation (H13) is then evaluated using a deformed space similar to the evaluation of previous integrals over \( p \) space. The result is

\[ G(\mathbf{r}) = (4\pi)^{-1} |\mathbf{a}|^{-1/2} \mathbf{r}^{-1+} \mathbf{r}^{-1+} \]

\[ \times \exp\{i(k_0 \cdot \mathbf{r}) + i[(\mathbf{k} - \mathbf{k}_0) \cdot \mathbf{a}(\mathbf{k} - \mathbf{k}_0)]^{1/2} (\mathbf{r} \cdot \mathbf{a} - |\mathbf{r}|)^{1/2} \}. \]  

Dividing Eq. (H2) by \( |\psi_\pi(0)|^2 \) and using Eqs. (H15) and (H12) for \( |\psi_\pi(0)|^2 \) yields
$$\left| \frac{2\pi}{\hbar^2} \right| \left| \hat{a} \right|^{-1/2} V(|\mathbf{r}'|) [\mathbf{r}' \cdot \hat{a}^{-1} \mathbf{r}']^{-1/2}$$
$$\times \exp \{i(\mathbf{k}_a - \mathbf{k}_0 \cdot \mathbf{r}') + i((\mathbf{k}_b - \mathbf{k}_0) \cdot \hat{a}(\mathbf{k}_a - \mathbf{k}_0))^{1/2}[\mathbf{r}' \cdot \hat{a}^{-1} \mathbf{r}']^{1/2} \}$$
$$\times d^3 r' \ll 1. \quad \text{(H16)}$$

The vectors $\mathbf{k}_a$ and $\mathbf{k}_b$ are both total vectors to the Fermi surface, $\mathbf{k}_a$ being the incident wave and $\mathbf{k}_b$ being in the direction away from the scatterer being considered. They correspond to the vectors $\mathbf{k}$ and $\mathbf{k}'$ of Section IV. Equation (H16) is the condition for the validity of the first Born approximation. Note that the wave vectors here are those measured from the origin of the ellipsoid at $\mathbf{k}_0$ to the Fermi surface. One can also write

$$(\mathbf{k}_b - \mathbf{k}_0) \cdot \hat{a}(\mathbf{k}_a - \mathbf{k}_0) = (8\pi^2 \varepsilon_f / \hbar^2). \quad \text{(H17)}$$

Equation (H16) can be evaluated directly, but to obtain a rough estimate, let

$$-\mathbf{r}' \cdot \hat{a}^{-1} \mathbf{r}' = \left| \hat{a} \right|^{-1} r'^{-2}, \quad \text{(H18)}$$
$$\left| \mathbf{k}_m \right| \equiv \left| \mathbf{k}_a - \mathbf{k}_0 \right| = (8\pi^2 \varepsilon_f) 1/2 - 1 \left| \hat{a} \right|^{-1/6}. \quad \text{(H19)}$$

Equations (H18) and (H19) are exact for spherical energy surfaces. They allow Eq. (H16) to have spherical symmetry. Using the results of Bohm for the integration of the screened coulomb potential in such an integral, and using the potential of Eq. (53) with $V_0 = e^2$, the validity condition becomes
The screening length is given by Kittel \(^21\) as

$$\lambda_s = \left( \frac{\varepsilon_f}{6\pi n_o e^2} \right)^{1/2},$$  \hspace{1cm} (H21)

where \(n_o\) is the carrier concentration. Using the values of
\(n_o = 10^{17}\) cm\(^{-3}\), \(m_o |\hat{\alpha}|^{1/3} = 29.1\), and \(\varepsilon_f = .025\) eV for bismuth, one obtains \(K = 12\). For bismuth telluride with \(n_o = 10^{19}\) cm\(^{-3}\), \(m_o |\hat{\alpha}|^{1/3} = 9.8\), and \(\varepsilon_f = .041\) eV, Eq. (H20) gives \(K = 2.2\).

For InSb (whose Fermi surface becomes slightly ellipsoidal under uniaxial stress) with \(n_o = 10^{16}\) cm\(^{-3}\), \(m^* = .0145 m_o\), and \(\varepsilon_f = .012\) eV, then \(K = 10.1\). Thus the first Born approximation should not be expected to give good quantitative results for these materials, although it could give fair results for bismuth telluride. (Since the potential resembles the coulomb potential for which the first Born approximation is exact, \(K \) could be greater than one before large errors occur.) The approximation is good (i.e. \(K\) is small) for materials with high carrier concentrations and small effective masses. In any case, the Born approximation leads to Eq. (72), thus showing in a qualitative way the effect of the mass tensor on the relaxation time tensor.
**XIV. APPENDIX I: ITERATIVE SOLUTION FOR f**

Equation (62) can be written as

$$e(3f_0/3\varepsilon)\bar{\nabla}\cdot\dot{E} = [q_0 - Q_0 - \gamma^{-1}q_1 + \gamma^{-1}Q_1]f_1,$$

(II)

where the operators are defined as

$$Q_0 f = B\int f_i d\Omega_i,$$

(I2)

$$q_0 = Q_0 f = 4\pi B,$$

(I3)

$$Q_1 f = B\int f_i (\xi - \xi_i) \cdot \alpha^{-1}(\xi - \xi_i) d\Omega_i,$$

(I4)

$$q_1 = Q_1 f = 4\pi B[\xi \cdot \alpha^{-1}\xi_i + (1/3)\text{Tr}(\alpha^{-1})].$$

