THE

PHYSICAL REVIEW

A journal of experimental and theoretical physics established by E. L. Nichols in 1893

SECOND SERIES, VOL. 155, NO. 3 — 15 MARCH 1967

Magnetoresistance Anisotropy in Metals due to Anisotropic Scattering of Electrons

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(Received 15 August 1966)

The elementary algebraic solution of the Boltzmann equation in the theory of metals, for the case where the kernel is of finite rank, is extended to the case where an external magnetic field of arbitrary strength is present. A closed expression is derived for the magnetoresistance tensor which is valid for arbitrary form of the energy surfaces and which does not depend on the relaxation-time approximation. As an illustrative study of the effects of scattering anisotropy, the high-field longitudinal magnetoresistance is calculated for cubic metals with spherical Fermi surfaces, when fourth-order terms are kept in the expansion of the scattering probability in powers of the wave-vector components. The results suggest that experiments on magnetoresistance in single crystals of the alkali metals may give information on the form of the scattering probability.

1. INTRODUCTION

THE magnetoresistance of metals in high magnetic fields has been extensively studied in recent years as a useful indicator of the topological structure of the Fermi surface.[1] Now that the form of the Fermi surface can be determined experimentally by a variety of methods, in some cases with considerable accuracy, interest is turning to the possibility of determining experimentally other important parameters characterizing electron transport processes—in particular, the relaxation time for scattering, or, more generally, the transition probability $p(\mathbf{k},\mathbf{k}')$ for scattering between states $\mathbf{k}$ and $\mathbf{k}'$ on the Fermi surface. Pippard,[2] in particular, has pointed out the striking sensitivity of the longitudinal magnetoresistance to the form of $p(\mathbf{k},\mathbf{k}')$ in the noble metals.

Standard magnetoresistance theory[3] is based on a Boltzmann equation in which a constant time of relaxation is assumed to exist, so that scattering anisotropy is ignored. Approximate solutions under more general conditions may be obtained by the variational method,[4] by assuming that an anisotropic relaxation time can be defined,[5] or by direct numerical solution of the Boltzmann equation.[6] However, it is difficult in practice to estimate the accuracy of the results obtained by these methods. In the present paper, we study the exact solution of the Boltzmann equation in the case where $p(\mathbf{k},\mathbf{k}')$ can be written as a finite sum of products of a function of $\mathbf{k}$ with a function of $\mathbf{k}'$. Sondheimer[7] has recently pointed out that for this form of $p(\mathbf{k},\mathbf{k}')$, the Boltzmann equation reduces to a set of linear equations with a singular matrix; his method of solution was subsequently simplified by Chambers.[8] The work of Sondheimer and Chambers referred to zero magnetic field, and in Sec. 2 of the present paper we extend their algebraic method of solution to the case where an applied magnetic field $\mathbf{H}$ of arbitrary magnitude is present. We derive an exact formal expression for the magnetoresistivity tensor $\hat{\rho}$ [Eq. (2.18)] which is valid for arbitrary energy surfaces and all values of $\mathbf{H}$. (In a recent note on the same problem,[9] the equation given is singular.)

The theory allows $\hat{\rho}$ to be calculated by quadratures for different forms of $p(\mathbf{k},\mathbf{k}')$ if the Fermi-surface geometry is known. Ideally, one would like to work backwards from measurements of the anisotropy of $\hat{\rho}$ to deduce the form of $p(\mathbf{k},\mathbf{k}')$. We have not, however,

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found any way of doing this systematically, and it seems that in practice one will have to proceed by trial and error, evaluating $\hat{\rho}$ for various assumed forms of $p(\mathbf{k},\mathbf{k}')$, until agreement with experiment is obtained. This is likely to be a very laborious task.

Equation (2.18) has a wide variety of possible applications. In general, the anisotropy of the components of $\hat{\rho}$ depends in a complicated way on both the Fermi-surface geometry and the form of the scattering probability. For an illustrative study of the effects of scattering anisotropy alone, we consider, in Sec. 3, the simplest special case in which nontrivial results are obtained. We use (2.18) to calculate the longitudinal magnetoresistance, in the limit of high magnetic fields, for a cubic metal with a spherical Fermi surface, using an expansion of $p(\mathbf{k},\mathbf{k}')$ in powers of the components of $\mathbf{k}$ and $\mathbf{k}'$, in which terms beyond fourth powers are neglected. For this model, which is applicable to the alkali metals, there can be no large effects of the type of those studied by Pippard[2] for copper, which depend on the presence of "necks" on the Fermi surface. Nevertheless, we find in Sec. 4 that measurements of the anisotropy of the longitudinal magnetoresistance may give useful information on the coefficients in the expansion of $p(\mathbf{k},\mathbf{k}')$. We make no attempt in this paper to discuss the physical mechanisms which lead to particular forms of $p(\mathbf{k},\mathbf{k}')$, but regard this function as one to be determined by experiment. We conclude in Sec. 5 by comparing the exact solutions with the results obtained in the relaxation-time approximation.

2. A GENERAL EXPRESSION FOR THE MAGNETORESISTIVITY TENSOR

The electron distribution function in the presence of uniform electric and magnetic fields $\mathbf{E}$ and $\mathbf{H}$ is $f_0(\epsilon_\mathbf{k}) + g(\mathbf{k})\partial f_0/\partial\epsilon_\mathbf{k}$, where f_0 is the equilibrium distribution, and where, to linear accuracy in $\mathbf{E}$, g satisfies the Boltzmann equation

$$-\frac{e}{\hbar c}\mathbf{v}\times\mathbf{H}\cdot\frac{\partial g}{\partial\mathbf{k}}+\int\{g(\mathbf{k})-g(\mathbf{k}')\}p(\mathbf{k},\mathbf{k}')\frac{dS'}{\hbar v'}=e\mathbf{v}\cdot\mathbf{E}. \quad (2.1)$$

Here, $\epsilon_\mathbf{k}$ is the one-electron energy, $\mathbf{k}$ the wave vector, and $\mathbf{v}=\hbar^{-1}\partial\epsilon/\partial\mathbf{k}$ the electronic velocity. The scattering is assumed to be elastic, and $p(\mathbf{k},\mathbf{k}')$ is the probability per unit time for the transition from a state $\mathbf{k}$ on the energy surface $\epsilon_\mathbf{k}=$constant, to a state $\mathbf{k}'$ in the region dS' of the same surface where the magnitude of the velocity is v'.

