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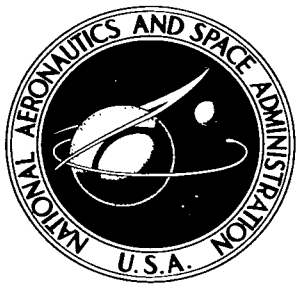

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EXACT SEMICLASSICAL THEORY FOR GALVANOMAGNETIC EFFECTS IN METALS

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NATIONAL AERONAUTICS AND SPACE ADMINISTRATION • WASHINGTON, D. C. • SEPTEMBER 1967

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EXACT SEMICLASSICAL THEORY FOR GALVANOMAGNETIC EFFECTS IN METALS*

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SUMMARY

From the linearized Boltzmann equation for the distribution function of conduction electrons under the influence of uniform electric and magnetic fields, a solution in closed form is obtained for the conductivity tensor which is valid for any magnetic field strength. This result is obtained without assuming the existence of a scattering relaxation time and is valid for an arbitrary Fermi surface, including those surfaces which support open electron trajectories for some orientations of the magnetic field. The starting point for this theory is the definition of an anisotropic vector mean free path and the assumption that this function may be expanded in powers of the magnetic field strength. The resulting power series for the electron current may be summed exactly by considering the complete set of eigenfunctions of a magnetic scattering operator.

INTRODUCTION

One of the most common experiments performed to study the nature of the Fermi surface in metals is the measurement of the galvanomagnetic properties of the metal. The primary usefulness of this technique is the information obtained about the anisotropy of the Fermi surface, and particularly, on the existence of directions in the crystal which support open electron trajectories.

So far there has been no comprehensive theory available that is capable of giving enough results to enable a detailed comparison with the experiments. The usual theories have been phenomenological and generally treat only one of the galvanomagnetic properties, such as the longitudinal magnetoresistance or the Hall effect. This report describes the formalism of an exact semiclassical theory giving the entire conductivity tensor as a function of magnetic field strength and orientation.

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*Supported in part by the U.S. Atomic Energy Commission.

**Case Institute of Technology.

ANALYSIS

The treatment described in this report is semiclassical, since it starts from a solution of the Boltzmann equation, but no a priori assumption is made about the nature of the Fermi surface or the existence of a relaxation time.

The semiclassical treatment of conduction electrons in metals is based on the assumption that these electrons can be described by a momentum-space distribution function f_k, which satisfies the Boltzmann equation. The linearized Boltzmann equation for the distribution function, including the effects of an applied electric field $\vec{E}$ and magnetic field $\vec{H}$, can be written (ref. 1) as

$$e\vec{v}_k \cdot \vec{E} \frac{\partial f_k^0}{\partial \epsilon_k} + \frac{e}{\hbar c} (\vec{v}_k \times \vec{H}) \cdot \nabla_k f_k = \frac{df_k}{dt} \tag{1}$$

where f_k is the distribution function (i.e., the probability of occupation of the electronic state of wave vector $\vec{k}$, energy ϵ_k, and group velocity $\vec{v}_k$). The group velocity is the $\vec{k}$-space gradient of the energy, so that

$$\hbar\vec{v}_k = \nabla_k \epsilon_k$$

The term df_k/dt formally represents the time rate of change of f_k due to collision processes. The metal is assumed to be in thermal equilibrium, and the Boltzmann equation represents the balance between the driving forces $\vec{E}$ and $\vec{H}$ and the scattering mechanisms in the metal. The function f_k^0 is the value of f_k in the absence of fields and is given by the usual Fermi-Dirac function.

At sufficiently low temperatures, it is a reasonable approximation to assume that the electron scattering is by elastic collisions. This assumption is not essential to the theory but simplifies the discussion of the formalism. The case of inelastic scattering can be treated by essentially the same methods as presented herein.

