Electron Transport with Arbitrarily Oriented Ellipsoidal Fermi Surfaces

H. J. MACKEY AND J. R. SYBERT
Department of Physics, North Texas State University, Denton, Texas
(Received 5 February 1968)

General expressions for the kinetic coefficients of electron transport are obtained for the case of an ellipsoidal Fermi surface arbitrarily oriented with respect to the applied magnetic field, in terms of the coefficients derived for the case of spherical surfaces. The utility of the technique is illustrated by application to a particular case commonly occurring in the treatment of the semimetals.

INTRODUCTION

SEMICONDUCTORS and semimetals are known to have Fermi surfaces which are well represented by sets of symmetry-related ellipsoids. It is therefore useful to obtain expressions for the elements of kinetic coefficient tensors for the case of a Fermi ellipsoid of arbitrary orientation relative to the applied electric, magnetic, and thermal gradient vectors.[1] The problem has been solved by Sondheimer and Wilson[2] for the case of spherical Fermi surfaces. The Sondheimer-Wilson theory has been modified by Grenier *et al.*[1] to discuss both the case of magnetic field directed along one of the principal axes of an ellipsoid as well as the case of magnetic field directed at an arbitrary angle in the plane of two principal axes of the ellipsoid.

In that which follows, explicit expressions are derived for the kinetic coefficient tensors for the most general orientation of a Fermi ellipsoid. The transformation technique of Ham and Mattis[3] is employed to simplify the algebra relating to the ellipsoidal surfaces. The concise tensor notation of Parrott[4] is employed throughout the development of the theory. General expressions are given for the isothermal conductivity tensor $\hat{\sigma}$ and the thermoelectric coefficient tensor $\hat{\epsilon}''$. The utility of the technique is demonstrated by a special case: Using the Sondheimer-Wilson theory, the conductivity tensor $\hat{\sigma}$ is written explicitly in terms of the elements of the reciprocal effective mass tensor $\hat{\alpha}$ for the case of three Fermi ellipsoids symmetrically distributed about a trigonal axis, the principal ellipsoid being tilted through an angle about a single axis perpendicular to the axis of threefold symmetry. This model is particularly applicable to the semimetals arsenic, antimony, and bismuth. It is shown that expressions for the other kinetic coefficients, the Peltier tensor $\hat{\pi}''$ and thermal conductivity $\hat{\lambda}''$, are also obtainable by this technique: This is accomplished simply by demonstrating the validity of the Onsager relation[5] $\hat{\pi}''=T\hat{\epsilon}''$ (T is the absolute temperature) and the Wiedemann-Franz law.

[1] Notation for the kinetic coefficients is given in C. G. Grenier, J. M. Reynolds, and J. R. Sybert, Phys. Rev. **132**, 58 (1963).
[2] A. H. Wilson, *The Theory of Metals* (Cambridge University Press, Cambridge, England, 1959), pp. 208ff.
[3] F. S. Ham and D. C. Mattis, IBM J. Res. Develop. **4**, 143 (1960).
[4] J. E. Parrott, Proc. Phys. Soc. (London) **87**, 1000 (1966).
[5] L. Onsager, Phys. Rev. **37**, 405 (1931); **38**, 2265 (1931).

TRANSFORMATION OF BOLTZMANN EQUATION

The surfaces of constant energy in $\mathbf{p}$ space are taken to be ellipsoids of arbitrary orientation (see Fig. 1) described by

$$2\epsilon=\mathbf{p}\cdot\hat{\alpha}\mathbf{p}, \tag{1}$$

where ϵ is the energy and $\hat{\alpha}$ is the constant inverse effective mass tensor. The transformation

$$\mathbf{w}\equiv\alpha_0^{-1/2}\hat{\alpha}^{1/2}\mathbf{p}=\hat{A}\mathbf{p} \tag{2}$$

reduces Eq. (1) to the form

$$2\epsilon=\alpha_0\mathbf{w}\cdot\mathbf{w}, \tag{3}$$

where α_0 is an arbitrary constant with the dimensions of $\hat{\alpha}$. Thus in $\mathbf{w}$ space the surfaces of constant energy are spheres (see Fig. 2). Use has been made of the fact that $\hat{A}$ is symmetric, which implies the identity

$$\mathbf{p}_1\cdot\hat{A}\mathbf{p}_2\equiv\hat{A}\mathbf{p}_1\cdot\mathbf{p}_2. \tag{4}$$

