VII. CONCLUSION

It has been shown how a nonlocal pseudopotential can be set up and parameterized in such a way as to give a very precise description of the Fermi surface of beryllium. Calculated and observed dHvA frequencies agree in most cases to within 1%. The effective masses computed for the various orbits indicate an electron mass enhancement due to many-body interactions of about 20%. The model also provides much other useful information on the behavior of electrons in beryllium. For example, the detailed knowledge of the shape of the Fermi surface yields caliper dimensions and allows some understanding of magnetic breakdown between orbits. The electronic specific heat also comes out of the calculation.

Further uses of the model include adapting it for computing pressure and strain variations of the band structure. With increased precision in calculation and alternative assumptions concerning the changes in pseudopotential under conditions of strain, the agreement with experimental values should improve, since the present approach yields reasonable results. Finally, this model may also be applied to the case of dilute alloys where the simplest procedure is to combine the effects of lattice-dimension changes with changes in the Fermi surface due to variation in electron density. Within this approximation, the Fermi-surface topology is more easily changed by altering the electron concentration than by application of pressure alone. This interesting problem remains to be discussed in a later publication.

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Magnetoconductivity of a Fermi Ellipsoid with Anisotropic Relaxation Time

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An extremely simple expression is obtained for the isothermal conductivity tensor for an arbitrarily oriented Fermi ellipsoid in an arbitrarily oriented magnetic field. The relationship between a simple kinetic equation and a vector form of the Boltzmann equation is demonstrated, and this relationship is used to show how to include the relaxation time as a tensor quantity. One again obtains a simple result which possesses the general characteristics shown to be required by other workers dealing in a different approximation.

INTRODUCTION

IN a previous paper,[1] the authors have utilized the Ham-Mattis transformation[2] to obtain a tensor relationship between the kinetic coefficients of electron transport calculated for an arbitrarily oriented Fermi ellipsoid with magnetic field **H** directed along the 3 axis and the corresponding coefficients calculated for a Fermi sphere with **H** along the 3 axis. The resulting expressions are functions of the elements of the reciprocal effective-mass tensor $\hat{\alpha}=\hat{m}^{-1}$ and the magnitude of **H**. This paper discusses the form taken by the isothermal-conductivity tensor $\hat{\sigma}$ of an arbitrarily oriented Fermi ellipsoid with **H** not restricted to any specific direction relative to experimental coordinates. The result is of an extremely simple form and is a function of the elements of the mass tensor $\hat{m}$ directly along with the components of **H**. Herring and Vogt[3] have treated the problem of allowing for anisotropy in the scattering by introducing tensor relaxation times $\hat{\tau}^{(i)}$, defined for each ellipsoidal piece of the Fermi surface such that $\hat{\tau}^{(i)}$ is simultaneously diagonal with its corresponding mass tensor $\hat{m}^{(i)}$. Working in this approximation with emphasis on Maxwellian distributions, they have shown that the diagonal elements $m^{(i)}{}_{jj}$, which occur in isotropic scalar τ theory, are simply replaced by $m^{(i)}{}_{jj}/\tau^{(i)}{}_{jj}$; i.e., the tensor $\hat{\tau}$ formalism weights the diagonal mass elements with corresponding $\hat{\tau}$ elements. They obtain expressions for the various conductivity elements by an iterative technique which generates a series valid at low magnetic field. The present paper deals with a highly degenerate system at very low temperatures such that emphasis is on a Fermi distribution. Hence the results are applicable to the metals and semimetals. In the present approximation, results are obtained in closed form, valid for all values of magnetic field. Korenblit[4] has dealt with the case where there is a single $\hat{\tau}$ seen by all the ellipsoids such that $\hat{\tau}$ does not belong to the principal axes of any ellipsoid. He has shown how to introduce $\hat{\tau}$ directly into the Boltzmann equation. The present work indicates how this modified Boltzmann equation may be reduced

[1] H. J. Mackey and J. R. Sybert, Phys. Rev. **172**, 603 (1968).
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to a vector form which is related to a simple kinetic equation for the drift velocity. It is found as a general result that $\hat{\tau}$ and $\hat{m}$ enter the Boltzmann equation as the product $\hat{\tau}^{-1}\hat{m}$ in agreement with Herring and Vogt.[3] Korenblit[4] uses the Onsager reciprocal relations to constrain the $\hat{\tau}$ tensor. This paper questions the validity of this constraint. As an example of the simplicity and usefulness of the present results, $\hat{\sigma}$ is calculated for a set of three ellipsoids symmetrically placed about a trigonal axis with $\mathbf{H}$ along the symmetry direction. The relaxation time is taken isotropic in the basal plane with a distinct value along the trigonal direction.

