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Magnetotransport in Simple Metals. An Exactly Soluble Model

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The magnetoconductivity tensors of a metal with a weakly anisotropic Fermi surface are determined from analytic solutions to the Boltzmann equation without any restrictions on the magnitude of the cyclotron frequency compared to the collision rate. Results are given for both a two- and a three-dimensional model, the former being analytically simpler to handle. The Hall coefficient and magnetoresistance are obtained as functions of the magnetic field, and we show by explicit calculation how the thermoelectric coefficients at high magnetic fields are determined by the thermodynamic entropy.

KEY WORDS: Anisotropic Fermi surface; Boltzmann equation; relaxation-time approximation; magnetoresistance; Hall coefficient; thermopower.

1. INTRODUCTION

Although transport phenomena in magnetic fields play a prominent role in solid state physics, there is a remarkable lack of analytically soluble models that may yield insight into the important effects of band anisotropy on these phenomena. The qualitative effects of the shape of the Fermi surface are readily appreciated from the pioneering work of Lifshitz, Azbel, and Kaganov,[1] who demonstrated how purely topological arguments may be used to predict the high-field behavior of the magnetoconductivity tensors relating an electric field or a temperature gradient to an electric or thermal current. A detailed calculation of the conductivity tensors is extremely difficult for a realistic Fermi surface, even in the simple relaxation time approximation for the effects of collisions. As a result, the discussion of the

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transport properties of metals in magnetic fields is usually restricted to the high-field limit, in which simple expressions for, e.g., the Hall coefficient may be obtained. Alternatively one introduces isotropic two-band models that possess nontrivial magnetotransport properties. Such models do not, of course, apply to simple metals like sodium or potassium, and they yield no insight into the role of anisotropy in magnetotransport.

In this paper we shall discuss a soluble model of an anisotropic Fermi surface, which is appropriate to simple metals. We demonstrate how the various magnetoconductivity tensors may be calculated analytically to second order in the anisotropy parameters. The model allows one to study explicitly the difference between the high-field and low-field Hall coefficient, the former depending on the total number of electrons only, and yields an expression for the transverse and longitudinal magnetoresistance which shows the expected saturation behavior in high magnetic fields. The off-diagonal part of the thermoelectric tensor in high magnetic fields is proportional to the thermodynamic entropy, contrary to the situation at low or intermediate fields, where it has a much more complicated dependence on the Fermi surface parameters.

In the following we solve this anisotropic single band model explicitly and demonstrate how the electronic distribution function and the related transport coefficients are obtained as functions of the magnetic field. The model is in principle applicable to the alkali metals, which have nearly spherical Fermi surfaces. However, as is well known, the standard semiclassical transport theory fails to account for the observed high-field magnetoresistance of materials like potassium. Rather than saturating at a small value in accordance with semiclassical theory, the experimentally observed magnetoresistance of potassium continues to rise with magnetic field, exhibiting a linear dependence on $\omega_c\tau$, the product of the cyclotron frequency ω_c and the collision time τ. The linear rise persists to fields corresponding to $\omega_c\tau \gtrsim 100$.[2] This linear magnetoresistance is generally attributed to macroscopic inhomogeneities, which distort the current flow, though no definitive explanation that applies to realistic situations has yet been given.

The aim of this paper is therefore not to explain the magnetoresistive behavior of the alkali metals, but rather to elucidate the effects originating from an anisotropic band structure in a case where analytic solutions may be obtained, and, in particular, to analyze the high-field properties. The model Fermi surface we shall study was introduced by Jones and Zener[3] and studied by Davis,[4] who calculated the low field magnetoresistance and Hall coefficient. The analysis of this model was later extended by Ah-Sam, Højgaard Jensen, and Smith,[5] who used variational methods to calculate the longitudinal magnetoresistance for all magnetic fields. These authors showed how to derive upper and lower bounds on the longitudinal magnetoresistance and found that their calculated upper and lower bounds coincided for this particular model, constituting in effect an exact model solution for the longitudinal magnetoresistance. The variational method does not, however, apply to the off-diagonal components of the conductivity tensor, and cannot therefore yield, e.g., the Hall coefficient.

To obtain the complete conductivity tensor we therefore use a more direct approach and expand the driving term of the kinetic equation in terms of a Fourier series in the phase variable that describes the location of an electron on an orbit specified by its energy ϵ and the value of the wave vector, k_z, along the direction of the magnetic field. The resulting first-order differential equation may be solved exactly by a Fourier expansion method.

The plan of the paper is as follows. In Section 2 we describe the model Fermi surface. The following section contains the solution of the transport equation and the calculation of the conductivity tensor, valid to second order in the anisotropy constants. The final section contains a brief discussion of the thermomagnetic properties of the model.

A number of mathematical details are collected in Appendix A.

2. THE MODEL FERMI SURFACE

In this section we summarize the equilibrium properties of our Fermi surface model. We consider both a two-dimensional and three-dimensional model, the latter being the case which describes nearly free electron metals like the alkali metals. The two-dimensional model possesses many features in common with the three-dimensional one, and it is somewhat simpler to analyze from a mathematical point of view.

The relationship between the energy ϵ and wave vector $\mathbf{k}$ of a Bloch electron is in three dimensions taken to be

$$k = k_0(\epsilon) + k_1(\epsilon) Y(\cos\theta, \phi) \tag{2.1}$$

where θ and ϕ are the polar and azimuthal angles of $\mathbf{k}$, and $k_0(\epsilon)$ and $k_1(\epsilon)$ given functions of ϵ. The anisotropy enters through Y, which is a cubic harmonic of fourth order, given by

$$Y = g(\cos\theta) + f(\cos\theta)\cos 4\phi = P_4(\cos\theta) + P_4^4(\cos\theta)(\cos 4\phi)/168 \tag{2.2}$$

Here $g = P_4$ is a Legendre polynomial, $P_4(x) = (35x^4 - 30x^2 + 3)/8$, while $f = P_4^4/168$ is given by the associated Legendre function, $P_4^4(x) = 105(1 - x^2)^2$. At $\theta = \pi/2$ one has

$$Y(0, \phi) = \tfrac{3}{8} + \tfrac{5}{8}\cos 4\phi \tag{2.3}$$

Note the cubic symmetry, which is evident from the presence of $\cos 4\phi$ in

Y. In two dimensions we may use the simpler expression

$$k = k_0(\epsilon) + k_1(\epsilon)\cos 4\phi \tag{2.4}$$

Physically the constant energy surfaces (2.4) correspond to a metal with a (noncircular) cylindrical Fermi surface. As we shall see, by taking the magnetic field along the cylinder axis, it is possible to derive simple expressions for the conductivity tensors from (2.4).