It is highly convenient simultaneously to transform the experimental coordinate space ($\mathbf{x}$ space) by[3]

$$\mathbf{y}=\hat{A}^{-1}\mathbf{x}. \tag{5}$$

Then one has the following relations:

$$d^3w=|\hat{A}|\,d^3p, \tag{6a}$$

$$d^3y=|\hat{A}^{-1}|\,d^3x, \tag{6b}$$

and the total Jacobian is

$$\partial(\mathbf{w},\mathbf{y})/\partial(\mathbf{p},\mathbf{x})=|\hat{A}|\,|\hat{A}^{-1}|=1, \tag{6c}$$

such that

$$d^6(w,y)=d^6(p,x). \tag{6d}$$

Thus phase volume is invariant and the distribution function f is appropriate to both spaces. The Boltzmann

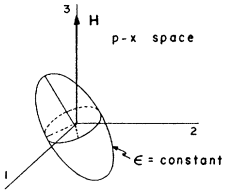

FIG. 1. Ellipsoidal energy surfaces, ϵ=const, are taken in an arbitrary orientation relative to the experimental coordinates (p-x space) which are chosen such that the magnetic field H is directed along the 3 axis.

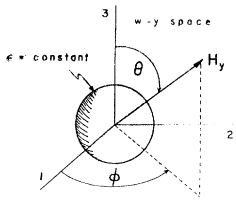

FIG. 2. Energy surfaces, ϵ=const, of Fig. 1 are mapped into spheres in **w** space. The transformed magnetic field $\mathbf{H}_y$ generally has three components in **y** space.

equation[6] in the experimental space is

$$[-e\mathbf{E}-(e/c)\mathbf{v}\times\mathbf{H}]\cdot\nabla_p f+\mathbf{v}\cdot\nabla_x f = -(f-f_0)/\tau=-f_1/\tau. \quad (7)$$

Here $\mathbf{E}=(E_1,E_2,E_3)$ is the electric field, $\mathbf{H}=(0,0,H)$ is the magnetic field, f_0 is the equilibrium Fermi function, and f_1 is the perturbation to f_0. The relaxation time $\tau(\epsilon)$ is taken to depend on **p** only through the energy. Making use of Eqs. (2) and (5), and the symmetry of $\hat{A}$, one has the relations[3]

$$\nabla_y f=\hat{A}\nabla_x f, \quad (8a)$$

$$\nabla_w f=\hat{A}^{-1}\nabla_p f, \quad (8b)$$

$$(\mathbf{v}\times\mathbf{H})\cdot\nabla_p f=\hat{A}(\mathbf{v}\times\mathbf{H})\cdot\nabla_w f, \quad (8c)$$

$$\hat{A}(\mathbf{v}\times\mathbf{H})\equiv(\hat{A}^{-1}\mathbf{v})\times(|\hat{A}|\hat{A}^{-1}\mathbf{H}). \quad (8d)$$

The identity expressed in Eq. (8d) may be easily verified in a coordinate system in which $\hat{A}$ is diagonal; such a system exists since $\hat{A}$ is symmetric. Then by effecting an arbitrary orthogonal transformation one may easily show that the relation is valid in an arbitrary coordinate system.

Now define the transformed electric field, magnetic field, and velocity by[6]

$$\mathbf{E}_y\equiv\hat{A}\mathbf{E}, \quad (9a)$$

$$\mathbf{H}_y\equiv|\hat{A}|\hat{A}^{-1}\mathbf{H}, \quad (9b)$$

$$\mathbf{u}\equiv\hat{A}^{-1}\mathbf{v}. \quad (9c)$$

Note that the relation

$$\mathbf{v}=\nabla_p\epsilon \quad (10a)$$

becomes

$$\mathbf{u}=\nabla_w\epsilon. \quad (10b)$$

Using the above relations, Eq. (7) becomes

$$[-e\mathbf{E}_y-(e/c)\mathbf{u}\times\mathbf{H}_y]\cdot\nabla_w f+\mathbf{u}\cdot\nabla_y f=-f_1/\tau. \quad (11)$$