THEORY

A. Isotropic Relaxation Time

The Boltzmann equation in the relaxation time approximation is

$$\nabla_x f\cdot\mathbf{v}+\nabla_p f\cdot[-e\mathbf{E}-(e/c)\mathbf{v}\times\mathbf{H}]+f_1/\tau=0, \quad (1)$$

where $f_1=f-f_0$, f_0 is the equilibrium Fermi function, and τ is the relaxation time taken here to depend on the momentum $\mathbf{p}$ only through the energy ϵ. Following Sondheimer and Wilson,[5] a solution for f_1 is sought in the form

$$f_1=-(\mathbf{C}\cdot\mathbf{p})\partial f_0/\partial\epsilon, \quad (2)$$

where $\mathbf{C}$ is taken to be a function of ϵ. Assume isothermal conditions and sample dimensions large compared to the mean free path such that $\nabla_x f=0$. Taking ellipsoidal energy surfaces

$$2\epsilon=\mathbf{p}\cdot\hat{\alpha}\mathbf{p}=\mathbf{p}\cdot\hat{m}^{-1}\mathbf{p}, \quad (3)$$

one may use Eqs. (2) and (3) to reduce Eq. (1) to a vector equation for $\mathbf{C}$:

$$-e\mathbf{E}+(e/c)\mathbf{H}\times\mathbf{C}-\hat{m}\mathbf{C}/\tau=0. \quad (4)$$

Equation (4) may be written

$$\mathbf{C}=c\tilde{G}\mathbf{E}, \quad (5a)$$

where $\tilde{G}$ is the transpose of $\hat{G}$, which is defined by

$$(\tilde{G})^{-1}=\hat{H}-\hat{H}^s, \quad (5b)$$

$$\hat{H}=\begin{bmatrix}0 & -H_3 & H_2\\ H_3 & 0 & -H_1\\ -H_2 & H_1 & 0\end{bmatrix}, \quad (5c)$$

$$\hat{H}^s=\hat{m}c/e\tau. \quad (5d)$$

The current density is computed as

$$\mathbf{J}=-2eh^{-3}\int\mathbf{v}f_1 d^3p, \quad (6a)$$

which becomes

$$\mathbf{J}=\left[2ech^{-3}\int\mathbf{v}(\hat{G}\mathbf{p})\left(\frac{\partial f_0}{\partial\epsilon}\right)d^3p\right]\cdot\mathbf{E}. \quad (6b)$$

[5] A. H. Wilson, *The Theory of Metals* (Cambridge University Press, Cambridge, 1959), p. 208ff.

The isothermal conductivity tensor $\hat{\sigma}$ is identified from Eq. (6b) as

$$\hat{\sigma}=2ech^{-3}\int(\hat{\alpha}\mathbf{p})(\hat{G}\mathbf{p})\left(\frac{\partial f_0}{\partial\epsilon}\right)d^3p. \quad (7)$$

Now change variables in order to facilitate integration of Eq. (7). Define a transformed momentum $\mathbf{w}$ by

$$\mathbf{w}=\alpha_0^{-1/2}\hat{\alpha}^{1/2}\mathbf{p}, \quad (8)$$

where α_0 is an arbitrary constant with the dimensions of $\hat{\alpha}$. This transformation deforms the ellipsoid of Eq. (3) into a sphere in $\mathbf{w}$ space given by

$$2\epsilon=\alpha_0\mathbf{w}\cdot\mathbf{w}. \quad (9)$$

The following relations are obtained from Eq. (9):

$$\mathbf{v}=\alpha_0^{1/2}\hat{\alpha}^{1/2}\mathbf{w}, \quad (10a)$$

$$d^3p=\alpha_0^{3/2}(\alpha_1\alpha_2\alpha_3)^{-1/2}d^3w. \quad (10b)$$

Substitution of Eqs. (10) into Eq. (7) yields

$$\hat{\sigma}=2ech^{-3}\alpha_0^{5/2}(\alpha_1\alpha_2\alpha_3)^{-1/2}\int\hat{\alpha}^{1/2}\mathbf{w}\hat{G}\hat{\alpha}^{-1/2}\mathbf{w}\left(\frac{\partial f_0}{\partial\epsilon}\right)d^3w. \quad (11)$$