For later use we now specify the relation between the band parameters and the total number of electrons, the density of states at the Fermi energy and the Fermi energy itself. The density of states (per unit volume $V = 1$) $g(\epsilon)$ in three dimensions is given by

$$g(\epsilon) = \sum_{\mathbf{k}\sigma} \delta(\epsilon - \epsilon(\mathbf{k})) = \frac{1}{4\pi^3} \int_{S(\epsilon)} \frac{dS}{v} \tag{2.5}$$

where the integration in (2.5) is extended over the two-dimensional surface $S(\epsilon)$ of constant energy ϵ. The magnitude of the group velocity $\mathbf{v} = (1/\hbar)(\partial\epsilon/\partial\mathbf{k})$ is denoted by v. The surface element dS is related to the solid angle element $d\Omega$, where $d\Omega = \sin\theta\, d\theta\, d\phi$, through

$$\cos\psi\, dS = k^2\, d\Omega \tag{2.6}$$

with $\cos\psi = \mathbf{k}\cdot\mathbf{v}/kv$, ψ being the angle between the group velocity $\mathbf{v}$ and the Bloch vector $\mathbf{k}$. The relation (2.6) is a consequence of the fact that $\mathbf{v}$ is perpendicular to the surface element dS. We use from here on units such that $\hbar = 1$.

We shall need, in the following, expressions for the velocity $\mathbf{v}$ given by

$$\mathbf{v} = \frac{\partial\epsilon}{\partial\mathbf{k}} \tag{2.7}$$

in terms of the derivatives of k with respect to ϵ, θ and ϕ. For the x component of the velocity we use

$$\frac{\partial k}{\partial k_x} = \frac{\partial k}{\partial\epsilon}\frac{\partial\epsilon}{\partial k_x} + \frac{\partial k}{\partial\theta}\frac{\partial\theta}{\partial k_x} + \frac{\partial k}{\partial\phi}\frac{\partial\phi}{\partial k_x} \tag{2.8}$$

which, together with the elementary expressions for $\partial k/\partial k_x$, $\partial\theta/\partial k_x$, and $\partial\phi/\partial k_x$, yields

$$v_x = \frac{1}{\partial k/\partial\epsilon}\left(\sin\theta\cos\phi - \frac{1}{k}\frac{\partial k}{\partial\theta}\cos\theta\cos\phi + \frac{1}{k\sin\theta}\frac{\partial k}{\partial\phi}\sin\phi\right) \tag{2.9}$$

For the y and z components we get similarly

$$v_y = \frac{1}{\partial k/\partial\epsilon}\left(\sin\theta\sin\phi - \frac{1}{k}\frac{\partial k}{\partial\theta}\cos\theta\sin\phi - \frac{1}{k\sin\theta}\frac{\partial k}{\partial\phi}\cos\phi\right) \tag{2.10}$$

$$v_z = \frac{1}{\partial k/\partial\epsilon}\left(\cos\theta + \frac{1}{k}\frac{\partial k}{\partial\theta}\sin\theta\right) \tag{2.11}$$

It follows that $\mathbf{v} \cdot \mathbf{k} = k/(\partial k/\partial \epsilon)$, allowing one to transform (2.6) into

$$dS = vk^2(\partial k/\partial \epsilon)\, d\Omega \tag{2.12}$$

The density of states $g(\epsilon)$ is in general given by the surface integral (2.5). Using (2.12) we transform (2.5) into

$$g(\epsilon) = (1/\pi^2)\langle k^2\, \partial k/\partial \epsilon\rangle \tag{2.13}$$

where $\langle \cdots \rangle$ is defined as the spherical average

$$\langle \cdots \rangle = \int \frac{d\Omega}{4\pi} \cdots = \int_{-1}^{1} \frac{d(\cos\theta)}{2} \int_0^{2\pi} \frac{d\phi}{2\pi} \cdots \tag{2.14}$$

In two dimensions ($d = 2$) one finds similarly

$$g(\epsilon) = (1/\pi)\langle k\, \partial k/\partial \epsilon\rangle \qquad \text{for} \quad d = 2$$

where the angular average only involves integration over ϕ according to $\langle \cdots \rangle = \int (d\phi/2\pi) \cdots$.

In the absence of anisotropy, $k = k_0(\epsilon)$, and the density of states in three dimensions is

$$g = g_0(\epsilon) = \frac{1}{\pi^2} k_0^2 \frac{\partial k_0}{\partial \epsilon} = \frac{1}{\pi^2} k_0^2 k_0' \tag{2.15}$$

where here and in the following the prime denotes differentiation with respect to ϵ. The Fermi momentum is $k_0(\epsilon_F)$. It is natural to introduce an effective mass m_0 by the definition

$$m_0 = k_0 k_0'|_{\epsilon=\epsilon_F} \tag{2.16}$$

such that in analogy to the case of free electrons

$$g_0(\epsilon_F) = \frac{1}{\pi^2} m_0 k_0(\epsilon_F) \tag{2.17}$$

Next we express the number of electrons and the density of states at the Fermi energy in terms of the parameters of the model. First we shall relate the number of electrons n to the Fermi energy. One has

$$n = \int_0^{\epsilon_F} d\epsilon\; g(\epsilon) = \frac{1}{3\pi^2} \langle (k(\epsilon_F))^3 \rangle \tag{2.18}$$

taking the zero of energy at the bottom of the band. We introduce the anisotropy parameters

$$\beta = \frac{k_1(\epsilon_F)}{k_0(\epsilon_F)} \tag{2.19}$$

and

$$\gamma = \frac{k_1'(\epsilon_F)}{k_0'(\epsilon_F)} \tag{2.20}$$

Then one finds readily

$$n = n_0\left(1 + \tfrac{4}{7}\,\beta^2\right) \tag{2.21}$$

where $n_0 = k_0^3/3\pi^2$. Similarly the density of states at the Fermi energy becomes

$$g(\epsilon_F) = g_0(\epsilon_F)\left(1 + \tfrac{4}{21}\,\beta^2 + \tfrac{8}{21}\,\beta\gamma\right) \tag{2.22}$$

In two dimensions (2.21) and (2.22) become respectively,

$$n = n_0\left(1 + \tfrac{1}{2}\,\beta^2\right) \tag{2.21$'$}$$

with $n_0 = k_0^2/2\pi$ and

$$g(\epsilon_F) = g_0(\epsilon_F)(1 + \tfrac{1}{2}\,\beta\gamma) \tag{2.22$'$}$$

with $g_0(\epsilon_F) = m_0/\pi$.