TRANSFORMATION OF KINETIC EQUATIONS

The definition of electric current density in differential form is

$$d\mathbf{J}=-dn(\mathbf{v})e\mathbf{v}, \quad (12)$$

where $dn(\mathbf{v})$ is the number of electrons per unit **x** volume with velocity infinitesimally near **v**. The corresponding quantity in **y** space is, by Eq. (6b),

$$dn'(\mathbf{u})\equiv|\hat{A}|dn(\mathbf{v}). \quad (13)$$

This, along with Eq. (9c), reduces Eq. (12) to

$$d\mathbf{J}=|\hat{A}^{-1}|\hat{A}(-dn'e\mathbf{u})=|\hat{A}^{-1}|\hat{A}d\mathbf{J}_y, \quad (14a)$$

where

$$d\mathbf{J}_y\equiv-dn'e\mathbf{u} \quad (14b)$$

is the transformed differential current density. Now consider the transport equation[1]

$$\mathbf{J}=\hat{\sigma}\mathbf{E}^*-\hat{\epsilon}''\mathbf{G}, \quad (15a)$$

where

$$\mathbf{E}^*=\mathbf{E}-(1/e)(\partial\zeta/\partial T)\mathbf{G}, \quad (15b)$$

$$\mathbf{G}\equiv-\nabla_x T, \quad (15c)$$

and where ζ is the chemical potential. Define

$$\mathbf{G}_y\equiv\hat{A}\mathbf{G}=-\nabla_y T, \quad (16a)$$

$$\mathbf{E}_y{}^*\equiv\hat{A}\mathbf{E}^*=\mathbf{E}_y-(1/e)(\partial\zeta/\partial T)\mathbf{G}_y. \quad (16b)$$

Then Eq. (15a) becomes

$$\mathbf{J}_y=\hat{\sigma}^*\mathbf{E}_y{}^*-\hat{\epsilon}^*\mathbf{G}_y, \quad (17a)$$

with

$$\hat{\sigma}^*\equiv|\hat{A}|\hat{A}^{-1}\hat{\sigma}\hat{A}^{-1}, \quad (17b)$$

$$\hat{\epsilon}^*\equiv|\hat{A}|\hat{A}^{-1}\hat{\epsilon}''\hat{A}^{-1}. \quad (17c)$$

From the definition of thermal current density,[7]

$$d\mathbf{W}^*=(\epsilon-\zeta)dn(\mathbf{v})\mathbf{v}, \quad (18)$$

the transformed differential thermal current density is

$$d\mathbf{W}_y{}^*\equiv|\hat{A}|\hat{A}^{-1}d\mathbf{W}^*. \quad (19)$$

The other transport equation[1]

$$\mathbf{W}^*=-\hat{\pi}''\mathbf{E}^*+\hat{\lambda}''\mathbf{G} \quad (20a)$$

becomes

$$\mathbf{W}_y{}^*=-\hat{\pi}^*\mathbf{E}_y{}^*+\hat{\lambda}^*\mathbf{G}_y, \quad (20b)$$

where

$$\hat{\pi}^*=|\hat{A}|\hat{A}^{-1}\hat{\pi}''\hat{A}^{-1}, \quad (20c)$$

$$\hat{\lambda}^*=|\hat{A}|\hat{A}^{-1}\hat{\lambda}''\hat{A}^{-1}. \quad (20d)$$