The integro-differential equation (2.1) is singular, since the homogeneous equation obtained by writing zero on the right-hand side has the nonzero solution $g(\mathbf{k})=$constant. The solubility condition, however, is satisfied,[7] and we obtain a nonsingular equation[8] by retaining in (2.1) only those parts which are odd in $\mathbf{k}$. This gives the equation

$$-\frac{e}{\hbar c}\mathbf{v}\times\mathbf{H}\cdot\frac{\partial g_1}{\partial\mathbf{k}}+g_1(\mathbf{k})\int p_0(\mathbf{k},\mathbf{k}')\frac{dS'}{\hbar v'} -\int g_1(\mathbf{k}')p_1(\mathbf{k},\mathbf{k}')\frac{dS'}{\hbar v'}=e\mathbf{v}\cdot\mathbf{E}, \quad (2.2)$$

where $g_1(\mathbf{k})=\frac{1}{2}\{g(\mathbf{k})-g(-\mathbf{k})\}$ is the odd part of g, and

$$\left.\begin{aligned} p_0(\mathbf{k},\mathbf{k}')&=\tfrac{1}{2}\{p(\mathbf{k},\mathbf{k}')+p(\mathbf{k},-\mathbf{k}')\},\\ p_1(\mathbf{k},\mathbf{k}')&=\tfrac{1}{2}\{p(\mathbf{k},\mathbf{k}')-p(\mathbf{k},-\mathbf{k}')\}\end{aligned}\right\} \quad (2.3)$$

are the parts of $p(\mathbf{k},\mathbf{k}')$ which are, respectively, even in both $\mathbf{k}$ and $\mathbf{k}'$, and odd in both $\mathbf{k}$ and $\mathbf{k}'$. Here, it is assumed that $p(\mathbf{k},\mathbf{k}')$ is independent of the magnetic field, and therefore[8] satisfies the symmetry relation $p(\mathbf{k},\mathbf{k}')=p(-\mathbf{k},-\mathbf{k}')$, which follows from the principle of microscopic reversibility $p(\mathbf{k},\mathbf{k}')=p(\mathbf{k}',\mathbf{k})$, and the reciprocity theorem $p(\mathbf{k},\mathbf{k}')=p(-\mathbf{k}',-\mathbf{k})$.

We assume that $p_1(\mathbf{k},\mathbf{k}')$ can be written as a finite sum of products of a function of $\mathbf{k}$ with a function of $\mathbf{k}'$. Since $p_1(\mathbf{k},\mathbf{k}')=p_1(\mathbf{k}',\mathbf{k})$, $p_1(\mathbf{k},\mathbf{k}')$ thus has the form

$$p_1(\mathbf{k},\mathbf{k}')=\sum_{i,j=1}^{N} b_{ij}q_i(\mathbf{k})q_j(\mathbf{k}'), \quad (2.4)$$

where $b_{ij}=b_{ji}$, and $q_i(\mathbf{k})$ ($i=1, 2, \ldots, N$) is a set of N arbitrary functions of $\mathbf{k}$ of integrable square. We write this in algebraic notation as

$$p_1(\mathbf{k},\mathbf{k}')=\langle q(\mathbf{k})|B|q(\mathbf{k}')\rangle, \quad (2.5)$$

where $|q\rangle$ is the column vector with components q_i and B is the $N\times N$ symmetric matrix with elements b_{ij} ($i, j=1, 2, \ldots, N$). With

$$P_0(\mathbf{k})=\int p_0(\mathbf{k},\mathbf{k}')\frac{dS'}{\hbar v'},\quad M=-\frac{e}{\hbar c}\mathbf{v}\times\mathbf{H}\cdot\frac{\partial}{\partial\mathbf{k}}, \quad (2.6)$$

Eq. (2.2) becomes

$$(M+P_0)g_1-\langle q|B|C\rangle=e\mathbf{v}\cdot\mathbf{E}, \quad (2.7)$$

where

$$|C\rangle=\int|q\rangle g_1\frac{dS}{\hbar v}, \quad (2.8)$$

and is independent of $\mathbf{k}$ and $\mathbf{k}'$. Equation (2.7) can be solved formally for g_1 to give

$$g_1=(M+P_0)^{-1}\{e\mathbf{v}\cdot\mathbf{E}+\langle q|B|C\rangle\}, \quad (2.9)$$

and, substituting this back into (2.8), we obtain the finite system of linear equations

$$|C\rangle=e|\mathbf{W}\rangle\cdot\mathbf{E}+AB|C\rangle, \quad (2.10)$$

where[10]

$$|\mathbf{W}\rangle=\int|q\rangle(M+P_0)^{-1}\mathbf{v}\frac{dS}{\hbar v},$$
$$A=\int|q\rangle(M+P_0)^{-1}\langle q|\frac{dS}{\hbar v}. \tag{2.11}$$

It is shown in Appendix A that it follows from the condition $p(\mathbf{k},\mathbf{k}')\geqslant 0$ that the matrix $I-AB$ (where I is the unit $N\times N$ matrix) is nonsingular if the functions $q_i(\mathbf{k})$ are linearly independent. The system (2.10), therefore, may be solved for $|C\rangle$ to give

$$|C\rangle=e(I-AB)^{-1}|\mathbf{W}\rangle\cdot\mathbf{E}, \tag{2.12}$$

and substituting this into (2.9), we obtain, as the solution of (2.7),

$$g_1=e(M+P_0)^{-1}\mathbf{v}\cdot\mathbf{E}+e(M+P_0)^{-1}\langle q|B(I-AB)^{-1}|\mathbf{W}\rangle\cdot\mathbf{E}. \tag{2.13}$$

The conductivity tensor $\hat{\sigma}$ is defined by $\mathbf{J}=\hat{\sigma}\cdot\mathbf{E}$, where, for a metal,

$$\mathbf{J}=\frac{e}{4\pi^3}\int g_1\mathbf{v}\frac{dS}{\hbar v}, \tag{2.14}$$

the surface integral going over the Fermi surface. Combining (2.13) and (2.14), we have

$$\hat{\sigma}=\hat{s}+\langle\mathbf{S}|B(I-AB)^{-1}|\mathbf{W}\rangle, \tag{2.15}$$

where

$$\hat{s}=\frac{e^2}{4\pi^3}\int\mathbf{v}(M+P_0)^{-1}\mathbf{v}\frac{dS}{\hbar v}, \tag{2.16}$$

and

$$\langle\mathbf{S}|=\frac{e^2}{4\pi^3}\int\mathbf{v}(M+P_0)^{-1}\langle q|\frac{dS}{\hbar v}. \tag{2.17}$$

It is usually more convenient to express $\mathbf{E}$ in terms of $\mathbf{J}$ by the magnetoresistivity tensor $\hat{\rho}$, which is the inverse of $\hat{\sigma}$. It is shown in Appendix A that the matrices $\hat{s}$ and $I-AB+|\mathbf{W}\rangle\cdot\hat{r}\cdot\langle\mathbf{S}|B$ (where $\hat{r}=\hat{s}^{-1}$) are nonsingular. From (2.15) it is then easily verified that the inverse of $\hat{\sigma}$ is given explicitly by

$$\hat{\rho}=\hat{r}-\hat{r}\cdot\langle\mathbf{S}|B\{I-AB+|\mathbf{W}\rangle\cdot\hat{r}\cdot\langle\mathbf{S}|B\}^{-1}|\mathbf{W}\rangle\cdot\hat{r}. \tag{2.18}$$