3. THE TRANSPORT EQUATION

Starting with the semiclassical transport equation we shall now demonstrate how it is solved and obtain complete expressions for the conductivity tensor valid to second order in the anisotropy parameters β and γ. As mentioned in the introduction, the effect of collisions is treated in the relaxation time approximation. When the collision probability is independent of the initial and final wave vectors, as in the case of s-wave scattering, the relaxation time approximation is justified, since the scattering-in term does not contribute.

We first discuss the three-dimensional case, in which the dispersion relation is defined by (2.1)–(2.2). The standard Boltzmann equation for the electron distribution function $f(\mathbf{r}, \mathbf{k}, t)$ is in the relaxation time approximation given by

$$\frac{\partial f}{\partial t} + \dot{\mathbf{r}} \cdot \frac{\partial f}{\partial \mathbf{r}} + \dot{\mathbf{k}} \cdot \frac{\partial f}{\partial \mathbf{k}} = -\frac{f - f^0}{\tau} \tag{3.1}$$

where f^0 denotes the equilibrium Fermi function $f^0 = [\exp(\epsilon - \mu)/k_B T + 1]^{-1}$ and τ is a relaxation time, which we take to be a constant.

For Bloch electrons in a magnetic field $\mathbf{B}$ and an electric field $\mathbf{E}$ the semiclassical equations of motion are

$$\begin{aligned} \dot{\mathbf{r}} &= \mathbf{v} = \frac{\partial \epsilon}{\partial \mathbf{k}} \\ \dot{\mathbf{k}} &= -e(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \end{aligned} \tag{3.2}$$

where the charge of the electron is denoted by $-e$. In the presence of an electric field or a temperature gradient the kinetic equation (3.1) may be linearized in the usual manner. For the purpose of keeping the discussion simple we shall first consider the case of an electric field alone, since the other transport coefficients may be readily obtained from the electrical conductivity, as shown in the following section. The operator involving the magnetic field may be written most conveniently in terms of the phase variable $\tilde{\phi}$, which specifies the position of an electron on the orbit defined by the two constants of the motion, the energy ϵ and the component of the **k** vector along the axis of the magnetic field. Taking the field to be along the z axis the new variables are $(\epsilon, k_z, \tilde{\phi})$ where

$$\tilde{\phi} = \frac{1}{m_c} \int \frac{dl}{v_\perp} \tag{3.3}$$

with the cyclotron effective mass m_c defined by

$$m_c = \frac{1}{2\pi} \oint \frac{dl}{v_\perp} \tag{3.4}$$

and $v_\perp = (v_x^2 + v_y^2)^{1/2}$.

The integrals in (3.3)–(3.4) are line integrals along the orbit specified by ϵ and k_z, the integral in (3.4) running over the entire orbit. In terms of these new variables the linearized Boltzmann equation becomes

$$-e\mathbf{E} \cdot \mathbf{v} \frac{\partial f^0}{\partial \epsilon} + \omega_c \frac{\partial}{\partial \tilde{\phi}} g = -\frac{g}{\tau} \tag{3.5}$$

where $g = f - f^0$ is the deviation from equilibrium and

$$\omega_c = \frac{eB}{m_c} \tag{3.6}$$

is the cyclotron frequency, which depends on k_z and ϵ. When evaluating (3.3)–(3.4) we need to express the line element dl in terms of the angle Φ between the components of **k** and **v** in the plane perpendicular to **B**, $dl = k \sin\theta \, d\phi / \cos\Phi$, where $\cos\Phi = \hat{k}_\perp \cdot \hat{v}_\perp$ with $\mathbf{v}_\perp$ and $\mathbf{k}_\perp$ being the perpendicular components $\mathbf{k}_\perp = (k_x, k_y, 0)$ and $\mathbf{v}_\perp = (v_x, v_y, 0)$. Using the expressions (2.9)–(2.10) for the velocity components in spherical coordinates one finds

$$m_c = \frac{1}{2\pi} \int_0^{2\pi} \Omega \, d\phi \tag{3.7}$$

where

$$\Omega = \frac{\partial k}{\partial \epsilon} \left(\frac{1}{k} - \frac{\cos\theta}{k \sin\theta} \frac{\partial k / \partial \theta}{k} \right)^{-1} \tag{3.8}$$

To second order in β and γ the function Ω becomes

$$\Omega \simeq m_0 \left[1 + \beta(Y - \cos\theta Y') + \beta^2 \cos^2\theta Y'^2 + \gamma Y + \beta\gamma Y(Y - \cos\theta Y') \right] \tag{3.9}$$

with $Y' = \partial Y/\partial \cos\theta$. The result (3.9) is formally valid to second order in the anisotropy constants. When the integral (3.7) is performed, care must be taken to ensure the constancy of k_z, since the polar angle θ is not a constant of the motion, as the electron traverses a given orbit. From the two relations $k_z = k\cos\theta$ and $k = k_0(1+\beta Y)$ one finds for an orbit of energy $\epsilon = \epsilon_F$, to second order in β,

$$\cos\theta = x_0\left[1 - \beta Y_0 + \beta^2\left(Y_0^2 + x_0 Y_0 Y_0'\right)\right] \tag{3.10}$$

where $Y_0 = g(x_0) + f(x_0)\cdot\cos 4\phi = g_0 + f_0\cos 4\phi$, $Y_0' = \partial Y_0/\partial x_0$ and $x_0 = k_z/k_0(\epsilon_F)$. The phase angle $\tilde{\phi}$ and the azimuthal angle ϕ are in general related by

$$\frac{d\tilde{\phi}}{d\phi} = \frac{1}{m_c}\Omega \tag{3.11}$$

When evaluating the conductivity we need to expand this relation only to first order in β and γ,

$$\phi \simeq \tilde{\phi} + \beta\tfrac{1}{4}\left[x_0 f_0'(x_0) - f_0\right]\sin 4\tilde{\phi} - \tfrac{1}{4}\gamma f_0 \sin 4\tilde{\phi} \tag{3.12}$$