Now write

$$d^3w=dS(\epsilon)d\epsilon/|\nabla_w\epsilon|=dS(\epsilon)d\epsilon/(\alpha_0 w), \quad (12)$$

where $dS(\epsilon)$ is an element of area on the sphere described in Eq. (9). Integration over the energy is now made in the highly degenerate approximation valid at low temperatures, where $-\partial f_0/\partial\epsilon$ is the δ function $\delta(\epsilon-\zeta)$, and ζ is the Fermi energy. This operation yields

$$\hat{\sigma}=-2ech^{-3}\alpha_0^{3/2}(\alpha_1\alpha_2\alpha_3)^{-1/2}w_F^{-1}\times\int\hat{\alpha}^{1/2}\mathbf{w}\hat{G}\hat{\alpha}^{-1/2}\mathbf{w}dS(\zeta). \quad (13)$$

Writing Eq. (13) in component form, one finds

$$\sigma_{ij}=-2ech^{-3}\alpha_0^{3/2}(\alpha_1\alpha_2\alpha_3)^{-1/2}w_F^{-1}\sum_k\alpha_i^{1/2}\alpha_k^{-1/2}G_{jk}\times\int w_j w_k dS(\epsilon), \quad (14)$$

where τ contained in $\hat{G}$ is now evaluated at $\epsilon=\zeta$. Noting the result

$$\int w_i w_k dS(\zeta)=\tfrac{4}{3}\pi w_F^4\delta_{jk}, \quad (15)$$

Eq. (13) becomes

$$\sigma_{ij}=-nec\tilde{G}_{ij}, \quad (16a)$$

where

$$n=(2h^{-3})(\tfrac{4}{3}\pi w_F^3)[\alpha_0^{3/2}(\alpha_1\alpha_2\alpha_3)^{-1/2}] \quad (16b)$$

is the number of electrons per unit crystal volume in

the ellipsoid, $2\zeta=\mathbf{p}\cdot\hat{\alpha}\mathbf{p}$. Equations (5) may be combined with Eq. (16a) to obtain a compact expression for $\hat{\sigma}$:

$$\hat{\sigma}=nec(\hat{H}^s-\hat{H})^{-1}. \tag{17}$$

Combining Eqs. (5a) and (16a) one finds

$$\mathbf{J}=\hat{\sigma}\mathbf{E}=-nec\tilde{G}\mathbf{E}, \tag{18a}$$

$$\mathbf{J}=-ne\mathbf{C}(\zeta). \tag{18b}$$

Equation (18b) shows that $\mathbf{C}(\zeta)$ is the drift velocity established by the applied fields.

B. Anisotropic Relaxation Time

Imagine an electron to move under the influence of $\mathbf{E}$ and $\mathbf{H}$ in an isotropic viscous medium. A kinetic description is given by

$$\dot{\mathbf{p}}=-e\mathbf{E}-(e/c)\mathbf{v}\times\mathbf{H}-\mathbf{p}/\tau. \tag{19}$$

At equilibrium, $\dot{\mathbf{p}}=0$ and the drift momentum is given by

$$-e\mathbf{E}+(e/c)\mathbf{H}\times\mathbf{v}_d-\mathbf{p}_d/\tau=0. \tag{20}$$

Anisotropic mass may be introduced by writing $\mathbf{p}=\hat{m}\mathbf{v}$ such that Eq. (20) becomes

$$-eE+(e/c)\mathbf{H}\times\mathbf{v}_d-\hat{m}\mathbf{v}_d/\tau=0. \tag{21}$$

Comparison of Eq. (21) with Eq. (4) indicates why the simple kinetic model generally gives the same result as the solution to the Boltzmann equation if one considers τ to be characteristic of electrons on the Fermi surface: The Boltzmann equation may be reduced to a vector equation [Eq. (4)] equivalent to Eq. (21) in which $\mathbf{C}$ plays the part of the drift velocity.

Now imagine a medium which is characterized by different viscosities in three orthogonal directions. A correct kinetic description is given by

$$\dot{\mathbf{p}}=-e\mathbf{E}-(e/c)\mathbf{v}\times\mathbf{H}-\hat{\tau}^{-1}\hat{m}\mathbf{v}. \tag{22}$$

Comparison of $\mathbf{C}$ to $\mathbf{v}_d$ as above shows that Eq. (4) should be replaced by

$$-e\mathbf{E}+(e/c)\mathbf{H}\times\mathbf{C}-\hat{\tau}^{-1}\hat{m}\mathbf{C}=0 \tag{23}$$

in the Boltzmann description.