[10] We use boldface letters to denote vectors in 3 dimensions, carets for 3×3 matrices (tensors), and Greek suffixes to denote vector and tensor components in 3 dimensions. In N dimensions the bra, ket notation is used for vectors, ordinary capitals for $N\times N$ matrices, and Latin subscripts for vector and matrix components. Thus, in (2.11), $|\mathbf{W}\rangle$ is an $N\times3$ matrix with elements $W_{i\alpha}$, and A is an $N\times N$ matrix with elements A_{ij} ($i,j=1,2,\ldots,N;\alpha=x,y,z$), where

$$W_{i\alpha}=\int q_i(M+P_0)^{-1}v_\alpha\frac{dS}{\hbar v},\quad A_{ij}=\int q_i(M+P_0)^{-1}q_j\frac{dS}{\hbar v}.$$

A dot [as in (2.10)] denotes an inner product in 3 dimensions; $\langle\mathbf{S}|A|\mathbf{W}\rangle$ is a 3×3 matrix whose $\alpha\beta$ element is $\sum_{ij}S_{\alpha i}A_{ij}W_{j\beta}$, and $|\mathbf{W}\rangle\cdot\hat{r}\cdot\langle\mathbf{S}|$ is an $N\times N$ matrix whose ij element is

$$\sum_{\alpha\beta}W_{i\alpha}r_{\alpha\beta}S_{\beta j}.$$

This formula represents an exact formal expression for the magnetoresistivity tensor, based on the Boltzmann equation (2.1) and the expression (2.4) for the scattering probability.

We note for later use that the $N\times N$ matrix $I-AB+|\mathbf{W}\rangle\cdot\hat{r}\cdot\langle\mathbf{S}|B$, whose inverse occurs in Eq. (2.18), is particularly simple to invert explicitly when $p_1(\mathbf{k},\mathbf{k}')$ has the special form

$$p_1(\mathbf{k},\mathbf{k}')=\alpha\mathbf{v}(\mathbf{k})\cdot\mathbf{v}(\mathbf{k}')+\beta\{\mathbf{v}(\mathbf{k})\cdot\mathbf{u}(\mathbf{k}')+\mathbf{v}(\mathbf{k}')\cdot\mathbf{u}(\mathbf{k})\}, \tag{2.19}$$

where $\mathbf{u}$ is an arbitrary vector function of $\mathbf{k}$. In this case, $N=6$, and we have, in an obvious notation,

$$\langle q(\mathbf{k})|=(\mathbf{v}(\mathbf{k}),\mathbf{u}(\mathbf{k})), \tag{2.20}$$

$$B=\begin{pmatrix}\alpha\hat{I} & \beta\hat{I}\\ \beta\hat{I} & 0\end{pmatrix},\qquad A=\begin{pmatrix}(4\pi^3/e^2)\hat{s} & (4\pi^3/e^2)\hat{S}\\ \hat{W} & \hat{A}\end{pmatrix}, \tag{2.21}$$

$$\langle\mathbf{S}|=(\hat{s},\hat{S}),\qquad |\mathbf{W}\rangle=\begin{pmatrix}(4\pi^3/e^2)\hat{s}\\ \hat{W}\end{pmatrix}, \tag{2.22}$$

where $\hat{I}$ is the unit 3×3 matrix and, from (2.11) and (2.17), $\hat{W}$, $\hat{A}$, and $\hat{S}$ are the 3×3 matrices:

$$\hat{W}=\int\mathbf{u}(M+P_0)^{-1}\mathbf{v}\frac{dS}{\hbar v},\quad \hat{A}=\int\mathbf{u}(M+P_0)^{-1}\mathbf{u}\frac{dS}{\hbar v},$$
$$\hat{S}=\frac{e^2}{4\pi^3}\int\mathbf{v}(M+P_0)^{-1}\mathbf{u}\frac{dS}{\hbar v}. \tag{2.23}$$

In terms of these,

$$\{I-AB+|\mathbf{W}\rangle\cdot\hat{r}\cdot\langle\mathbf{S}|B\}^{-1}=\begin{pmatrix}\hat{I} & 0\\ -\beta(\hat{A}-\hat{W}\cdot\hat{r}\cdot\hat{S}) & \hat{I}\end{pmatrix}^{-1}=\begin{pmatrix}\hat{I} & 0\\ \beta(\hat{A}-\hat{W}\cdot\hat{r}\cdot\hat{S}) & \hat{I}\end{pmatrix}, \tag{2.24}$$

and Eq. (2.18) becomes

$$\hat{\rho}=\hat{r}-(4\pi^3\alpha/e^2)\hat{I}-(4\pi^3/e^2)\beta\hat{r}\cdot\hat{S}-\beta\hat{W}\cdot\hat{r}-(4\pi^3\beta^2/e^2)(\hat{A}-\hat{W}\cdot\hat{r}\cdot\hat{S}). \tag{2.25}$$

3. HIGH-FIELD LONGITUDINAL MAGNETORESISTANCE FOR METALS WITH SPHERICAL FERMI SURFACES

To evaluate (2.18) or (2.25) explicitly, we require the result of operating with $(M+P_0)^{-1}$ on a given function of $\mathbf{k}$. Now, if P_0 is identified with τ^{-1}, the differential equation

$$(M+P_0)F(\mathbf{k})=G(\mathbf{k}) \tag{3.1}$$

is the Boltzmann equation of the standard theory of magnetoresistance, in which it is assumed that a relaxation time $\tau(\mathbf{k})$ exists. As is well known,[11] the solution of this equation is conveniently expressed in terms of variables defining orbits $\epsilon_\mathbf{k}$=constant, $\mathbf{k}\cdot\mathbf{H}$ constant on the Fermi surface. For closed orbits, the solution is a periodic function of a phase angle ϕ defining position in the orbit and takes the explicit form

$$F(\phi)\equiv(M+P_0)^{-1}G$$
$$=\frac{1}{\omega_c}\int_{-\infty}^{\phi}G(\phi')\exp\left\{\frac{1}{\omega_c}\int_{\phi}^{\phi'}P_0(\phi'')d\phi''\right\}d\phi', \quad (3.2)$$

where ω_c is the cyclotron frequency for the orbit. For a completely closed Fermi surface, then, $\hat{s}$, $\langle\mathbf{S}|$, $|\mathbf{W}\rangle$, and A may be explicitly expressed as integrals over the Fermi surface and evaluated by quadrature if the Fermi-surface geometry is known.

To proceed further we make the following simplifying assumptions:

(i) The energy surfaces are spherical, with

$$\epsilon_\mathbf{k}=\hbar^2|\mathbf{k}|^2/2m, \quad \mathbf{v}=\hbar\mathbf{k}/m, \quad (3.3)$$

where m is an effective mass. $|\mathbf{v}|$ and $|\mathbf{k}|$ thus have constant values, v_0 and k_0 say, on the Fermi surface. It is well known[12] that a degenerate electron gas with the energy spectrum (3.3) has zero magnetoresistance if the relaxation time is constant, so that with the assumption (3.3) both the existence and the anisotropy of a nonzero magnetoresistance effect are entirely ascribable to the scattering anisotropy. The assumption of a spherical Fermi surface seems to hold with considerable accuracy for the alkali metals.[13]