Returning to the kinetic equation (3.5) we express the velocity occurring in the driving term proportional to the electric field **E** in terms of $\cos\tilde{\phi}$ and $\sin\tilde{\phi}$ and their higher harmonics. The result of this evaluation is given in Appendix A. In the present case where the anisotropy is considered to be weak it is sufficient to include the first, third, and fifth harmonics in the transverse case, and the zeroth and fourth one in the longitudinal case, corresponding to our treatment of the cubic harmonic as a small perturbation.

Thus we get to second order in the anisotropy parameters β and γ

$$v_x = \sum_{n=0,1,2} P_n \cos(2n+1)\tilde{\phi} \tag{3.13}$$

and

$$v_y = \sum_{n=0,1,2} (-1)^n P_n \sin(2n+1)\tilde{\phi} \tag{3.14}$$

where P_n is given in Eqs. (A1)–(A3). The velocity component along the magnetic field is

$$v_z = \sum_{n=0,4} Q_n \cos n\tilde{\phi} \tag{3.15}$$

with Q_n given by (A4)–(A5).

Once the expansion in Fourier coefficients has been performed the solution of the kinetic equation is straightforward. In the transverse case with **E** along the x axis, $\mathbf{E} = (E, 0, 0)$, the kinetic equation is

$$\left(\frac{1}{\tau} + \omega_c \frac{\partial}{\partial \tilde{\phi}}\right) g = eE \frac{\partial f^0}{\partial \epsilon} \sum_{n=0,1,2} P_n \cos(2n+1)\tilde{\phi} \tag{3.16}$$

with the solution

$$g = \sum_{n=0}^{2} a_n \cos(2n+1)\tilde{\phi} + b_n \sin(2n+1)\tilde{\phi} \tag{3.17}$$

The Fourier coefficients a_n and b_n are given by

$$a_n = \tau e E \frac{\partial f^0}{\partial \epsilon} \frac{P_n}{1 + (2n+1)^2 \omega_c^2 \tau^2} \tag{3.18}$$

and

$$b_n = \tau e E \frac{\partial f^0}{\partial \epsilon} \frac{P_n (2n+1)\omega_c \tau}{1 + (2n+1)^2 \omega_c^2 \tau^2} \tag{3.19}$$

as seen by inserting the solution (3.17) in (3.16).

Once the distribution function has been determined the remaining task is to calculate the current.

The electrical current **j** is

$$j_i = -e \int \frac{d\mathbf{k}}{4\pi^3} v_i g = -\frac{e}{4\pi^3} \int d\epsilon \int dk_z \int d\tilde{\phi}\, m_c v_i g \tag{3.20}$$

As usual the integration over ϵ may be done at zero temperature, using $\partial f^0/\partial \epsilon = -\delta(\epsilon - \epsilon_F)$. To complete the integral over k_z it is necessary to express all quantities in terms of x_0, using (3.10). The resulting expression becomes algebraically complicated but readily integrable. The details are outlined in Appendix A. In three dimensions the conductivity tensor σ_{ij} relating the current to the electric field through $j_i = \sigma_{ij} E_j$ is given by

$$\sigma_{xx} = \sigma_0 \left\{ \frac{1}{1+\alpha^2} \left[1 + c_1 + \frac{\alpha^2}{1+\alpha^2} c_2 + \left(\frac{\alpha^2}{1+\alpha^2} \right)^2 c_3 \right] + \frac{1}{1+9\alpha^2} c_4 + \frac{1}{1+25\alpha^2} c_5 \right\} \tag{3.21}$$

$$\sigma_{yx} = \sigma_0 \left\{ \frac{\alpha}{1+\alpha^2} \left[1 + d_1 + \frac{\alpha^2}{1+\alpha^2} d_2 + \left(\frac{\alpha^2}{1+\alpha^2} \right)^2 c_3 \right] - \frac{3c_4\alpha}{1+9\alpha^2} + \frac{5c_5\alpha}{1+25\alpha^2} \right\} \tag{3.22}$$

$$\sigma_{zz} = \sigma_0 \left[1 + \frac{4}{21}(21\beta^2 - 2\beta\gamma + \gamma^2) - \frac{\alpha^2}{1+16\alpha^2} \frac{80}{231} (3\beta - \gamma)^2 \right] \tag{3.23}$$

and $\sigma_{yy} = \sigma_{xx}$, $\sigma_{xy} = -\sigma_{yx}$, $\sigma_{xz} = \sigma_{zx} = 0$. Here $\sigma_0 = n_0 e^2 \tau / m_0$ with $n_0 = k_0^3/3\pi^2$ and m_0 is given by (2.16). We have furthermore introduced the important dimensionless parameter α as

$$\alpha = \omega_0 \tau, \qquad \omega_0 = eB/m_0 \tag{3.24}$$

The coefficients in (3.21) and (3.22) are as follows:

$$\begin{aligned}
c_1 &= \frac{2663}{1232}\beta^2 + \frac{93}{1232}\gamma^2 - \frac{419}{1848}\beta\gamma \\
c_2 &= -\frac{582}{77}\beta^2 - \frac{95}{231}\gamma^2 + \frac{152}{231}\beta\gamma \\
c_3 &= \frac{492}{77}\beta^2 + \frac{76}{231}\gamma^2 + \frac{24}{77}\beta\gamma \\
c_4 &= \frac{2655}{2464}\beta^2 + \frac{75}{2464}\gamma^2 + \frac{435}{1232}\beta\gamma \\
c_5 &= \frac{1875}{2464}\beta^2 + \frac{625}{2464}\gamma^2 - \frac{625}{1232}\beta\gamma \\
d_1 &= \frac{905}{176}\beta^2 + \frac{887}{3696}\gamma^2 - \frac{157}{264}\beta\gamma \\
d_2 &= -\frac{828}{77}\beta^2 - \frac{19}{33}\gamma^2 + \frac{116}{231}\beta\gamma
\end{aligned} \tag{3.25}$$

The longitudinal magnetoconductivity, σ_{zz}, agrees with that calculated by Ah-Sam et al.[5] using variational methods.

