Geometrical Interpretation of the Magnetoconductivity of a Fermi Ellipsoid*

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The Sondheimer-Wilson approximation to the magnetoconductivity tensor of metals has recently been extended by Mackey and Sybert to the model of an arbitrarily oriented Fermi ellipsoid with an anisotropic relaxation time. A study of their results shows that a straightforward geometrical interpretation can be attached to the parameters which appear in the transverse-magnetoconductivity and Hall-conductivity expressions derived from this quasiclassical model at arbitrary strengths of the applied magnetic field. It is suggested that the geometrical relationships may be more general than their limited derivation and could lead to quantitative predictions of the galvanomagnetic coefficients of some metals with a complex Fermi surface.

INTRODUCTION

A tractable analytical calculation of the magnetoconductivity tensor of metals appears to require rather drastic specializations and simplifying assumptions. One such case is the calculation by Sondheimer and Wilson[1] of the transverse magnetoconductivity tensor due to independent bands of electronic carriers represented by spherical sheets of the Fermi surface with an isotropic scalar relaxation time. Grenier *et al.*[2] extended the Sondheimer-Wilson results to ellipsoidal surfaces, and Mackey and Sybert[3] have recently succeeded in adapting the Sondheimer-Wilson approach to arbitrarily oriented ellipsoids with a tensor relaxation time. The latter is about the most general case that has been worked to conclusion. Nonellipsoidal Fermi surfaces have been treated by other formalisms, but the results obtained are limited. The Jones-Zener expansion[4] is useful only at very weak magnetic fields, while the vector mean free path method[5] leaves the results in quadratures. Another possibility is the graphical method, in which the correct Fermi surface is simulated by a planar-faced model,[6] but this method, like that of Jones and Zener, seems to be an inherently weak-field approximation. How does one calculate the magnetoconductivities of nonellipsoidal Fermi surfaces in a manner suitable for comparison with experiments not restricted to weak- or strong-field limits?

The breaking of a similar impasse which existed for energy-band calculations was largely due to recognition of the physical significance of certain geometrical features of the Fermi surface. Perhaps it is also true for transport effects, that features of the results obtained for an ellipsoidal surface have a geometrical interpretation which transcends the ellipsoidal limitations of the calculation.

In this paper, it is shown that there exists a simple geometrical interpretation of the results of Mackey and Sybert when applied to tilted ellipsoids symmetrically arrayed about the direction of the applied magnetic field. Reasonable quantitative success has been obtained in developing a band model based upon this geometrical interpretation which predicts the galvanomagnetic coefficients of tungsten at effectively arbitrary field strength.[7]

THEORY

It is well known that an appropriate description of the dispersion relation of a degenerate energy band at the Fermi energy is, in some cases, given in terms of a mass tensor. It *may* also be appropriate, as proposed by Herring and Vogt,[8] to describe some scattering processes in terms of a relaxation-time tensor. Mackey and Sybert[3] have derived a very compact form for the isothermal electrical magnetoconductivity tensor $\overleftrightarrow{\sigma}$ of a model of the above type. In Gaussian units, their results for a single electron band with spatial charge density ne are

$$\overleftrightarrow{\sigma} = nec(\overleftrightarrow{H}^{s} - \overleftrightarrow{H})^{-1}, \tag{1}$$

$$\overleftrightarrow{H} \equiv (c/e)\overleftrightarrow{\tau}^{-1}\overleftrightarrow{m}, \tag{2}$$

where $\overleftrightarrow{H}$ is the magnetic part of the applied field tensor. For a uniform steady field H, one can always, as is customary, describe $\overleftrightarrow{\sigma}$ in a laboratory coordinate system oriented such that

$$\overleftrightarrow{H} = \begin{bmatrix} 0 & -H & 0 \\ H & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} . \tag{3}$$

In this same system, $\overleftrightarrow{m}$ and $\overleftrightarrow{\tau}$ are the mass and relaxation-time tensors. The laboratory system

is not generally the principal-axis system, but is obtained from the principal-axis system by an orthogonal transformation $\overleftrightarrow{x}$. Explicitly,

$$\overleftrightarrow{m}_p \equiv \begin{bmatrix} m_1 & 0 & 0 \\ 0 & m_2 & 0 \\ 0 & 0 & m_3 \end{bmatrix} \quad \text{and} \quad \overleftrightarrow{m} = \overleftrightarrow{x}^{-1} \overleftrightarrow{m}_p \overleftrightarrow{x}, \tag{4}$$

$$\overleftrightarrow{\tau}_p \equiv \begin{bmatrix} \tau_1 & 0 & 0 \\ 0 & \tau_2 & 0 \\ 0 & 0 & \tau_3 \end{bmatrix} \quad \text{and} \quad \tau = \overleftrightarrow{x}^{-1} \overleftrightarrow{\tau}_p \overleftrightarrow{x} . \tag{5}$$