(ii) We assume that $p(\mathbf{k},\mathbf{k}')$ has cubic symmetry, and expand it in powers of the products of the direction cosines κ_α, κ_α' of $\mathbf{k}$ and $\mathbf{k}'$ relative to the cubic axes, keeping powers up to and including the fourth. (This is the lowest order in which anisotropic effects appear.) Since $\sum_\alpha \kappa_\alpha^2$ is constant on the sphere [Eq. (3.3)], the most general form of $p(\mathbf{k},\mathbf{k}')$ is, to this order,

$$p(\mathbf{k},\mathbf{k}')=a_0+\sum_\alpha\{c_2\kappa_\alpha\kappa_\alpha'+a_4(\kappa_\alpha^4+\kappa_\alpha'^4)+b_4\kappa_\alpha^2\kappa_\alpha'^2$$
$$+c_4(\kappa_\alpha^3\kappa_\alpha'+\kappa_\alpha\kappa_\alpha'^3)\}+\sum_{\alpha\neq\beta}e_4\kappa_\alpha\kappa_\beta\kappa_\alpha'\kappa_\beta', \quad (3.4)$$

where a_0, c_2, a_4, b_4, c_4, and e_4 are constants. This expression is sufficiently general to represent a variety of possible scattering functions $p(\mathbf{k},\mathbf{k}')$, provided that the variation with $\mathbf{k}$ and $\mathbf{k}'$ is not too singular.

(iii) We confine attention to the saturation value ρ_∞ of the longitudinal magnetoresistance coefficient for large magnetic fields. For arbitrary directions of the applied magnetic field $\mathbf{H}$ this is

$$\rho_\infty=\lim_{H\to\infty}\mathbf{H}\cdot\hat{\rho}\cdot\mathbf{H}/H^2, \quad (3.5)$$

where H is the magnitude of $\mathbf{H}$. There is no difficulty in principle in calculating for the present model all the components of the magnetoresistance tensor (including those representing Hall effects) for arbitrary values of $\mathbf{H}$. The quantity (3.5) is, however, both the simplest to calculate and—provided sufficiently large magnetic fields are available—is likely to be the most useful in practice for the purpose of relating measurements of magnetoresistance to the form of $p(\mathbf{k},\mathbf{k}')$. Resistivities are easier to measure accurately than are Hall fields, and, since the "two-band" effect in conduction leads to a non-zero transverse, but zero longitudinal, magnetoresistance effect,[14] small departures of the Fermi surface from the spherical form (3.3) are more likely in the case of the transverse than in the case of the longitudinal magnetoresistance to mask the effects which arise from the anisotropy of $p(\mathbf{k},\mathbf{k}')$.

With the assumptions (i) and (ii), the calculation of ρ_∞ as a function of the orientation of $\mathbf{H}$ is straightforward. The odd part of (3.4) is

$$p_1(\mathbf{k},\mathbf{k}')=\sum_\alpha\{c_2\kappa_\alpha\kappa_\alpha'+c_4(\kappa_\alpha^3\kappa_\alpha'+\kappa_\alpha\kappa_\alpha'^3)\}. \quad (3.6)$$

This is of the form of Eq. (2.19) with

$$c_2=\alpha(\hbar k_0/m)^2, \quad c_4=\beta\hbar k_0/m, \quad \mathbf{u}=(\kappa_x^3,\kappa_y^3,\kappa_z^3), \quad (3.7)$$

so that $\hat{\rho}$ is given by (2.25). To obtain ρ_∞, we require the orders in $1/H$, in the limit $H\to\infty$, of the components of the tensors $\hat{r}$, $\hat{S}$, $\hat{W}$, and $\hat{A}$ which appear in (2.25). These may be obtained by well-known arguments[15] which are summarized in Appendix B. It is found that

$$(e^2/4\pi^3)\rho_\infty=(e^2/4\pi^3)r_\infty-\alpha-\beta r_\infty S_\infty-(e^2/4\pi^3)\beta W_\infty r_\infty$$
$$-\beta^2(A_\infty-W_\infty r_\infty S_\infty), \quad (3.8)$$

where, for any matrix $\hat{T}$, T_∞ is defined as in (3.5).

In Appendix C the quantities r_∞, S_∞, W_∞, and A_∞ are calculated for the case when $\epsilon_\mathbf{k}$ is given by (3.3), and $p(\mathbf{k},\mathbf{k}')$ by (3.4). Substitution of the results into (3.8) gives, after some rearrrangement, the final result

$$\frac{\rho_\infty}{G}=\frac{\{1-\nu I_2(\mu,s_4)\}^2}{I_1(\mu,s_4)}-\lambda-\nu^2 I_3(\mu,s_4). \quad (3.9)$$

Here

$$G=\frac{4\pi^3L}{e^2v_0^2}, \quad \lambda=\frac{c_2}{L}, \quad \mu=\frac{a_4}{L}, \quad \nu=\frac{c_4}{L},$$
$$L=a_0+\tfrac{3}{5}a_4+\tfrac{1}{3}b_4 \quad\text{and}\quad s_4=\sum_\alpha h_\alpha^4, \quad (3.10)$$

[11] See Ref. 3, p. 515.
[12] See Ref. 3, p. 494.
[13] C. C. Grimes and A. F. Kip, Phys. Rev. **132**, 1991 (1963); D. Shoenberg and P. J. Stiles, Proc. Roy. Soc. (London) **A281**, 62 (1964); H. J. Foster, P. H. E. Meijer, and E. V. Mielczarek, Phys. Rev. **139**, A1849 (1965).
[14] R. G. Chambers, Proc. Phys. Soc. (London) **A65**, 903 (1952).
[15] I. M. Lifshitz, M. Y. Azbel', and M. I. Kaganov, Zh. Eksperim. i Teor. Fiz. **31**, 63 (1956) [English transl.: Soviet Phys.—JETP **4**, 41 (1957)]; Ref. 3, p. 517.

where $h_\alpha(\alpha=x,y,z)$ are the direction cosines of **H** relative to the cubic axes. I_1, I_2, and I_3 are functions of μ and s_4 defined in Appendix C.

4. EVALUATION AND DISCUSSION OF THE FORMULA FOR ρ_∞

A complete evaluation of Eq. (3.9) for all values of the parameters will not be attempted, and we discuss only some of the more interesting features of the result. We note that ρ_∞ depends on the orientation of **H** only through the quantity s_4, which varies between $\frac{1}{3}$ (when **H** is parallel to a $\langle 111\rangle$ direction) and 1 (when **H** is parallel to a cubic axis). We define the *anisotropy* $f(s_4)$ and the *relative anisotropy* $r(s_4)$ of ρ_∞ as

$$f(s_4)=\frac{\rho_\infty(s_4)}{\rho_\infty(\frac{1}{3})},\quad r(s_4)=\frac{f(s_4)-f(1)}{f(\frac{1}{3})-f(1)},\qquad (4.1)$$

and, on the assumption that $f(s_4)$ has a single maximum $f_{\max}$, and a single minimum $f_{\min}$ as a function of s_4, we define the *total variation* t as $f_{\max}-f_{\min}$; this provides a convenient measure of the over-all degree of anisotropy of ρ_∞.