Let us consider some simple limits of these rather complicated expressions. In the zero field limit ($\alpha \to 0$) one has

$$\sigma_{xx} = \sigma_{xx}^0 = \sigma_{zz}^0 = \sigma_0\left[1 + 4\beta^2 - \tfrac{8}{21}\beta\gamma + \tfrac{4}{21}\gamma^2\right] \tag{3.26}$$

while at high fields ($\alpha \to \infty$)

$$\sigma_{xx} = \sigma_{xx}^\infty = \sigma_0 \frac{1}{\alpha^2}\left(1 + \frac{8}{7}\beta^2 + \frac{16}{21}\beta\gamma\right) \tag{3.27}$$

and

$$\sigma_{yx} = \sigma_{yx}^\infty = \sigma_0 \frac{1}{\alpha}\left(1 + \frac{4}{7}\beta^2\right) \tag{3.28}$$

The result (3.28) for σ_{yx} involves as expected simply the total number of electrons n, given by (2.21), or

$$\sigma_{yx} = \frac{ne}{B}, \qquad \alpha \to \infty \tag{3.29}$$

The high-field limit of the diagonal resistivity element ρ_{xx} is correspondingly

$$\rho_{xx} = \rho_{xx}^\infty = \frac{1}{\sigma_0}\left(1 + \frac{16}{21}\beta\gamma\right) \tag{3.30}$$

whereas in zero field

$$\rho_{xx} = \rho_{xx}^0 = \frac{1}{\sigma_0}\left(1 - 4\beta^2 + \frac{8}{21}\beta\gamma - \frac{4}{21}\gamma^2\right) \tag{3.31}$$

Note that the difference $\rho_{xx}^\infty - \rho_{xx}^0 = (1/\sigma_0)[80\beta^2/21 + 4(\beta+\gamma)^2/21]$ is always positive, regardless of the sign of β and γ, corresponding to a positive magnetoresistance. The low-field magnetoresistance is given by

$$\rho_{xx} - \rho_{xx}^0 = \sigma_0^{-1}\tfrac{4}{77}\alpha^2(597\beta^2 + 37\gamma^2 - 46\beta\gamma) \tag{3.32}$$

whereas the low-field Hall coefficient is

$$R_H = R_H^0 = \frac{\rho_{yx}}{H} = -\frac{1}{n_0 e}\left(1 - \frac{16}{7}\beta^2 + \frac{4}{21}\gamma^2 - \frac{24}{7}\beta\gamma\right) \tag{3.33}$$

In Figures 1 and 2 we plot the field dependence of ρ_{xx} and the Hall coefficient R_H for various values of β and γ. It is illuminating to compare (3.33) with the high-field Hall coefficient $R_H^\infty = -1/ne$, where according to (2.21) $n = n_0(1 + \frac{4}{7}\beta^2)$. We see that $R_H^0/R_H^\infty = 1 - \frac{12}{7}(\beta+\gamma)^2 + \gamma^2\frac{40}{21}$. Note that the Hall coefficient exhibits a maximum at $\alpha \simeq 1$ as shown in Figure 2.

In two dimensions the calculation of σ_{xx} and σ_{xy} is much simpler. Details are given in Appendix A. The results are obtained with a magnetic field along the cylinder axis,

$$\sigma_{xx} = \sigma_0\left\{\frac{1}{1+\alpha^2}\left[1 + \frac{31}{32}\beta^2 - \frac{\gamma^2}{32} + \frac{7}{16}\beta\gamma + \frac{\alpha^2}{1+\alpha^2}\beta\gamma\right] + \frac{1}{1+9\alpha^2}\left(\frac{15}{8}\beta + \frac{3}{8}\gamma\right)^2 + \frac{1}{1+25\alpha^2}\left(\frac{15}{8}\beta - \frac{5}{8}\gamma\right)^2\right\} \tag{3.34}$$

and

$$\sigma_{yx} = \sigma_0\left\{\frac{\alpha}{1+\alpha^2}\left[1 + \frac{31}{32}\beta^2 - \frac{\gamma^2}{32} - \frac{\beta\gamma}{16} + \frac{\alpha^2}{1+\alpha^2}\beta\gamma\right] - \frac{3\alpha}{1+9\alpha^2}\left(\frac{15}{8}\beta + \frac{3}{8}\gamma\right)^2 + \frac{5\alpha}{1+25\alpha^2}\left(\frac{15}{8}\beta - \frac{5}{8}\gamma\right)^2\right\} \tag{3.35}$$

where $\sigma_0 = n_0 e^2\tau/m_0$, $m_0 = k_0 k_0'$ and $n_0 = k_0^2/2\pi$ [cf. (2.21′)], while $\alpha = eB\tau/m_0$ as before. The corresponding resistivity and Hall coefficient are shown in Figures 3 and 4.

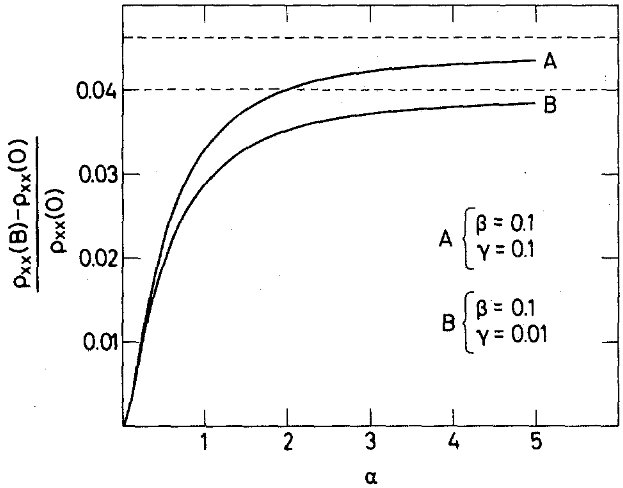

Fig. 1. A: Transverse magnetoresistance as a function of $\alpha = (eB/m_0)\tau$, for $\beta = 0.1$ and $\gamma = 0.1$. The saturation value in the high-field limit is indicated by the dashed line. B: As in Fig. 1A except that $\beta = 0.1$ and $\gamma = 0.01$.