For the specific example of an ellipsoid tilted away from the laboratory 3 (field) direction by a rotation through an angle ψ about the 1 principal axis, the preceding definitions imply

$$\overleftrightarrow{H}^s = c/e \begin{bmatrix} m_1\tau_1^{-1} & 0 & 0 \\ 0 & [m_2\tau_2^{-1}\cos^2\psi + m_3\tau_3^{-1}\sin^2\psi] & [(m_2\tau_2^{-1} - m_3\tau_3^{-1})\sin\psi\cos\psi] \\ 0 & [(m_2\tau_2^{-1} - m_3\tau_3^{-1})\sin\psi\cos\psi] & [m_2\tau_2^{-1}\sin^2\psi + m_3\tau_3^{-1}\cos^2\psi] \end{bmatrix} . \tag{6}$$

It was shown by Onsager[9] that, if the laboratory 3 direction defines an axis of at least threefold rotational symmetry in the metal, the only nonzero elements of the magnetoconductivity tensor are $\sigma_{11} = \sigma_{22}$, $\sigma_{12} = -\sigma_{21}$, and σ_{33}, as in the isotropic case. A specific example which satisfies this condition is that of three tilted ellipsoids symmetrically placed about the 3 direction. The discussion that follows will focus upon σ_{11}^T and σ_{12}^T, the total transverse magnetoconductivity and Hall conductivity due to the three ellipsoids. Following Mackey and Sybert, the results are

$$\sigma_{11}^T = 3nec a_i H_i/(H^2 + H_i^2), \tag{7}$$

$$\sigma_{12}^T = -3necH/(H^2 + H_i^2), \tag{8}$$

$$H_i^2 \equiv H_{11}^s[H_{22}^s - (H_{23}^s)^2/H_{33}^s], \tag{9}$$

$$a_i \equiv H_i/2H_{11}^s + H_{11}^s/2H_i, \tag{10}$$

where the subscript i would denote the ith such band of carriers in a multiband model. The above result is formally indentical to that of Mackey and Sybert, but the elements of their $\overleftrightarrow{H}^s$ are different due to their use of a $\overleftrightarrow{\tau}$ which was diagonal in the laboratory coordinate system.

The object is to now indicate the geometrical significance on a Fermi surface of the quantities H_i and a_i. Direct substitution for the elements of $\overleftrightarrow{H}^s$ in terms of the principal-axis tensors $\overleftrightarrow{m}_p$ and $\overleftrightarrow{\tau}_p$ yields

$$H_i = \frac{c}{e}\left(\frac{m_1m_2m_3}{\tau_1\tau_2\tau_3}\right)^{1/2}(m_2\tau_2^{-1}\sin^2\psi + m_3\tau_3^{-1}\cos^2\psi)^{-1/2}, \tag{11}$$

$$a_i = \frac{1}{2}\left(\frac{\tau_1 m_1^{-1}}{\tau_3 m_3^{-1}\sin^2\psi + \tau_2 m_2^{-1}\cos^2\psi}\right)^{1/2} + \frac{1}{2}\left(\frac{\tau_3 m_3^{-1}\sin^2\psi + \tau_2 m_2^{-1}\cos^2\psi}{\tau_1 m_1^{-1}}\right)^{1/2} . \tag{12}$$

The actual scattering anisotropy should be expected to fall between two limiting cases of these last expressions.

Limiting Case (i): Complete Scattering Isotropy

Isotropic scattering is defined here as that scattering which is independent of the direction of the $\vec{k}$ vector on the Fermi surface. It is characterized by the condition $\tau_1 = \tau_2 = \tau_3 \equiv \tau_i$. The interpretation of H_i and a_i is unambiguous for this case of the ellipsoidal model.