For elastic scattering, the right side of equation (1) can be written as

$$\frac{df_k}{dt} = \int Q(\vec{k}, \vec{k}')(f_k - f_{k'})\, d\vec{k} \tag{2}$$

where $Q(\vec{k}, \vec{k}')$ is the probability per unit time that an electron which is known to be initially in the state $\vec{k}$ is scattered into the originally empty state $\vec{k}'$. This probability is symmetric, $Q(\vec{k}, \vec{k}') = Q(\vec{k}', \vec{k})$. The integral in equation (2) is symbolic for a summation over all k-states. The symbol $d\vec{k}$ is defined in the notation of Ziman (ref. 1) such

that $d\vec{k} = [V/(2\pi)^3]d^3k$ where V is the volume of the sample.

It was shown originally in reference 2 that a solution to equation (1), with the substitution of equation (2) for df_k/dt, could be obtained by assuming a trial solution of the form

$$f_k - f_k^0 = -e\vec{E} \cdot \vec{\Lambda}(\vec{k}) \frac{\partial f_k^0}{\partial \epsilon_k} \tag{3}$$

where the trial function $\vec{\Lambda}(\vec{k})$ has the appearance of a vector mean free path and is independent of $\vec{E}$. The assumption of this trial function is equivalent to linearizing the Boltzmann equation, since equation (3) explicitly states that the deviation from equilibrium is taken to be linear in the electric field. This assumption is then equivalent to making the restriction that Ohm's law must hold in the metal (i.e., that the electron current is linear in $\vec{E}$). The conductivity tensor then has the following form (ref. 2):

$$\sigma = -e^2 \int \vec{v}_k \vec{\Lambda}(\vec{k}) \frac{\partial f_k^0}{\partial \epsilon_k} d\vec{k} \tag{4}$$

Substituting equation (3) into equation (1) results in the following equation for $\vec{\Lambda}(\vec{k})$:

$$\vec{v}_k - \left(\frac{e}{\hbar c}\right)(\vec{v}_k \cdot \vec{H} \times \vec{\nabla}_k)\vec{\Lambda} = (q - Q)\vec{\Lambda} \tag{5}$$

where Q is defined as the scattering operator

$$Q\vec{\Lambda}(\vec{k}) \equiv \int Q(\vec{k}, \vec{k}')\vec{\Lambda}(\vec{k}')d\vec{k}' \tag{6a}$$

and q is the scalar function

$$q(\vec{k}) \equiv \int Q(\vec{k}, \vec{k}')d\vec{k}' \tag{6b}$$

The method used to solve equation (4) is to expand $\vec{\Lambda}$ in a power series in $\vec{H}$

$$\vec{\Lambda}(\vec{k}) = \sum_{n=0}^{\infty} \vec{\Lambda}^{(n)}(\vec{k}) \tag{7}$$

where each term $\vec{\Lambda}^{(n)}$ is proportional to $(H)^n$. This series is substituted into equa-

tion (5), and the result is a set of equations, infinite in number, which is obtained by separating the coefficients of each power of $\vec{H}$:

$$\left.\begin{aligned} \vec{v}_k &= (q - Q)\vec{\Lambda}^{(0)} \\ -\frac{eH}{\hbar c}(\vec{v}_k \cdot \hat{h} \times \nabla_k)\vec{\Lambda}^{(n)} &= (q - Q)\vec{\Lambda}^{(n+1)} \end{aligned}\right\} \tag{8}$$

where $\hat{h}$ is a unit vector such that $\vec{H} = H\hat{h}$. The first equation of (8) was derived in reference 2 to calculate the electrical resistance of a metal in the absence of a magnetic field. The remaining equations (also derived in ref. 2) describe the effect that the magnetic field has on the electronic properties.