One now proceeds to obtain a solution to Eq. (11) and then computes the current densities

$$\mathbf{J}_y=-2eh^{-3}\int f_1\mathbf{u}d^3w, \quad (21a)$$

$$\mathbf{W}_y{}^*=2h^{-3}\int f_1(\epsilon-\zeta)\mathbf{u}d^3w \quad (21b)$$

for the case of spherical energy surfaces. The coefficients of $\mathbf{E}_y{}^*$ and $\mathbf{G}_y$ are identified as the kinetic coefficients $\hat{\sigma}^*$, $\hat{\epsilon}^*$, $\hat{\pi}^*$, and $\hat{\lambda}^*$. The **p**-**x**-space parameters $\hat{\sigma}$, $\hat{\epsilon}''$, $\hat{\pi}''$, and $\hat{\lambda}''$ are then obtained by inverting Eqs. (17b), (17c), (20c), and (20d). There is no loss in generality by taking $\mathbf{H}=(0,0,H)$ in the experimental **x** space. Then Eq. (9b) gives

$$\mathbf{H}_y=|\hat{A}|H[(A^{-1})_{13},(A^{-1})_{23},(A^{-1})_{33}], \quad (22)$$

[6] Subscripts on gradient operators are meant to indicate the space in which the operator is defined. Subscripts to vectors (boldface) and to vector magnitudes (light face) indicate the space in which the vector is defined and do not indicate Cartesian components.

[7] H. B. Callen, *Thermodynamics* (John Wiley & Sons, Inc., New York, 1960).

where $(A^{-1})_{ij}$ is an element of the tensor $\hat{A}^{-1}$. Writing out the components of $\mathbf{H}_y$ in spherical polar form gives

$$\sin\theta = r/t, \tag{23a}$$

$$\cos\theta = (A^{-1})_{33}/t, \tag{23b}$$

$$\sin\phi = (A^{-1})_{23}/r, \tag{23c}$$

$$\cos\phi = (A^{-1})_{13}/r, \tag{23d}$$

$$r = [(A^{-1})_{23}^2 + (A^{-1})_{13}^2]^{1/2}, \tag{23e}$$

$$t \equiv [(A^{-1})_{13}^2 + (A^{-1})_{23}^2 + (A^{-1})_{33}^2]^{1/2} = (A^{-2})_{33}^{1/2}, \tag{23f}$$

where θ and ϕ are defined in Fig. 2. Although the problem is now reduced to the simpler situation involving spherical energy surfaces, it is of further convenience to perform an orthogonal transformation from **y** space to **y′** space such that the magnetic field $\mathbf{H}_{y'}$ is directed along the y_3' axis. This may be accomplished by using

$$\hat{T} \equiv \hat{Y}(\theta)\hat{Z}(\phi), \tag{24}$$

where $\hat{Z}(\phi)$ is a right-handed rotation through angle ϕ about the y_3 axis and $\hat{Y}(\theta)$ is a subsequent right-handed rotation through angle θ about the new y_2' axis (see Figs. 2 and 3). The necessary elements of $\hat{Z}(\phi)$ and $\hat{Y}(\theta)$ are given in Eqs. (23). Denote all variables in the **y′** space by the addition of primes. Then

$$\hat{\sigma}^* = \hat{T}^{-1}\hat{\sigma}^{*\prime}\hat{T} \tag{25a}$$

and

$$\hat{\sigma} = |\hat{A}^{-1}|\hat{A}\hat{T}^{-1}\hat{\sigma}^{*\prime}\hat{T}\hat{A}, \tag{25b}$$

with the other kinetic coefficients transforming similarly. Thus the problem has been reduced to computing Eqs. (21a) and (21b) for the case of spherical energy surfaces with magnetic field directed along the 3 axis (y_3' axis). Then the tensor multiplication indicated in Eqs. (25) handles the job of representing the kinetic coefficients in the experimental coordinates (**x** space).

RESULTS OF SONDHEIMER-WILSON THEORY

The Sondheimer-Wilson approximation[2] to the solutions of Eqs. (21) for the case of spherical energy surfaces with magnetic field directed along the y_3' axis yields

$$\hat{\sigma}^{*\prime} = n'ec\begin{bmatrix} H_{y'i}L' & \mp H_{y'}L' & 0 \\ \pm H_{y'}L' & H_{y'i}L' & 0 \\ 0 & 0 & 1/H_{y'i} \end{bmatrix}, \tag{26a}$$

$$\hat{\epsilon}^{*\prime} = \tfrac{1}{3}\pi^2k^2cTZ'\begin{bmatrix} \pm H_{y'i}L' & -H_{y'}L' & 0 \\ H_{y'}L' & \pm H_{y'i}L' & 0 \\ 0 & 0 & \pm 1/H_{y'i} \end{bmatrix}, \tag{26b}$$