(a) Equation (3.9) contains the three parameters λ, μ, and ν which correspond, respectively, to the second-order term in $p(\mathbf{k},\mathbf{k}')$ with coefficient c_2, the even fourth-order term with coefficient a_4, and the odd fourth-order term with coefficient c_4. λ, however, is merely a constant additive term, so that (3.9) is essentially a two-parameter expression, and the anisotropy of ρ_∞ arises entirely from the two fourth-order terms in $p(\mathbf{k},\mathbf{k}')$. The existence of the term λ, however, is important, since it influences the range of possible values of μ and ν (see below). Note that the term with coefficient e_4 in $p(\mathbf{k},\mathbf{k}')$ does not contribute at all to ρ_∞, and that the terms with coefficients a_0 and b_4 only affect the value of L and hence of λ, μ, ν.

(b) The parameters λ, μ, and ν in (3.9) cannot vary arbitrarily but are restricted by the condition that the transition probability (3.4) must be non-negative. A complete discussion of these restrictions is difficult, although various necessary conditions are easily obtained; for example, μ cannot lie in the interval $(-15, -5/7)$. A number of conditions of this type are derived in Appendix D. In our calculations however, we have also admitted values of λ, μ, ν which do not satisfy these conditions, in the belief that the model studied may have a semiempirical validity wider than its literal interpretation would allow.

(c) A simple explicit result is obtained in the special case when $\mu=0$, so that P_0 is constant, and the anisotropy in ρ_∞ is due entirely to the odd term $\sum(\kappa_\alpha{}^3\kappa_\alpha{}' + \kappa_\alpha\kappa_\alpha{}'^3)$ in $p(\mathbf{k},\mathbf{k}')$. In this case, (C12), (C13), and (C14) reduce to

$$I_1=\tfrac{1}{3},\quad I_2=\tfrac{1}{5},\quad I_3=(1/35)(6-6s_4+5s_4{}^2),\qquad (4.2)$$

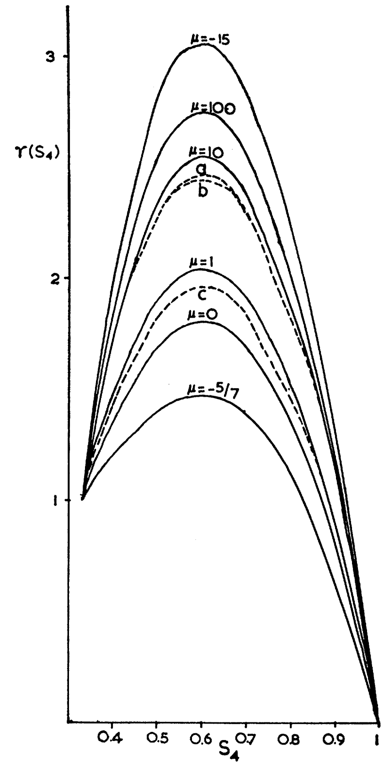

FIG. 1. Relative longitudinal magnetoresistance anisotropy. Solid curves $\lambda=\nu=0$, broken curves explained in text. [λ and ν are defined by Eqs. (3.4) and (3.10), and measure, respectively, the strengths of the second-order term and the odd fourth-order term in $p(\mathbf{k},\mathbf{k}')$.]

and with these values, (3.9) and (4.1) give

$$f(s_4)=\frac{3-(6/5)\nu-(\nu^2/175)(3-5s_4)^2-\lambda}{3-(6/5)\nu-(16\nu^2/1575)-\lambda}.\qquad (4.3)$$

Thus $f(s_4)$ varies parabolically with s_4, with a maximum at $s_4=0.6$, and a minimum (in the range $\frac{1}{3}\leqslant s_4\leqslant 1$) at $s_4=1$. The total variation is

$$t=\frac{(4\nu^2/175)}{3-(6/5)\nu-(16\nu^2/1575)-\lambda},\qquad (4.4)$$

and we see that, while the term λ does not itself produce any anisotropy of ρ_∞, it may, by diminishing the denominator of (4.4), greatly enhance the value of t. The relative anisotropy is, for all ν and λ, the unique parabola

$$r(s_4)=(9/4)(1-s_4)(5s_4-1);\qquad (4.5)$$

this is the curve labelled $\mu=0$ in Fig. 1.

We have also evaluated ρ_∞ for the case of constant P_0, and a scattering probability given by the odd sixth-order terms $\sum\kappa_\alpha{}^3\kappa_\alpha{}'^3$, and $\sum(\kappa_\alpha{}^5\kappa_\alpha{}'+\kappa_\alpha\kappa_\alpha{}'^5)$. In

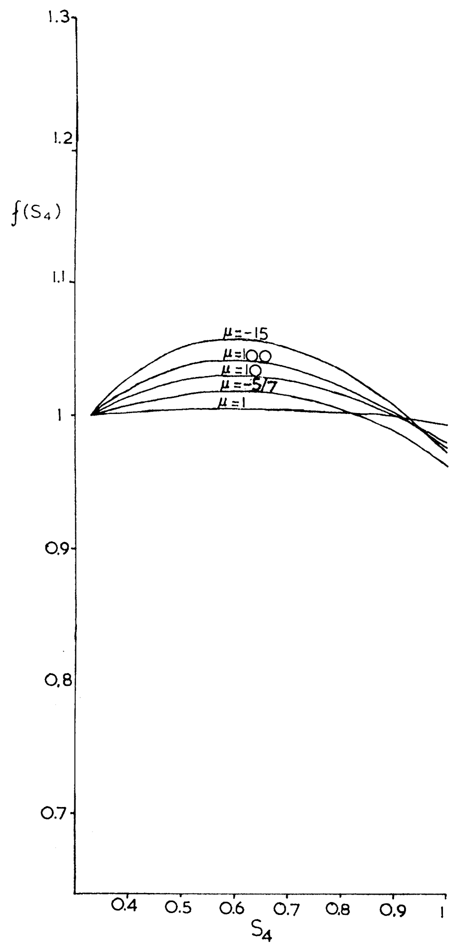

FIG. 2. Longitudinal magnetoresistance anisotropy with $\lambda=\nu=0$.

these cases ρ_∞ depends on both s_4 and s_6, where $s_6=\sum h_\alpha{}^6$. The presence of such terms in $p(\mathbf{k},\mathbf{k}')$ could be investigated by employing different orientations of $\mathbf{H}$ which correspond to the same value of s_4, but different values of s_6. Numerical estimates of these effects, however, indicate that the anisotropy of ρ_∞ in fact differs only slightly from that given by the parabolic law (4.3), so that it is unlikely that these effects could be observed in practice, and we shall not present the results in detail.

(d) For nonzero values of μ, the integrals I_1, I_2, and I_3 have been evaluated numerically as functions of s_4 for a number of values of μ in the permissible ranges $\mu<-15$ and $\mu>-5/7$. Consider first the special case when $\nu=\lambda=0$, which corresponds to the existence of a $\mathbf{k}$-dependent relaxation time (see Sec. 5 below). In this case (3.9) and (4.1) give

$$f(s_4)=\frac{I_1(\mu,\frac{1}{3})}{I_1(\mu,s_4)}. \quad (4.6)$$

This function is shown in Fig. 2 for several values of μ. The curve for $\mu=-15$ shows a total variation of about 9%. As μ decreases through $-\infty$ (equivalent to $+\infty$) towards zero the curves flatten out, and when $\mu=0$ there is no anisotropy; they then start to broaden again and for $\mu=-5/7$ reach a total variation of about 6%. All show a maximum very close to $s_4=0.6$. If the relative anisotropy $r(s_4)$ is plotted as in Fig. 1, there is a more uniform behavior as μ varies, the curves becoming steadily less peaked as μ passes over its allowed range of values.