Equation (23) has the solution given in Eqs. (5) if $\hat{H}^s$ is generalized from that form given in Eq. (5d) to

$$\hat{H}^s=\hat{\tau}^{-1}\hat{m}c/e. \tag{24}$$

With this change in the definition of the "saturation field tensor" $\hat{H}^s$, the calculation of $\mathbf{J}$ is identical to that given above, and one arrives again at Eqs. (17) and (18), where the elements of $\hat{\tau}$ are to be evaluated at $\epsilon=\zeta$.

Korenbilt[4] has shown that the collision term in the Boltzmann equation may be replaced by

$$(\partial f/\partial t)_{\text{coll}}=-\nabla_p f\cdot\hat{m}\hat{\tau}^{-1}\mathbf{v}. \tag{25a}$$

Using Eq. (2), where $f_1=f-f_0$, Eq. (25a) may be approximated by

$$(\partial f/\partial t)_{\text{coll}}=\tilde{\tau}^{-1}\hat{m}\mathbf{C}\cdot\mathbf{v}(\partial f_0/\partial\epsilon). \tag{25b}$$

This approximation has the property that for the case of isotropic scattering, where $\hat{\tau}=\tau$, Eq. (25b) reduces to

$$(\partial f/\partial t)_{\text{coll}}=\tau^{-1}\mathbf{C}\cdot\mathbf{p}(\partial f_0/\partial\epsilon)=-f_1/\tau, \tag{25c}$$

so that the formalism will reduce to the results obtained from the approximation

$$(\partial f/\partial t)_{\text{coll}}=-(f-f_0)/\tau \tag{25d}$$

as used in Eq. (1). Insertion of Eq. (26b) into Eq. (1) yields Eq. (23) with $\hat{\tau}^{-1}$ replaced by $\tilde{\tau}^{-1}$. This replacement follows into Eq. (24). However, if there exists a coordinate system such that $\hat{\tau}$ is diagonal, then $\hat{\tau}$ is symmetric and $\tilde{\tau}^{-1}=\hat{\tau}^{-1}$. It is to be noted that in this case $\hat{\tau}$ and $\hat{m}$ appear in $\hat{\sigma}$ through $\hat{H}^s$ in the combination $\hat{\tau}^{-1}\hat{m}$, in agreement with Herring and Vogt.[3] It is to be emphasized that Eq. (25b) follows from Eq. (25a) in an approximation in which three terms proportional to $\mathbf{v}$ have been neglected. Although it is difficult to judge quantitatively the degree of this approximation, it appears emminently reasonable for the formalism to reduce to Eq. (25d) for the case of isotropic scattering. Neglect of these terms is necessary for this connection to be made between the ordinary scalar τ approximation and the Korenblit approximation.

DISCUSSION

The resistivity tensor for a single ellipsoid is obtained from Eq. (17) as

$$\hat{\rho}=(nec)^{-1}(\hat{H}^s-\hat{H}). \tag{26}$$

Although Eq. (17) was derived for a coordinate system in which $\hat{m}$ is diagonal, it is clear that the form of Eq. (26), and therefore the form of Eq. (17), is invarient under orthogonal similarity transformation. Therefore, Eq. (17) may be used for any coordinate system so long as $\hat{H}^s$ and $\hat{H}$ are represented in that system. If the total Fermi surface consists of a single ellipsoid, then one expects $\hat{\tau}$ to be diagonal simultaneously with $\hat{\alpha}$ such that $\hat{H}^s$ is diagonal. Then the Onsager relation

$$\rho_{ij}(+H)=\rho_{ji}(-H) \tag{27}$$

follows from Eq. (26) because $\hat{H}$ is antisymmetric; this is the case considered by Herring and Vogt.[3] Examination of Eqs. (17) or (26) shows that for the Onsager relations to hold for a single ellipsoid, $\hat{H}^s$ must be symmetric; i.e., the product $\hat{\tau}^{-1}\hat{m}$ must be symmetric. This is obviously the case of $\hat{\tau}$ and $\hat{m}$ are simultaneously diagonal. If the Fermi surface consists of a set of ellipsoids which do not belong to a common set of principal axes, then $\hat{\tau}$, which refers to the crystal symmetry, will not likely be simultaneously diagonal with any of the various $\hat{m}$. Then the conductivity tensor

belonging to a single ellipsoid will not generally obey the Onsager relation

$$\sigma_{ij}(H)=\sigma_{ji}(-H). \tag{28}$$

However, if there exists a three-, four- or sixfold symmetry axis, one may expect $\hat{\tau}$ to be diagonal in a coordinate system having one axis in the symmetry direction with $\hat{\tau}$ exhibiting isotropy in the plane perpendicular to this direction. Then the total conductivity given by the sum of the individual conductivities as computed from Eq. (17) should obey Eq. (28). In the problem treated by Korenblit,[4] he has required the product $\hat{\tau}^{-1}\hat{m}$ to be symmetric in order to have the Onsager relations hold for the partial conductivity due to one of a group of ellipsoids. It is not clear to the authors that this constraint is necessary. As will be shown in an example below, it is quite possible to have the partial conductivities not obey the Onsager relations individually while the total conductivity given by their sum does obey these relations. In any event, the $\hat{\tau}$ explicity considered by Korenblit is such that $\hat{\tau}^{-1}\hat{m}$ is symmetric.