The semiaxes of each ellipsoid are given by $(2m_1\zeta_0)^{1/2}$, $(2m_2\zeta_0)^{1/2}$, and $(2m_3\zeta_0)^{1/2}$, where ζ_0 is the Fermi energy. The extremal intersection between one of the ellipsoids and a family of planes normal to the direction of the applied field is an elliptical extremal orbit, the enclosed area A_e of which determines the de Haas–van Alphen frequency. Elementary mensuration formulas give

$$A_e = 2\pi\zeta_0(m_1m_2m_3)^{1/2}(m_2\sin^2\psi + m_3\cos^2\psi)^{-1/2}.$$

For a quadratic dispersion law, the cyclotron effective mass is given by

$$m_i^* = (2\pi)^{-1}\frac{\partial A_e}{\partial \zeta_0} = (2\pi)^{-1}\frac{A_e}{\zeta_0} .$$

Therefore, we have

$$H_i = cA_e/2\pi e\tau_i\zeta_0 = m_i^* c/e\tau_i, \tag{13}$$

which is a standard result.[2]

The equivalent result for a_i is not standard. Consider the ratio P_{orb}/P_{cir}. In this ratio, P_{orb} is the perimeter of the extremal orbit, and P_{cir} is the perimeter of a circle which would enclose the same area A_e as that enclosed by the extremal

ellipse. Application of elementary mensuration formulas in order to determine this ratio yields the very simple result

$$a_i = (P_{\text{orb}}/P_{\text{cir}})^2 . \tag{14}$$

This result leads one to interpret a_i as a geodesic factor in the magnetoconductivity, which partially describes the shape of the path a typical carrier traverses upon the Fermi surface as the momentum of the carrier is reversed by collisions.

Limiting Case (2): Complete Scattering Anisotropy

Completely anisotropic scattering is defined here as that scattering in which the tensor $\overleftrightarrow{\tau}_p$ is scaled in direct proportion to the tensor $\overleftrightarrow{m}_p$. It is characterized by the condition

$$\tau_1/m_1 = \tau_2/m_2 = \tau_3/m_3 \equiv \tau_i^*/m_i^* ,$$

where m_i^* is the cyclotron effective mass as defined earlier, and τ_i^* is now defined by the above condition as the effective relaxation time of the band for the stated field configuration. In this case, one immediately obtains the results

$$H_i = m_i^* c/e\tau_i^*, \tag{15}$$

$$a_i = 1 . \tag{16}$$

The assumption of completely anisotropic scattering on an anisotropic Fermi surface has led, as a little reflection will show it should, to the standard result for isotropic scattering on a spherical Fermi surface.

From the two limiting cases, one can now speculate about an interpolation form for the intermediate case. The simplest possibility is

$$H_i = m_i^* c/e\tau_i^*, \tag{17}$$

$$a_i = (P_{\text{orb}}/P_{\text{cir}})^\gamma , \qquad 0 \le \gamma \le 2. \tag{18}$$

CONCLUSION

The perimeter rule [Eq. (18)] is the focal point of this work. It is interesting that the coefficient a_i has such an interpretation. Interest in Eq. (18) should not be great, however, unless it can be shown that Eqs. (17) and (18) along with Eqs. (7) and (8) are applicable to more complex and unsolved problems. Equations (17) and (18) with $\gamma = 1$ have been applied to the complex Fermi surface of tungsten,[10] and this will be detailed in the following paper.[7] The quantitative success achieved in that application was sufficient to prompt this separate report.

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[1]A. H. Wilson, *Theory of Metals* (Cambridge U. P., Cambridge, England, 1953), p. 208 ff.

[2]C. G. Grenier, J. M. Reynolds, and J. R. Sybert, Phys. Rev. 132, 58 (1963).

[3]H. J. Mackey and J. R. Sybert, Phys. Rev. 180, 678 (1969).

[4]J. M. Ziman, *Electrons and Phonons* (Oxford U. P., Oxford, England, 1960), p. 501 ff.

[5]G. Fair and P. L. Taylor, Bull. Am. Phys. Soc. 15, 252 (1970).

[6]R. S. Allgaier, Phys. Rev. 165, 775 (1968); and C. C. Evans, T. A. Reglein, and R. S. Allgaier, Phys. Rev. B (to be published).

[7]J. R. Long, Bull. Am. Phys. Soc. 15, 252 (1970); following paper, Phys. Rev. B 3, 1209 (1971).

[8]C. Herring and E. Vogt, Phys. Rev. 101, 944 (1956).

[9]L. Onsager, Phys. Rev. 37, 405 (1931); 38, 2265 (1931).

[10]See, for instance, R. F. Girvan, A. V. Gold, and R. A. Phillips, J. Phys. Chem. Solids 29, 1485 (1968).