$$\hat{\pi}^{*\prime} = T\hat{\epsilon}^{*\prime}, \tag{26c}$$

$$\hat{\lambda}^{*\prime} = (\pi^2k^2T/3e^2)\hat{\sigma}^{*\prime}, \tag{26d}$$

$$L' \equiv (H^2_{y'} + H^2_{y'i})^{-1}, \tag{26e}$$

$$H_{y'i} \equiv c/e\tau\alpha_0, \tag{26f}$$

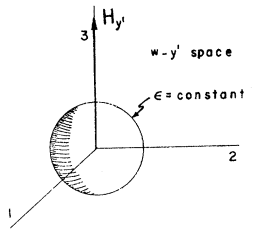

FIG. 3. Orthogonal transformation from **y** space to **y′** space transforms $\mathbf{H}_y$ into $\mathbf{H}_{y'}$, which is directed along the 3 axis.

where the upper signs are for electrons, the lower signs are for holes, $\tau = \tau(\zeta)$, and k is Boltzmann's constant.[8] Now rewrite these equations in terms of **x**-space parameters. Z' is the number of states per unit **y′** volume, per unit energy interval. Let Z be the density of states in **x** space. Then, by analogy to Eq. (13),

$$Z' = |\hat{A}|Z. \tag{27}$$

Combining Eqs. (22), (23f), (26e), and (26f), one finds

$$H_{y'} = |\hat{A}|tH, \tag{28a}$$

$$L' = (|\hat{A}|t)^{-2}L, \tag{28b}$$

$$L \equiv (H^2 + H_i^2)^{-1}, \tag{28c}$$

$$H_i \equiv c(\alpha_0 e\tau|\hat{A}|t)^{-1}. \tag{28d}$$

Combining Eqs. (13), (27), and (28) gives

$$\hat{\sigma}^{*\prime} = \frac{nec}{t}\begin{bmatrix} H_iL & \mp HL & 0 \\ \pm HL & H_iL & 0 \\ 0 & 0 & 1/H_i \end{bmatrix}, \tag{29a}$$

$$\hat{\epsilon}^{*\prime} = \frac{\pi^2k^2cTZ}{3t}\begin{bmatrix} \pm H_iL & -HL & 0 \\ HL & \pm H_iL & 0 \\ 0 & 0 & \pm 1/H_i \end{bmatrix}. \tag{29b}$$

Thus, given an explicit representation of $\hat{\alpha}$, Eqs. (29) along with Eqs. (28c) and (28d) may be inserted in Eq. (25) to obtain explicit expressions for $\hat{\sigma}$ and $\hat{\epsilon}''$. From Eqs. (26c) and (26d) one sees that in **x** space

$$\hat{\lambda}'' = (\pi^2k^2T/3e^2)\hat{\sigma}, \tag{30a}$$

$$\hat{\pi}'' = T\hat{\epsilon}'', \tag{30b}$$

such that expressions are obtained for all the kinetic coefficients.

EFFECTIVE MASS

The so-called saturation field H_i given in Eq. (28d) has the form[9,10]

$$H_i = m^*c/e\tau, \tag{31a}$$

with

$$m^* \equiv (\alpha_0|\hat{A}|t)^{-1}. \tag{31b}$$

[8] Equations (26a) and (26b) are applicable for the strongly degenerate approximation where integration over energy involves essentially the δ functions $\delta(\epsilon-\zeta)$, and therefore $\tau(\epsilon)$ is evaluated at the Fermi energy.

[9] D. E. Soule, Phys. Rev. **112**, 698 (1958).

[10] J. W. McClure, Phys. Rev. **112**, 715 (1958).

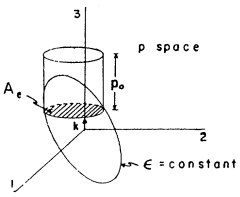

FIG. 4. Right elliptical cylinder of height p_0 is erected upon the elliptical base of area A_e defined by the intersection of a plane p_3=const and the constant energy surface shown in Fig. 1.