(e) Figure 3 shows a number of anisotropy curves for the same values of μ as in Fig. 2, but now allowing λ and ν to be nonzero. There are several points to be remarked.

(i) Considerable enhancement in the total variation of the anisotropy is achieved for some values of λ and ν. The greatest effect shown in Fig. 3 is for $\mu=-15$, $\lambda=30$, and $\nu=-30$, with a total variation of about 65%. However, Eqs. (D17) and (D18) of Appendix D show that, when $\mu=-15$, λ and ν must satisfy the relation $3\lambda+2\nu=0$, so that the values $\lambda=30$ and $\nu=-30$ are in fact not allowed on a rigorous interpretation of the model.

(ii) Curves having an inverted shape relative to those in Fig. 2 are obtained for some values of λ and ν; for example, $\mu=100$, $\lambda=0$, $\nu=-180$, and $\mu=-15$, $\lambda=0$, $\nu=-30$ in Fig. 3. Again these values are inconsistent with a positive $p(\mathbf{k},\mathbf{k}')$ and, while it is not certain whether or not this effect can occur for admissible values of the parameters, it will at best be considerably less marked than for the values shown.

(iii) Two quite different sets of values of λ, μ, ν may produce anisotropy curves which lie close together over a large part of the range of s_4; for example, those for $\mu=10$, $\lambda=12$, $\nu=-12$, and $\mu=1$, $\lambda=6$, $\nu=-6$ shown in Fig. 3. The *relative* anisotropy curves for these values, however, (the broken curves *a* and *c*, respectively, in Fig. 1) are quite distinct. This shows that it is important to employ a suitable type of analysis of experimental data.

(iv) Although the form of the anisotropy curves in Fig. 3 seems to bear no simple relation to the values of the parameters, the relative anisotropy curves obey the rule that, for a given μ, all curves with λ, $\nu\neq0$ fall below that with $\lambda=\nu=0$ (and are, for admissible values of λ and ν, quite close to the latter). In view of the regular variation with μ when $\lambda=\nu=0$, this shows that one could use an experimental curve of relative anisotopy to set a lower bound on μ.

5. THE RELAXATION-TIME APPROXIMATION

When the collision term in the Boltzmann equation (2.1) reduces to the form $g(\mathbf{k})/\tau(\mathbf{k})$, we say that a relaxation time $\tau(\mathbf{k})$ exists. For spherical Fermi surfaces, it is well known[16] that an isotropic relaxation

[16] See Ref. 3, p. 268.

time exists whenever $p(\mathbf{k},\mathbf{k}')$ only depends on the angle θ between $\mathbf{k}$ and $\mathbf{k}'$, and is given by

$$\frac{1}{\tau}=\int(1-\cos\theta)p(\mathbf{k},\mathbf{k}')\frac{dS'}{\hbar v'}; \tag{5.1}$$

in this case there is no magnetoresistance effect. More generally, a $\mathbf{k}$-dependent relaxation time exists whenever $p_1(\mathbf{k},\mathbf{k}')=0$ and is given by

$$\frac{1}{\tau(\mathbf{k})}=P_0(\mathbf{k})=\int p_0(\mathbf{k},\mathbf{k}')\frac{dS'}{\hbar v'}; \tag{5.2}$$

an example of this is the case $\mu\neq 0$, $\nu=\lambda=0$ studied in Sec. 4, where (see Appendix C)

$$1/\tau=(4\pi m k_0 L/\hbar^2)\{1+\mu(\kappa_x{}^4+\kappa_y{}^4+\kappa_z{}^4)\}. \tag{5.3}$$

If, following Ziman,[5] we assume that we can use a relaxation time given by (5.1) for arbitrary $p(\mathbf{k},\mathbf{k}')$, we obtain, on substituting (3.4) into (5.1), an expression for τ of the same form as (5.3), but with L and μ replaced by L' and μ', where

$$L'=L(1-\tfrac{1}{3}\lambda-\tfrac{1}{5}\nu),\quad \mu'=(\mu-\tfrac{1}{3}\nu)/(1-\tfrac{1}{3}\lambda-\tfrac{1}{5}\nu). \tag{5.4}$$

With this assumption, therefore, the anisotropy of ρ_∞ is obtained by putting $\lambda=\nu=0$, and replacing μ by μ' in Eq. (3.9), so that the results are given by the curves of Figs. 1 and 2 if the parameters are reinterpreted appropriately. For example, the sets of values $\mu=-15$, $\lambda=0$, $\nu=-30$, and $\mu=0$, $\lambda=6$, $\nu=-6$ in Fig. 3 correspond to $\mu'=-5/7$ and $\mu'=10$, respectively, but the curves are quite different from those for $\mu=-5/7$ and $\mu=10$ in Fig. 2. The curve $\mu=-15$, $\lambda=15$, $\nu=-15$ in Fig. 3, however, also corresponds to $\mu'=10$, and is similar to the $\mu=10$ curve in Fig. 2, as is corroborated by the relative anisotropy curve shown in Fig. 1—the broken curve b. This set of values of λ, μ, ν comes much closer to being realizable with $p(\mathbf{k},\mathbf{k}')\geqslant 0$ than the other two sets, though all three are not in fact allowed, and it is likely that the relaxation-time approximation is in fact quite good for permissible values of λ, μ, ν, though it differs from the exact theory in giving no anisotropy whenever $\nu=3\mu$.

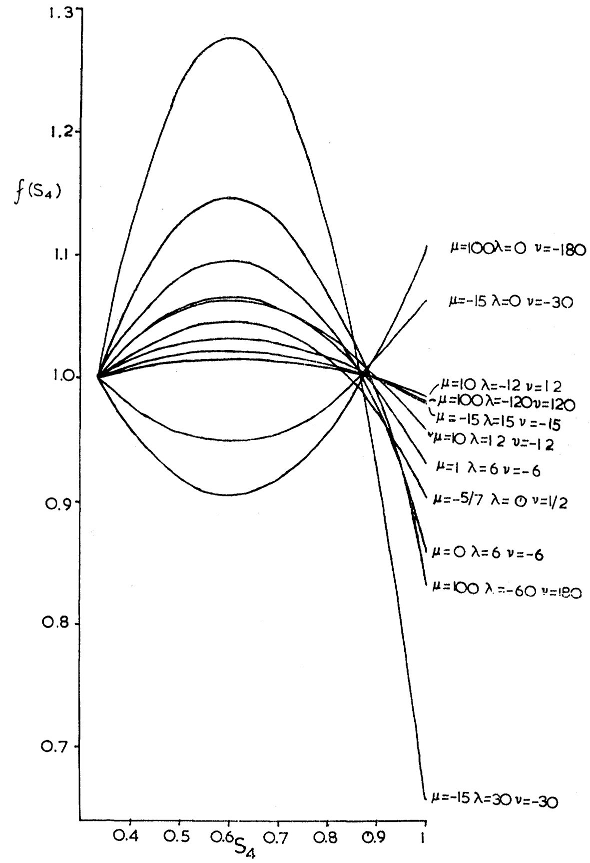

FIG. 3. Longitudinal magnetoresistance anisotropy with $\lambda,\nu\neq 0$.