(I5)

Dividing by $q_0$, and defining an inverse to the operation of the bracket in Eq. (II), one can write the formal solution to $f_1$ as

$$f_1 = (e/4\pi B)(3f_0/3\varepsilon)(1 - L_1 - \gamma^{-1}L_2)^{-1}\bar{\nabla}\cdot\dot{E},$$

(I6)

where

$$L_1 = (1/4\pi B)Q_0,$$

(I7)

and

$$L_2 = (1/3)\text{Tr}(\alpha^{-1}) + (\mu^2/2e) - (1/4\pi B)Q_1.$$  

(I8)

To solve for $f_1$ to the first order in the parameter $\gamma^{-1}$, and neglecting all higher order terms, Eq. (I6) can be
written as

\[ f_1 = \left( \frac{e}{4\pi B} \right) \left( \frac{\partial f}{\partial \xi} \right) \left( \frac{\partial \xi}{\partial f} \right) \left[ (1-L_1)^{-1} + \gamma^{-1} L_2 (1-L_1)^{-1} + \cdots \right] \vec{v} \cdot \vec{E}. \]  

(I9)

For the term \((1-L_1)^{-1} \vec{v} \cdot \vec{E}\), expand the inverse operator in a series as

\[ (1-L_1)^{-1} \vec{v} \cdot \vec{E} = \sum_{n=0}^{\infty} L_1^n \vec{v} \cdot \vec{E}. \]  

(Il0)

Noting that \(Q_0 \vec{v} \cdot \vec{E}\) is zero from symmetry considerations, one obtains

\[ L_1 (\vec{v} \cdot \vec{E}) = 0, \]

\[ L_1^n (\vec{v} \cdot \vec{E}) = 0, \]  

(Ill)

which gives

\[ (1-L_1)^{-1} \vec{v} \cdot \vec{E} = \vec{v} \cdot \vec{E}. \]  

(Il2)

Putting this into Eq. (I9) yields

\[ f_1 = \left( \frac{e}{4\pi B} \right) \left( \frac{\partial f}{\partial \xi} \right) \left( \frac{\partial \xi}{\partial f} \right) \left[ \vec{v} \cdot \vec{E} + \gamma^{-1} (1-L_1)^{-1} L_2 \vec{v} \cdot \vec{E} \right]. \]  

(Il3)

The \(L_2\) operation now gives

\[ L_2 \vec{v} \cdot \vec{E} = \vec{v} \cdot \left[ \left( \frac{1}{3} \right) \text{Tr} (\vec{a}^{-1}) + \left( \frac{p^2}{2\xi} \right) + \left( \frac{2}{3} \right) \vec{a}^{-1} \right] \vec{E}. \]  

(Il4)

The remaining \((1-L_1)^{-1}\) operator proceeds as in Eq. (Il2).
Thus

\[
\left(\frac{e}{4\pi B}\frac{\partial f_0}{\partial \epsilon}\right)^{-1} f_1
\]

\[
= \nabla \cdot \left(1 + \gamma^{-1}\left[\left(1/3\right)\text{Tr}(\hat{\alpha}^{-1}) + (2/3)\hat{\alpha}^{-1}\right]\right) E
\]

+ \gamma^{-1}(1-L_1)^{-1}(p^2/2\epsilon)\nabla \cdot \mathbf{E}.
\]  

(E15)

The term containing \((p^2/2\epsilon)\) yields

\[
\gamma^{-1}\sum L_1^n (p^2/2\epsilon) \nabla \cdot \mathbf{E} = \gamma^{-1}(p^2/2\epsilon)\nabla \cdot \mathbf{E}.
\]

(E16)

Thus one obtains from Eqs. (E15) and (E16)

\[
f_1 = e\left(\frac{\partial f_0}{\partial \epsilon}\right)\left[\nabla \cdot \hat{T} \mathbf{E} + (1/4\pi B)(p^2/2\epsilon)\nabla \cdot \mathbf{E}\right],
\]

(E17)

where

\[
\hat{T} = (1/4\pi B)\left[1 + \gamma^{-1}\left[\left(1/3\right)\text{Tr}(\hat{\alpha}^{-1}) + (2/3)\hat{\alpha}^{-1}\right]\right].
\]

(E18)

Equation (E17) is the same as Eq. (70), which was obtained by guessing the proper form of \(f_1\).
XV. REFERENCES


12. In Eq. (16) and following it is assumed that $\tau$ is independent of the magnetic field. The validity of this is discussed by P. N. Argyres, Phys. Rev. 117, 315 (1960).


16. Since the effective masses are anisotropic, they are not conserved during a collision. Thus the center of mass concept looses its value. The center of momentum denotes the coordinate system in which the total momentum is zero.

17. Using the constants given in Appendix H for bismuth, bismuth telluride, and indium antimonide, and using the smallest element of $\hat{a}$, one obtains for $(2\gamma \hat{a})^{-1}$ the values 2.92, .0485, and .189 respectively. For comparison, if the average mass $|\hat{a}|^{-1/3}$ is used, then $(2\gamma)^{-1} |\hat{a}|^{-1/3}$ is .206, .0167, and .189 respectively.