It is interesting to calculate the cyclotron mass m_c for comparison to Eq. (31b). The cyclotron-mass formula[11] is

$$m_c \equiv (1/2\pi)\partial A_e/\partial\epsilon, \tag{32}$$

where A_e is the area of the ellipse normal to the magnetic field $\mathbf{H}=(0,0,H)$ formed by the intersection of the plane

$$\mathbf{p}\cdot\mathbf{k}=p_3=\text{const} \tag{33a}$$

and the ellipsoid

$$2\epsilon=\mathbf{p}\cdot\hat{\alpha}\mathbf{p}. \tag{33b}$$

Here $\mathbf{k}$ is the unit vector along x_3. Using Eq. (2), the plane transforms to a plane in $\mathbf{w}$ space,

$$\mathbf{w}\cdot\mathbf{k}'=p_3'=\text{const}, \tag{34a}$$

where

$$p_3'=p_3(\mathbf{k}\cdot\hat{A}^{-2}\mathbf{k})^{-1/2}=p_3(A^{-2})_{33}^{-1/2} \tag{34b}$$

and

$$\mathbf{k}'=(A^{-2})_{33}^{-1/2}\hat{A}^{-1}\mathbf{k} \tag{34c}$$

is the unit vector normal to the transformed plane. Since the ellipsoid transforms to a sphere [see Eq. (3)], the ellipse of area A_e transforms to a circle of area A_c, where

$$A_c=2\pi\epsilon/\alpha_0-\pi p_3^2(A^{-2})_{33}^{-1}. \tag{35}$$

In order to determine A_e in terms of A_c one may use Eq. (6a) to advantage. Construct an elliptical cylinder of height p_0 on the ellipse in $\mathbf{p}$ space as indicated in Fig. 4. Then from Eqs. (34) one sees that this transforms into a circular cylinder in $\mathbf{w}$ space of height p_0' (see Fig. 5), where

$$p_0'=p_0(A^{-2})_{33}^{-1/2}. \tag{36}$$

Then

$$A_e=[2\pi\epsilon/\alpha_0-\pi p_3^2(A^{-2})_{33}^{-1}]|\hat{A}^{-1}|\,(A^{-2})_{33}^{-1/2}. \tag{37}$$

Equation (32) gives

$$m_c=(\alpha_0|\hat{A}|)^{-1}(A^{-2})_{33}^{-1/2}. \tag{38}$$

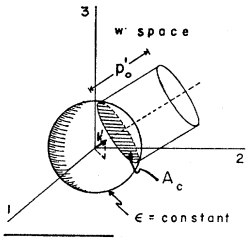

FIG. 5. Elliptical cylinder of Fig. 4 maps into a right circular cylinder of height p_0' and basal area A_c in $\mathbf{w}$ space.

[11] See, e.g., J. M. Ziman, *Electrons and Phonons* (Oxford University Press, London, 1960), p. 514.

Comparison to Eq. (31b) shows that $m^*=m_c$. Then

$$H/H_i=\omega_c\tau, \tag{39}$$

where ω_c is the cyclotron frequency.

AN APPLICATION

Consider a Fermi ellipsoid of electrons which has been rotated out of principal axes by a rotation through angle ψ about the 1 axis. Denote $\hat{\alpha}$ in a principal-axis system by $\hat{\alpha}_p$, where

$$\hat{\alpha}_p=\begin{bmatrix}\alpha_1 & 0 & 0\\ 0 & \alpha_2 & 0\\ 0 & 0 & \alpha_3\end{bmatrix}. \tag{40}$$

The above described ellipsoid is characterized by

$$\hat{\alpha}=\hat{X}(-\psi)\hat{\alpha}_p\hat{X}(\psi), \tag{41}$$

where

$$\hat{X}(\psi)\equiv\begin{bmatrix}1 & 0 & 0\\ 0 & c & s\\ 0 & -s & c\end{bmatrix}, \tag{42a}$$

$$c\equiv\cos\psi, \tag{42b}$$

$$s\equiv\sin\psi. \tag{42c}$$

Writing out Eq. (41) explicitly, one has

$$\hat{\alpha}=\begin{bmatrix}\alpha_1 & 0 & 0\\ 0 & \alpha_2c^2+\alpha_3s^2 & (\alpha_2-\alpha_3)sc\\ 0 & (\alpha_2-\alpha_3)sc & \alpha_2s^2+\alpha_3c^2\end{bmatrix}. \tag{43}$$