6. CONCLUDING REMARKS

The discussion given here shows that, already, with isotropic energy surfaces and minimum assumptions as to the form of the scattering probability, the anisotropy of the longitudinal magnetoresistance can show a considerable variety of behavior. While measurements of this effect by themselves cannot lead to a unique determination of the individual coefficients in the expression for $p(\mathbf{k},\mathbf{k}')$, it should be possible, with adequate data, to place drastic limits on the possible forms of this function. In a later paper we hope to study the extent to which a fuller knowledge of the components of the magnetoresistance tensor can lead to a more complete determination of $p(\mathbf{k},\mathbf{k}')$.

To our knowledge there are, at present, no measurements on single crystals of the alkali metals which could be compared with the present theory. The practical difficulties are to prepare sufficiently good and pure specimens, and to obtain magnetic fields large enough to ensure that saturation values of ρ are measured. A theoretical difficulty in using the present theory to analyze magnetoresistance data comes from the magnetoresistive effects which arise from nonsphericity of the Fermi surface, and which, if appreciable, could largely mask the effects of interest here. Nevertheless, it seems reasonable to conclude that measurements of high-field magnetoresistance in the alkalis could give some insight into the form of the electron-scattering processes.

ACKNOWLEDGMENTS

We wish to thank Professor R. G. Chambers for a useful discussion. Part of this work was supported by a grant from the Science Research Council.

APPENDIX A: PROOF THAT VARIOUS MATRICES ARE NONSINGULAR

Consider the inequality

$$\int\int\{\lambda(M+P_0)^{-1}\phi+\mu(M'+P_0')^{-1}\phi'\}^2 \times p(\mathbf{k},\mathbf{k}')\frac{dS}{\hbar v}\frac{dS'}{\hbar v'}>0. \quad \text{(A1)}$$

If ϕ does not vanish identically, this holds for all real λ and μ, such that $\lambda^2+\mu^2\neq 0$, since $p(\mathbf{k},\mathbf{k}')\geqslant 0$, and is nonzero over a finite part of the energy surface. If ϕ is an odd function of $\mathbf{k}$, (A1) is equivalent to

$$\int P_0\{(M+P_0)^{-1}\phi\}^2\frac{dS}{\hbar v}+\nu\int\int\{(M+P_0)^{-1}\phi\} \times\{(M'+P_0')^{-1}\phi'\}p_1(\mathbf{k},\mathbf{k}')\frac{dS}{\hbar v}\frac{dS'}{\hbar v'}>0, \quad \text{(A2)}$$

where $-1\leqslant\nu=2\lambda\mu/(\lambda^2+\mu^2)\leqslant 1$. Now,

$$\begin{aligned}\int[\phi(M+P_0)^{-1}\phi-P_0\{(M+P_0)^{-1}\phi\}^2]\frac{dS}{\hbar v} &=\int\{M(M+P_0)^{-1}\phi\}(M+P_0)^{-1}\phi\frac{dS}{\hbar v}\\ &=-\frac{1}{2}\frac{e}{\hbar c}\int \mathbf{v}\times\mathbf{H}\cdot\frac{\partial}{\partial\mathbf{k}}\{(M+P_0)^{-1}\phi\}^2\frac{dS}{\hbar v}\\ &=\frac{1}{2}\frac{e}{\hbar^2 c}\int d\mathbf{S}\cdot\frac{\partial}{\partial\mathbf{k}}\times[\mathbf{H}\{(M+P_0)^{-1}\phi\}^2], \quad \text{(A3)}\end{aligned}$$

since $d\mathbf{S}=\mathbf{v}dS/v$. For a closed surface, the right-hand side of (A3) vanishes by Stokes's theorem, and if the energy surface intersects the Brillouin-zone boundary, the right-hand side of (A3) again vanishes, since ϕ is periodic in the reciprocal lattice. Thus (A2) can be written

$$\int\phi(M+P_0)^{-1}\phi\frac{dS}{\hbar v}+\nu\int\int\{(M+P_0)^{-1}\phi\} \times\{(M'+P_0')^{-1}\phi'\}p_1(\mathbf{k},\mathbf{k}')\frac{dS}{\hbar v}\frac{dS'}{\hbar v'}>0. \quad \text{(A4)}$$

Putting

$$\phi=\sum_{i=1}^{N} y_i q_i(\mathbf{k})=\langle y|q\rangle, \quad \text{(A5)}$$

(A4) gives

$$\langle y|A+\nu A^T BA|y\rangle>0, \quad \text{(A6)}$$

so long as the q_i's are independent, where A^T is the transposed matrix. Hence $A+\nu A^TBA$ is positive-definite, and in particular A is positive-definite. Hence $A(A^{-1})^T(A^T+\nu A^TBA)A^{-1}$ is also positive-definite, and for $\nu=-1$ this is $I-AB$, which is therefore nonsingular. Similarly, putting $\phi=\mathbf{x}\cdot\mathbf{v}$, $\nu=0$, it follows that $\hat{s}$ is positive-definite, and so, therefore, is $\hat{r}=\hat{s}^{-1}$.

In order to show $I-AB+|\mathbf{W}\rangle\cdot\hat{r}\cdot\langle\mathbf{S}|B$ nonsingular, it is convenient to separate from $p_1(\mathbf{k},\mathbf{k}')$ its dependence on $\mathbf{v}$, and to write, instead of (2.5),

$$p_1(\mathbf{k},\mathbf{k}')=\mathbf{v}\cdot\hat{\alpha}\cdot\mathbf{v}'+\mathbf{v}\cdot\langle\boldsymbol{\beta}|q_0'\rangle +\langle q_0|\boldsymbol{\beta}\rangle\cdot\mathbf{v}'+\langle q_0|B_0|q_0'\rangle, \quad \text{(A7)}$$

where $\mathbf{x}\cdot\mathbf{v}+\langle y|q_0\rangle=0$ implies both $\mathbf{x}=0$ and $\langle y|=\langle 0|$. Then, putting $\phi=\langle y|q_0\rangle-\langle y|\mathbf{S}_0\rangle\cdot\hat{r}^T\cdot\mathbf{v}$ in (A4), we have, instead of (A6),

$$\langle y|D_0+\nu D_0{}^TB_0D_0|y\rangle>0, \quad \text{(A8)}$$

where $D_0=A_0-|\mathbf{W}_0\rangle\cdot\hat{r}\cdot\langle\mathbf{S}_0|$, and A_0, $|\mathbf{W}_0\rangle$ and $\langle\mathbf{S}_0|$ are given by Eqs. (2.11) and (2.17), with $\langle q_0|$ in place of $\langle q|$. We conclude, as before, that $D_0+\nu D_0{}^TB_0D_0$, and in particular D_0, are positive-definite, and so, therefore, is $I-D_0B_0$. Now, if $D=A-|\mathbf{W}\rangle\cdot\hat{r}\cdot\langle\mathbf{S}|$, the determinants of $I-D_0B_0$ and $I-DB$ are equal; hence $I-DB$ is nonsingular.