The operator $(q - Q)$ is singular, but an inverse operator may still be defined by the arguments in reference 2. Thus, if the cyclotron frequency is defined as $\omega = eH/mc$ where m is the free electron mass, equation (8) may be written as

$$\vec{\Lambda}^{(n)} = \left[\left(-\frac{m\omega}{\hbar}\right)(q - Q)^{-1}(\vec{v}_k \cdot \hat{h} \times \nabla_k)\right]^n \vec{\Lambda}^{(0)} \tag{9}$$

It is convenient to reduce the form of this equation by defining a magnetic scattering operator T.

$$T \equiv \left(\frac{im}{\hbar}\right)(q - Q)^{-1}(\vec{v}_k \cdot \hat{h} \times \nabla_k) \tag{10}$$

where the factor i and the symmetry of the scattering probability $Q(\vec{k}, \vec{k'})$ make T a Hermitian operator. Then equation (7) may be written as

$$\vec{\Lambda}(\vec{k}) = \sum_{n=0}^{\infty} (i\omega T)^n (q - Q)^{-1}\vec{v}_k \tag{11}$$

This geometric series may be summed to give as the conductivity

$$\sigma = -e^2 \int \vec{v}_k [1 - i\omega T]^{-1}(q - Q)^{-1}\vec{v}_k \left(\frac{\partial f_k^0}{\partial \epsilon_k}\right) d\vec{k} \tag{12}$$

This result, although formally correct for the conductivity, is not in a form useful for computations. This equation may be rewritten by considering the eigenfunctions of the magnetic operator defined by

$$Tb_l(\vec{k}) = \tau_l b_l(\vec{k}) \tag{13}$$

or, explicitly.

$$im(\vec{v}_k \cdot \hat{h} \times \nabla_k) b_l(\vec{k}) = \hbar\tau_l (q - Q) b_l(\vec{k}) \tag{14}$$

where the eigenvalues τ_l are real since T is Hermitian. Note, from the definition of T, that $Tb_l^* = -\tau_l b_l^*$. In the integral for the conductivity, the operator T acts on the zero-field mean free path $(q - Q)^{-1}\vec{v}_k$. This function is expanded in a complete set of the $b_l(\vec{k})$ as follows:

$$(q - Q)^{-1} v_\mu = \sum_l \beta_{l\mu} b_l(\vec{k}) \tag{15}$$

where v_μ is the μ^{th} component of v_k, defined with respect to the crystal axis system. This summation in equation (15) includes, for every term $\beta_{l\mu} b_l$, its complex conjugate term $\beta_{l\mu}^* b_l^*$, since the function $(q - Q)^{-1} v_\mu$ is real. Substituting this expansion into equation (12) results in

$$\sigma_{\nu\mu} = -e^2 \sum_l \frac{\beta_{l\mu}}{1 - i\omega\tau_l} \int v_\nu b_l \frac{\partial f_k^0}{\partial \epsilon_k} d\vec{k} \tag{16}$$

Although the solution for Λ which is used in equation (16) was derived using a power series expansion in H, the validity of this solution is not limited to the low-field region. This fact can be seen by noting that the solution for Λ, when substituted into equation (5), represents a solution of the Boltzmann equation for any value of H.

The main problem now becomes the calculation of the field-orientation-dependent eigenfunctions $b_l(\vec{k})$ and the expansion coefficients. Equation (14) represents an integral differential equation for the eigenfunctions, with the field direction $\hat{h}$ as a parameter. This problem may be simplified by making use of the scattering eigenfunctions as introduced in reference 2 and defined by the eigenvalue equation

$$q^{-1} Q a_n(\vec{k}) = \alpha_n a_n(\vec{k}) \tag{17}$$

These field-independent eigenfunctions have the orthogonality property that

$$\int a_r(\vec{k})q(\vec{k})a_n(\vec{k})\,d\vec{k} = \delta_{rn} \tag{18}$$

Now the magnetic eigenfunctions may be expanded in a complete set of the a_n, with expansion coefficients γ_{ln} that depend upon $\hat{h}$,

$$b_l(\vec{k}) = \sum_n \gamma_{ln}(\hat{h})a_n(\vec{k}) \tag{19}$$

This expansion makes it possible to eliminate the integral operator (q - Q) from equation (14). Substituting equation (19) for $b_l(\vec{k})$ in equation (14), multiplying by $a_r(\vec{k})$, and integrating the orthogonality condition (eq. (18)) over the Fermi surface yield

$$\hbar\tau_l(1 - \alpha_r)\gamma_{lr} = -im\hat{h} \cdot \sum_n \gamma_{ln} \int a_r(\vec{k})\left[\vec{v}_k \times (\nabla_k a_n(\vec{k}))\right]d\vec{k} \tag{20}$$