As an example, consider a Fermi surface consisting of three ellipsoids symmetrically placed about a trigonal axis with the magnetic field directed in the symmetry direction. Let the principal ellipsoid be rotated out of the principal axes by a rotation through angle ψ about the 1 axis. Then $\hat{m}$ for this ellipsoid has the form

$$\hat{m}=\begin{bmatrix} m_1 & 0 & 0 \\ 0 & m_2c^2+m_3s^2 & (m_2-m_3)sc \\ 0 & (m_2-m_3)sc & m_2s^2+m_3c^2 \end{bmatrix}, \tag{29a}$$

$$c=\cos\psi, \tag{29b}$$

$$s=\sin\psi, \tag{29c}$$

where m_i is a principal element of $\hat{m}$. As discussed above, take $\hat{\tau}$ to be isotropic in the basal plane as

$$\hat{\tau}=\begin{bmatrix} \tau & 0 & 0 \\ 0 & \tau & 0 \\ 0 & 0 & \tau_3 \end{bmatrix}. \tag{30}$$

Then one has

$$\hat{H}^s=\begin{bmatrix} m_{11}c/e\tau & 0 & 0 \\ 0 & m_{22}c/e\tau & m_{23}c/e\tau \\ 0 & m_{23}c/e\tau_3 & m_{33}c/e\tau_3 \end{bmatrix}, \tag{31a}$$

$$\hat{H}=\begin{bmatrix} 0 & -H & 0 \\ H & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{31b}$$

Substitution of Eqs. (31) into Eq. (17) gives the contribution of the principal ellipsoid to the conductivity as

$$\hat{\sigma}=\frac{nec}{\Delta}\begin{bmatrix} (H_{22}^sH_{33}^s-H_{23}^sH_{32}^s) & -HH_{33}^s & -HH_{23}^s \\ HH_{33}^s & H_{11}^sH_{33}^s & -H_{11}^sH_{23}^s \\ HH_{32}^s & -H_{11}^sH_{32}^s & (H_{11}^sH_{22}^s+H^2) \end{bmatrix}, \tag{32a}$$

$$\Delta=H_{33}^s(H_i^2+H^2), \tag{32b}$$

$$H_i^2=H_{11}^s(H_{22}^s-H_{23}^sH_{32}^s/H_{33}^s). \tag{32c}$$

The total conductivity $\hat{\sigma}^T$ due to all three ellipsoids is given by

$$\hat{\sigma}^T=\hat{\sigma}+\hat{Z}(\tfrac{2}{3}\pi)\hat{\sigma}\hat{Z}(-\tfrac{2}{3}\pi)+\hat{Z}(-\tfrac{2}{3}\pi)\hat{\sigma}\hat{Z}(\tfrac{2}{3}\pi), \tag{33}$$

where $\hat{Z}(\theta)$ is a right-handed rotation about the 3 axis. Combining Eqs. (32) and (33) gives

$$(\hat{\sigma}^T)_{11}=(\hat{\sigma}^T)_{22}=NecaH_iL, \tag{34a}$$

$$(\hat{\sigma}^T)_{12}=-(\hat{\sigma}^T)_{21}=-NecH_iL, \tag{34b}$$

$$(\hat{\sigma}^T)_{33}=Nec[1/H_{33}^s+H_{11}^sH_{23}^sH_{32}^sL/(H_{33}^s)^2], \tag{34c}$$

$$N=3n, \tag{34d}$$

$$a=\tfrac{1}{2}(H_i/H_{11}^s+H_{11}^s/H_i), \tag{34e}$$

$$L=(H_i^2+H^2)^{-1}. \tag{34f}$$

The other elements of $\hat{\sigma}^T$ are zero. One sees that, although the partial conductivities do not obey the Onsager theorem [see Eqs. (32)], the resulting total $\hat{\sigma}$ as given in Eqs. (33) does obey the reciprocal relations. This example should emphasize the simplicity of the result given in Eq. (17) and the ease with which the total conductivity due to many ellipsoids may be written down even in the case for **H** not along a symmetry direction.