Then

$$\hat{A}=\alpha_0^{-1/2}\begin{bmatrix}\sqrt{\alpha_1} & 0 & 0\\ 0 & c^2\sqrt{\alpha_2}+s^2\sqrt{\alpha_3} & (\sqrt{\alpha_2}-\sqrt{\alpha_3})sc\\ 0 & (\sqrt{\alpha_2}-\sqrt{\alpha_3})sc & c^2\sqrt{\alpha_3}+s^2\sqrt{\alpha_2}\end{bmatrix}. \tag{44}$$

From Eqs. (23) and (24), noting that the rotation ϕ about the y_3 axis is $\frac{1}{2}\pi$, one finds

$$\hat{T}=q^{-1/2}\begin{bmatrix}0 & A_{22} & A_{23}\\ -q^{1/2} & 0 & 0\\ 0 & -A_{23} & A_{22}\end{bmatrix}, \tag{45a}$$

$$|\hat{A}|t=A_{11}q^{1/2}, \tag{45b}$$

$$q\equiv(A_{22})^2+(A_{23})^2. \tag{45c}$$

Now writing out Eq. (25b) explicitly, one finds

$$\hat{\sigma}=necL\begin{bmatrix}d_1H_i & -H & -d_2H\\ H & d_1^{-1}H_i & d_3H_i\\ d_2H & d_3H_i & d_4H_i+d_5/H_iL\end{bmatrix}, \tag{46}$$

with

$$d_1\equiv(\alpha_{11}/\alpha_{22})^{1/2}, \qquad d_2\equiv\alpha_{23}/\alpha_{22},$$
$$d_3\equiv\alpha_{23}(\alpha_{11}\alpha_{22})^{-1/2}, \qquad d_4\equiv(\alpha_{23})^2(\alpha_{11})^{-1/2}(\alpha_{22})^{-3/2},$$
$$d_5\equiv\alpha_2\alpha_3(\alpha_{11})^{-1/2}(\alpha_{22})^{-3/2}, \qquad m^*=(\alpha_{11}\alpha_{22})^{-1/2},$$

where the α_{ij} are the elements of $\hat{\alpha}$ defined in Eq. (43). Now suppose there are three such ellipsoids located with trigonal symmetry about the x_3 axis. The total conductivity is

$$\hat{\sigma}_t=\hat{\sigma}+\hat{Z}(\tfrac{2}{3}\pi)\hat{\sigma}\hat{Z}(-\tfrac{2}{3}\pi)+\hat{Z}(-\tfrac{2}{3}\pi)\hat{\sigma}\hat{Z}(\tfrac{2}{3}\pi), \tag{47a}$$

$$\hat{\sigma}_i=\begin{bmatrix} \frac{3}{2}(\sigma_{11}+\sigma_{22}) & \frac{3}{2}(\sigma_{12}-\sigma_{21}) & 0 \\ -\frac{3}{2}(\sigma_{12}-\sigma_{21}) & \frac{3}{2}(\sigma_{11}+\sigma_{22}) & 0 \\ 0 & 0 & 3\sigma_{33} \end{bmatrix}. \quad (47b)$$

Then the conductivity related to experiment is

$$\hat{\sigma}_i=Nec\begin{bmatrix} a_iH_iL & -HL & 0 \\ HL & a_iH_iL & 0 \\ 0 & 0 & b_iH_iL+c_i \end{bmatrix}, \quad (48a)$$

where

$$a_i\equiv\tfrac{1}{2}[(\alpha_{11}/\alpha_{22})^{1/2}+(\alpha_{22}/\alpha_{11})^{1/2}], \quad (48b)$$

$$b_i\equiv(\alpha_{23})^2(\alpha_{11})^{-1/2}(\alpha_{22})^{-3/2}, \quad (48c)$$