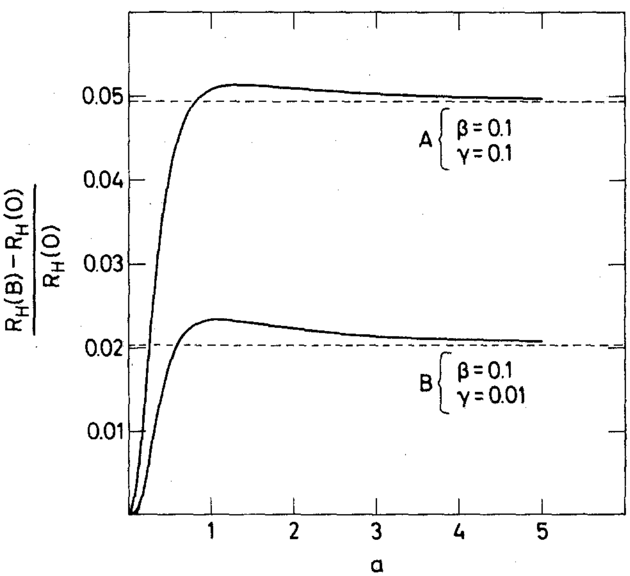

Fig. 2. A: Hall coefficient $[R_H(B) - R_H(0)]/R_H(0)$ as a function of $\alpha = (eB/m_0)\tau$, for $\beta = 0.1$ and $\gamma = 0.1$. $R_H(0)$ is the low-field Hall coefficient. The saturation value in the high-field limit is indicated by the dashed line. B: As in Fig. 2A except that $\beta = 0.1$ and $\gamma = 0.01$.

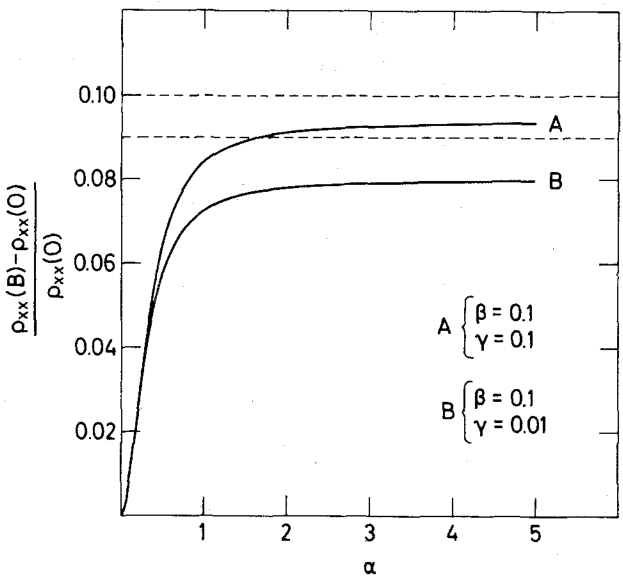

Fig. 3. As in Fig. 1 but in two dimensions, where ρ_{xx} is given by (3.34)–(3.35).

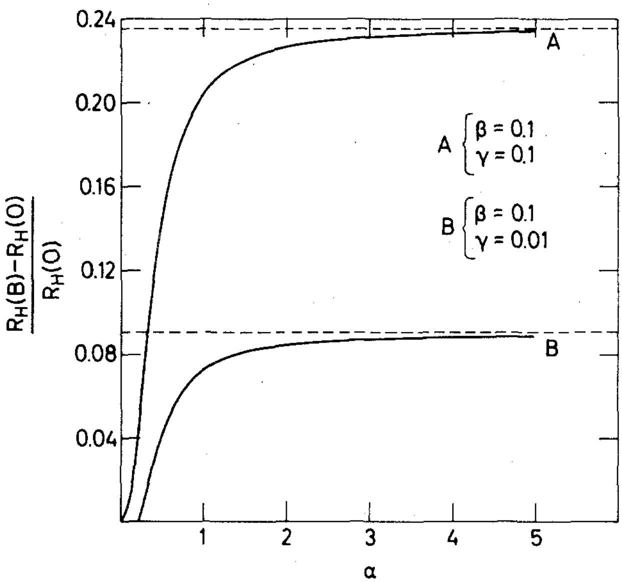

Fig. 4. As in Fig. 2 but in two dimensions, where ρ_{yx} is given by (3.34)–(3.35).

4. THERMAL TRANSPORT

The solution we have presented in the preceding section may be taken over immediately to discuss thermal effects. The Sommerfeld expansion which involves an integration over energy may always be performed after the integration over the angular variables has been completed as in the preceding section. In general we are interested in determining the tensors relating the electric field **E** and the temperature gradient ∇T to the electric current **j** and the heat current **u**,

$$\begin{aligned} \mathbf{j} &= \bar{\bar{\sigma}}\mathbf{E} - \bar{\bar{\beta}}\nabla T \\ \mathbf{u} &= \bar{\bar{\gamma}}\mathbf{E} - \bar{\bar{\lambda}}\nabla T \end{aligned} \tag{4.1}$$

According to Onsager's relations we have

$$\beta_{ij}(\mathbf{B}) = \frac{1}{T}\gamma_{ji}(-\mathbf{B}) \tag{4.2}$$

which may be explicitly verified from the kinetic equation. By employing the Sommerfeld expansion we find, e.g.,

$$\gamma_{ij} = -\frac{\pi^2}{3}\frac{(k_B T)^2}{e}\sigma'_{ij} \tag{4.3}$$

where $\sigma'_{ij} = \partial\sigma_{ij}/\partial\epsilon_F$. Similarly one finds

$$\lambda_{ij} = \frac{\pi^2}{3}\frac{k_B^2}{e^2}T\sigma_{ij} \tag{4.4}$$

which is the Wiedemann–Franz law.