Although equation (20) looks formidable, it may be better understood by defining the vector quantity $\vec{C}_{rn}$ as

$$\vec{C}_{rn} \equiv -\frac{im}{\hbar} \int a_r \vec{v}_k \times (\nabla_k a_n)d\vec{k} \tag{21}$$

With this definition, equation (20) becomes simply

$$\tau_l\gamma_{lr}(1 - \alpha_r) = \hat{h} \cdot \sum_n \vec{C}_{rn}\gamma_{ln} \tag{22}$$

This is a set of linear equations which may be solved for τ_l and γ_{lr} once the other quantities are known.

Combining equations (16) and (19) results in the final form for the conductivity tensor:

$$\sigma_{\nu\mu} = -e^2 \sum_{l,n} \frac{1}{1 - i\omega\tau_l} \beta_{l\mu}\gamma_{ln}g_{\nu n} \tag{23}$$

where

$$g_{\nu n} \equiv \int v_\nu a_n(\vec{k}) \frac{\partial f_k^0}{\partial \epsilon_k} d\vec{k} \tag{24}$$

To make this expression for the conductivity more resemble the usual forms found in the literature and to make explicit the role of the open orbits, equation (23) may be rewritten as

$$\sigma_{\nu\mu} = -e^2 \sum_{\substack{l,n \\ \tau_l=0}} \mathrm{Re}(\beta_{l\mu}\gamma_{ln})g_{\nu n} + e^2 \sum_{\substack{l,n \\ \tau_l\neq 0}} \frac{\omega\tau_l}{1+(\omega\tau_l)^2} \mathrm{Im}(\beta_{l\mu}\gamma_{ln})g_{\nu n}$$

$$-e^2 \sum_{\substack{l,n \\ \tau_l\neq 0}} \frac{1}{1+(\omega\tau_l)^2} \mathrm{Re}(\beta_{l\mu}\gamma_{ln})g_{\nu n} \tag{25}$$

Although the use of two eigenvalue expansions may appear unduly complicated, the second expression yields the advantage that most of the labor is put into the calculation of the coefficients $g_{\nu n}$, which are independent of the magnitude and direction of the applied magnetic field. Thus, the scattering eigenvalue problem is solved only once for each metal considered. Then, if the assumption is reasonable that the magnetic eigenfunction $b_l(\vec{k})$ is well approximated by only a small number of the a_n (i.e., if the series in equation (19) may be truncated after a few terms), solving for the $\beta_{l\mu}$ and γ_{ln} involves only solving a set of linear equations of a reasonable order. This part of the problem, which must be done anew for each field direction, then becomes easier to handle. This method certainly requires less work then solving equation (14) as an integral equation over the whole Fermi surface for each field direction.

CONCLUDING REMARKS

There are two main benefits of the formulation described herein for the conductivity. The first is the observation that all the integrals involved are well-defined integrals over the Fermi surface. It is not necessary to trace out all possible electron trajectories in the metal, such as is necessary in the Chambers method (ref. 3) for example. The

present method requires, in addition to the Fermi surface, only the velocity vectors at each point on the surface, for a mesh as small as the available machine time allows. The second benefit is that it is unnecessary to treat separately electron trajectories which may be open for some field directions. The contributions to the current for such open-orbit directions may be shown to be equivalent to including those eigenfunctions of T in equation (13) which correspond to $\tau_l = 0$. From the final form of the conductivity (eq. (25)), it is seen that this contribution to the conductivity is a constant, independent of the magnitude of the magnetic field. This conclusion is equivalent to the result obtained in the other theories, which must trace out such orbits in momentum space.

The work summarized herein indicates that the transport properties of conduction electrons in electric and magnetic fields may be obtained in a closed form, and a procedure for calculation is indicated. No assumption has been made about the existence of a relaxation time for the electron scattering or about the form of the Fermi surface of the metal.

Lewis Research Center,
National Aeronautics and Space Administration,
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NASA-Langley, 1967 —— 26 E-3883

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