$$c_i\equiv\alpha_2\alpha_3(\alpha_{22})^{-1}e\tau/c, \quad (48d)$$

$$N\equiv 3n. \quad (48e)$$

SUMMARY

The foregoing example illustrates the ease with which one may write the total conductivity tensor for a Fermi surface consisting of a set of ellipsoids symmetrically placed about the direction of the magnetic field. It should be clear, however, that even for a set of ellipsoids having no symmetry with respect to the direction of the magnetic field one may follow the above recipe to determine the total conductivity. One need only write the $\hat{\alpha}$ tensors describing the various ellipsoids in a common coordinate system chosen such that the magnetic field is along the 3 axis. The rest of the problem is simply to perform the indicated tensor multiplications and then to add up the individual conductivities. Corresponding expressions for $\hat{\epsilon}''$, $\hat{\lambda}''$, and $\hat{\pi}''$ are obtained in an obvious manner [see Eq. (26)]. One may choose to represent the spherical geometry solutions in an approximation different from that of the Sondheimer-Wilson theory,[2] but the method of obtaining the ellipsoidal geometry solutions remains the same.

PHYSICAL REVIEW VOLUME 172, NUMBER 3 15 AUGUST 1968

Anomalous Skin Effect for Specular Electron Scattering and Optical Experiments at Non-Normal Angles of Incidence*

K. L. Kliewer and Ronald Fuchs
Institute for Atomic Research and Department of Physics, Iowa State University, Ames, Iowa 50010
Received 14 March 1968

The anomalous skin effect for specular electron scattering at the metal surface is studied, permitting the impinging plane wave to have an arbitrary angle of incidence. It is shown that the expressions for the surface impedance for a non-normal angle of incidence obtained by Reuter and Sondheimer as a generalization from their work at normal incidence are correct for S polarization but incorrect for P polarization. The correct surface impedance for P polarization leads to an additional absorption peak in the frequency range $10^{-2}\omega_p\lesssim\omega\lesssim\omega_p$, where ω_p is the free-electron plasma frequency. This additional absorption, particularly pronounced for long electron lifetimes, is investigated in detail. One important conclusion drawn from this work is that, in general, optical experiments performed at non-normal angles of incidence cannot be analyzed in terms of a single complex frequency-dependent dielectric function. In the frequency range of the additional P absorption, two such dielectric functions are needed, one function for describing P polarization and a different function for describing S polarization.

I. INTRODUCTION

THE theory by which the anomalous skin effect was incorporated into the general theory of the optical properties of metals was developed in detail by Reuter and Sondheimer[1] and Dingle[2] for both specular and diffuse electron scattering at the metal surface. This work, utilizing the Boltzmann equation, treated the case of a plane wave incident normally on the metal surface, although conclusions were drawn concerning also the effect of non-normal incidence. A quantum-mechanical treatment of the anomalous skin effect at normal incidence with specular reflection was given by Mattis and Bardeen[3]; their result for the surface impedance was in agreement with that of Reuter and Sondheimer.

A recent study of the classical optical properties of an electron gas by the present authors[4] indicated that interesting absorption structure can occur at non-normal angles of incidence, structure that possesses no counterpart at normal incidence. This fact, together with the appearance of the striking results of optical studies performed by Mayer and his co-workers[5] on the alkali metals at large angles of incidence, suggested to us that a reexamination of the theory of the anomalous

* Work performed in the Ames Laboratory of the U. S. Atomic Energy Commission. Contribution No. 2269.
[1] G. E. H. Reuter and E. H. Sondheimer, Proc. Roy. Soc. (London) **A195**, 336 (1948).
[2] R. B. Dingle, Physica **19**, 311 (1953).
[3] D. C. Mattis and J. Bardeen, Phys. Rev. **111**, 412 (1958).
[4] K. L. Kliewer and R. Fuchs, Phys. Rev. **153**, 498 (1967).
[5] H. Mayer and B. Hietel, in *Optical Properties and Electronic Structure of Metals and Alloys*, edited by F. Abeles (North-Holland Publishing Co., Amsterdam, 1966), p. 47, and references cited therein.