The thermoelectric tensor $\bar{\bar{S}}$ is obtained by relating the electric field **E** to the temperature gradient ∇T under conditions when the particle current **j** vanishes,

$$\mathbf{E} = \bar{\bar{\sigma}}^{-1}\bar{\bar{\beta}}\nabla T = \bar{\bar{S}}\nabla T \tag{4.5}$$

or

$$\bar{\bar{S}} = \bar{\bar{\sigma}}^{-1}\bar{\bar{\beta}} \tag{4.6}$$

At high fields S_{xx} is given by

$$S_{xx} = \frac{\beta_{xy}}{\sigma_{xy}} = -\frac{\pi^2}{3}\frac{k_B^2 T}{e}\frac{\sigma'_{yx}}{\sigma_{yx}} \tag{4.7}$$

The energy dependence of σ'_{yx} is according to (3.28) determined by the combination $k_0^3 + \frac{4}{7}k_1^2 k_0$. Upon taking the derivative of this with respect to ϵ we get

$$\lim_{\alpha\to\infty}\frac{\sigma'_{yx}}{\sigma_{yx}} = \frac{g(\epsilon_F)}{n} \tag{4.8}$$

where $g(\epsilon_F)$ is the density of states given by (2.22). The result (4.8) is in agreement with the general property that the high-field limit of the thermoelectric tensor involves the entropy of the electrons.[6] At low and intermediate fields the calculation of the thermoelectric tensor introduces the second derivative of k_1 with respect to ϵ, evaluated at the Fermi energy.

APPENDIX A

In this appendix, we give expressions for the Fourier coefficients in the expansion of the velocity components (3.13)–(3.15), and we discuss the procedure for the derivation of the result (3.34)–(3.35).

From (3.12) we obtain

$$\cos n\phi = \cos n\tilde{\phi} + \frac{n}{2}(c\beta + d\gamma)\left[\cos(4-n)\tilde{\phi} - \cos(n+4)\tilde{\phi}\right] - \frac{n^2}{4}(c\beta + d\gamma)^2 \cos n\tilde{\phi}$$

where the coefficients c and d are given in terms of f_0 and g_0, defined below (3.10), as $c = \frac{1}{4}(f_0 - x_0 f_0')$, $d = \frac{1}{4} f_0$. A similar expression holds for $\sin n\phi$, where n is an integer. Upon substitution of (3.10) into (2.9)–(2.11) and using the expressions for $\cos n\phi$ and $\sin n\phi$ as above, we find

$$P_0 = \frac{1}{\partial k_0/\partial\epsilon}\left[\left(1 - x_0^2 + 2\beta x_0^2 g_0\right)^{1/2} + \beta g_0' \sin\theta_0 \cos\theta_0 + \gamma(-g\sin\theta_0) + \beta^2 A + \gamma^2 B + \beta\gamma C\right] \tag{A1}$$

$$P_1 = \frac{1}{\partial k_0/\partial\epsilon}\left[\beta\left(\frac{1}{2} f_0 \frac{\cos^2\theta_0}{\sin\theta_0} + \frac{c}{2}\sin\theta_0 + \frac{1}{2} f_0' \sin\theta_0 \cos\theta_0 - \frac{2 f_0}{\sin\theta_0}\right) + \gamma\left(\frac{d}{2}\sin\theta_0 - \frac{1}{2} f_0 \sin\theta_0\right)\right] \tag{A2}$$

$$P_2 = \frac{1}{\partial k_0/\partial\epsilon}\left[\beta\left(\frac{1}{2} f_0 \frac{\cos^2\theta_0}{\sin\theta_0} - \frac{c}{2}\sin\theta_0 + \frac{1}{2} f_0' \sin\theta_0 \cos\theta_0 + \frac{2 f_0}{\sin\theta_0}\right) + \gamma\left(-\frac{d}{2}\sin\theta_0 - \frac{1}{2} f_0 \sin\theta_0\right)\right] \tag{A3}$$

$$Q_0 = \frac{1}{\partial k_0/\partial\epsilon}\left[\cos\theta_0 + \beta(g_0'\cos^2\theta_0 - g_0\cos\theta_0 - g_0') + \gamma(-g_0\cos\theta_0) + \beta^2 D + \gamma^2 E + \beta\gamma F\right] \tag{A4}$$

$$Q_4 = \frac{1}{\partial k_0/\partial\epsilon}\left[\beta(f_0'\cos^2\theta_0 - f_0\cos\theta_0 - f_0') + \gamma(-f_0\cos\theta_0)\right] \tag{A5}$$

In writing (A1)–(A5) we have introduced $x_0 = k_z/k_0(\epsilon_F)$ explicitly in the first term of (A1) instead of the polar angle θ_0 of the undeformed Fermi sphere, $k = k_0(\epsilon_F)$, since after squaring P_0 this term should be integrated over the full range of x_0 from $-(1+\beta)$ to $(1+\beta)$. The remaining terms are expressed in terms of the angle θ_0, which runs from 0 to π, corresponding to $-1 < x_0 < 1$. The coefficients A, B, C, D, E, and F of the quadratic terms of P_0 and Q_0 need not be determined explicitly as shown below. The component σ_{xx} for example, is given by [see (3.20)]

$$\sigma_{xx} = \sigma_0 \int dx_0 \frac{3}{4}\left[\frac{m_c P_0^2}{1+\omega_c^2\tau^2} + \frac{m_c P_1^2}{1+9\omega_c^2\tau^2} + \frac{m_c P_2^2}{1+25\omega_c^2\tau^2}\right] \tag{A6}$$

where the integration limits of x_0 have been discussed above. The integrand contains polynomial functions of x_0, thus the integral above is easily done. The cyclotron mass m_c and $\omega_c\tau$ may be replaced with m_0 and α, respectively, in the last two terms of the integrand in (A6) since P_1^2 and P_2^2 are quadratic in β and γ, while the relationships

$$m_c = m_0(1 + m_1\beta + b_1\gamma + m_2\beta^2 + b_2\beta\gamma) \tag{A7}$$

and

$$\frac{1}{1+\omega_c^2\tau^2} = \frac{1}{1+\alpha^2}\left\{1 + \frac{\alpha^2}{1+\alpha^2}\left[2m_1\beta + 2b_1\gamma + 2m_2\beta^2 + 2b_2\beta\gamma - 3(m_1\beta + b_1\gamma)^2\right] + \left(\frac{\alpha^2}{1+\alpha^2}\right)^2 (2m_1\beta + 2b_1\gamma)^2\right\} \tag{A8}$$

have to be used in the first term. Here $m_1 = g_0 - x_0 g_0'$, $b_1 = g_0$, $m_2 = x_0^2(g_0 g_0'' + \frac{1}{2}f_0 f_0'' + g_0'^2 + \frac{1}{2}f_0'^2)$ and $b_2 = g_0^2 + \frac{1}{2}f_0^2 - 2x_0 g_0 g_0' - x_0 f_0 f_0'$.

The contribution from the nondetermined terms in (A1) is obtained by equating the zero field limit of (A6) with the result (3.26), which is easily calculated from the Boltzmann equation without change of variables. A similar procedure is applied in the case of σ_{xy} except that the contribution from the nondetermined coefficients in (A1) cannot be obtained by switching off the field. Instead we use the relationship

$$\int dx_0 \frac{m_c\omega_c\tau P_0^2}{1+\omega_c^2\tau^2} = \alpha \int dx_0 \frac{m_0 P_0^2}{1+\omega_c^2\tau^2}$$

$$= \alpha \int dx_0 \frac{m_c P_0^2}{1+\omega_c^2\tau^2} - \alpha \int dx_0 \frac{(m_c - m_0)P_0^2}{1+\omega_c^2\tau^2}$$

where $m_c - m_0$ is given by (A7). The first term in the last expression above is known from σ_{xx} and in the second we may neglect the second-order terms involving the unknown coefficients A, B, and C in (A1).

Since the procedure in two dimensions is similar to that in three dimensions, except that it is much easier in this case, we shall only give the results below and number them with primes of their equivalent result in three dimensions:

$$v_x = \frac{1}{\partial k/\partial \epsilon}\left(\cos\phi + \frac{1}{k}\frac{\partial k}{\partial \phi}\sin\phi\right) \tag{2.9'}$$

$$v_y = \frac{1}{\partial k/\partial \epsilon}\left(\sin\phi - \frac{1}{k}\frac{\partial k}{\partial \phi}\cos\phi\right) \tag{2.10'}$$

$$\tilde{\phi} = \frac{1}{m_c}\int \frac{dl}{v} \tag{3.3'}$$

$$m_c = \frac{1}{2\pi}\oint \frac{dl}{v} \tag{3.4'}$$

$$\frac{\mathbf{k}\cdot\mathbf{v}}{kv}\,dl = k\,d\phi \tag{2.6'}$$

The Boltzmann equation is given by (3.5). We find the following results analogous to (3.12)–(3.14)

$$\phi \simeq \tilde{\phi} - \tfrac{1}{4}(\beta + \gamma)\sin 4\tilde{\phi} \tag{3.12'}$$

$$v_x = \sum_{n=0,1,2} D_n \cos(2n+1)\tilde{\phi} \tag{3.13'}$$

$$v_y = \sum_{n=0,1,2} (-1)^n D_n \sin(2n+1)\tilde{\phi} \tag{3.14'}$$

where

$$D_0 = \frac{1}{\partial k_0/\partial \epsilon}\left(1 + \frac{31}{64}\beta^2 - \frac{1}{64}\gamma^2 - \frac{1}{32}\beta\gamma\right) \tag{A1'}$$

$$D_1 = \frac{1}{\partial k_0/\partial \epsilon}\left(-\frac{15}{8}\beta - \frac{3}{8}\gamma\right) \tag{A2'}$$

$$D_2 = \frac{1}{\partial k_0/\partial \epsilon}\left(\frac{15}{8}\beta - \frac{5}{8}\gamma\right) \tag{A3'}$$

Equations (3.16)–(3.19) are valid also in two dimensions,

$$j_i = -e\int \frac{d\mathbf{k}}{2\pi^2} v_i g = \frac{-e}{2\pi^2}\int d\epsilon \int d\tilde{\phi}\, m_c v_i g \tag{3.20'}$$

From (3.4′) we find

$$m_c = m_0(1 + \tfrac{1}{2}\beta\gamma) \tag{A7'}$$

and

$$\frac{1}{1+\omega_c^2\tau^2} = \frac{1}{1+\alpha^2}\left(1 + \frac{\alpha^2}{1+\alpha^2}\,\beta\gamma\right) \tag{A8'}$$

Finally we substitute the expressions for m_c, v_i, and g into (3.20′) and obtain

$$\sigma_{xx} = \sigma_0 m_c\left(\frac{D_0^2}{1+\omega_c^2\tau^2} + \frac{D_1^2}{1+9\omega_c^2\tau^2} + \frac{D_2^2}{1+25\omega_c^2\tau^2}\right)$$

$$\sigma_{yx} = \sigma_0 m_c\left(\frac{\omega_c\tau D_0^2}{1+\omega_c^2\tau^2} - \frac{3\omega_c\tau D_1^2}{1+9\omega_c^2\tau^2} + \frac{5\omega_c\tau D_2^2}{1+25\omega_c^2\tau^2}\right)$$

which gives (3.34) and (3.35), respectively. The limiting value at $B = 0$ is

$$\sigma_{xx}^0 = \sigma_0\left(1 + 8\beta^2 - \tfrac{1}{2}\beta\gamma + \tfrac{1}{2}\gamma^2\right) \tag{3.26'}$$

whereas the high-field limits are

$$\sigma_{yx}^\infty = \frac{ne}{B} \tag{3.29'}$$

$$S_{xx}^\infty = -\frac{\pi^2}{3}\frac{k_B^2 T}{e}\frac{g(\epsilon_F)}{n} \tag{4.7'}$$

where n and $g(\epsilon_F)$ are given by (2.21′) and (2.22′), respectively.

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