APPENDIX B: ASYMPTOTIC FORM OF LONGITUDINAL MAGNETORESISTANCE

Let $\hat{T}$ be any matrix of the form

$$\hat{T}=\int\mathbf{p}(\mathbf{k})(M+P_0)^{-1}\mathbf{q}(\mathbf{k})\frac{dS}{\hbar v}, \quad \text{(B1)}$$

where the integral is over a closed surface in $\mathbf{k}$ space. For an element $T_{\alpha\beta}$ of $\hat{T}$ we have, using (3.2) and the periodicity in ϕ of $(M+P_0)^{-1}q_\alpha$,

$$\begin{aligned}T_{\alpha\beta}&=\frac{1}{\omega_c}\int p_\alpha(\mathbf{k})\frac{dS}{\hbar v}\int_{-\infty}^{\phi}q_\beta(\phi')\exp\left\{\frac{1}{\omega_c}\int_{\phi}^{\phi'}P_0(\phi'')d\phi''\right\}d\phi'\\ &=\frac{1}{\omega_c}\int p_\alpha(\mathbf{k})\frac{dS}{\hbar v}\frac{\displaystyle\int_{\phi}^{\phi+2\pi}q_\beta(\phi')\exp\left\{\frac{1}{\omega_c}\int_{\phi}^{\phi'}P_0(\phi'')d\phi''\right\}d\phi'}{\exp(2\pi\bar{P}_0/\omega_c)-1}, \quad \text{(B2)}\end{aligned}$$

where

$$\bar{P}_0=\frac{1}{2\pi}\int_0^{2\pi}P_0(\phi)d\phi \quad \text{(B3)}$$

denotes the average value of $P_0(\mathbf{k})$ around the orbit considered. If Oa, Ob, and Oh are Cartesian axes with Oh parallel to $\mathbf{H}$, the component k_h of $\mathbf{k}$ parallel to $\mathbf{H}$ is constant for a particular orbit, and we have[17]

$$dS/\hbar v=(m^*/\hbar^2)dk_h d\phi\,, \tag{B4}$$

where m^* is the cyclotron mass. Hence, expanding (B2) in powers of $1/\omega_c$ and keeping only the leading term, we obtain

$$\lim_{H\to\infty} T_{\alpha\beta}=\int p_\alpha \frac{\bar{q}_\beta}{\bar{P}_0}\frac{dS}{\hbar v}=\frac{2\pi}{\hbar^2}\int \frac{m^*\bar{p}_\alpha\bar{q}_\beta}{\bar{P}_0}dk_h\,, \tag{B5}$$

where the bars denote orbit averages as in (B3). Thus, as $H\to\infty$, $T_{\alpha\beta}$ tends to a constant limit provided that $\bar{p}_\alpha$ and $\bar{q}_\beta$ are both nonzero. However, if $\bar{p}_\alpha$ or $\bar{q}_\beta$ vanishes, $T_{\alpha\beta}\to 0$ as $H\to\infty$, and, to obtain the leading term in $T_{\alpha\beta}$ for large H, it is necessary to keep higher-order terms in the expansion of (B2). In particular, if α denotes any direction perpendicular to $\mathbf{H}$, $\bar{v}_\alpha=0$. It is now easy to determine the asymptotic form of the matrices $\hat{r}=\hat{s}^{-1}$, $\hat{S}$, $\hat{W}$, and $\hat{A}$ defined by Eqs. (2.14) and (2.21), using the same arguments as in the theory of Lifshitz, Azbel', and Kaganov.[15] It is found that, referring to the coordinate system $Oabh$ introduced above, the limiting form of $\hat{s}$ is

$$\hat{s}=\begin{bmatrix} A/H^2 & B/H & C/H \\ -B/H & D/H^2 & E/H \\ -C/H & -E/H & F \end{bmatrix}, \tag{B6}$$

where A, B, C, D, E, and F are constants. Inverting this, it follows that the components of $\hat{r}$ are all of order 1 in H, except for the Hall components r_{ab} and r_{ba} which are of order H. Further, the components $S_{\alpha\beta}$ of $\hat{S}$ are of order $1/H$, except for $\alpha=h$, when they are of order 1; the components $W_{\alpha\beta}$ of $\hat{W}$ are of order $1/H$, except for $\beta=h$, when they are of order 1; and the components of $\hat{A}$ are all of order 1. The asymptotic form of $\hat{\sigma}$ obtained from these results is the same as Eq. (B6), which is the expression obtained when a time of relaxation is assumed to exist; both are in agreement with the general arguments of Lifshitz *et al.*[15] The quantity ρ_∞ in Sec. 3 is the high-field limit of $\mathbf{H}\cdot\hat{\rho}\cdot\mathbf{H}/H^2=\rho_{hh}$, and, on writing down this component of (2.25) and discarding all terms which are zero in the limit $H\to\infty$, Eq. (3.8) is obtained.

APPENDIX C: EVALUATION OF INTEGRALS FOR A SPHERICAL FERMI SURFACE

If $\hat{T}$ is given by (B1), and T_∞ is defined as in (3.5), we have from (B5), introducing spherical polar coordinates k_0, θ, and ϕ on the Fermi sphere with polar axis along $\mathbf{H}$,

$$T_\infty=\frac{2\pi mk_0}{\hbar^2}\int_0^\pi \frac{\bar{p}_h q_h}{\bar{P}_0}\sin\theta d\theta\,, \tag{C1}$$

[17] See Ref. 3, p. 517.

where p_h and q_h are the components of $\mathbf{p}$ and $\mathbf{q}$ parallel to $\mathbf{H}$.

The mean values required in the evaluation of s_∞, S_∞, W_∞, and A_∞ are $\bar{v}_h=(\hbar k_0/m)\bar{\kappa}_h$, u_h and $\bar{P}_0$, where $\mathbf{u}$ is given by (3.7) and where, using (2.4) and (3.4) and performing the elementary integrations over the Fermi sphere,

$$P_0=(4\pi mk_0/\hbar^2)L\{1+\mu(\kappa_x^4+\kappa_y^4+\kappa_z^4)\}\,, \tag{C2}$$

with

$$L=a_0+\tfrac{3}{5}a_4+\tfrac{1}{3}b_4, \quad\text{and}\quad \mu=a_4/L. \tag{C3}$$

If $\mathbf{p}$ is any vector with components $p_\alpha(\alpha=x,\,y,\,z)$ relative to the cubic axes, and if $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{h}$ are orthogonal unit vectors with $\mathbf{h}$ parallel to $\mathbf{H}$, we have

$$p_h=\mathbf{p}\cdot\mathbf{h}=\sum_\alpha p_\alpha h_\alpha;$$

hence $\bar{\kappa}_h$, u_h, and $\bar{P}_0$ can immediately be obtained from the formula

$$\langle\kappa_\alpha^n\rangle_{\rm av}=\frac{1}{2\pi}\int_0^{2\pi}(a_\alpha\cos\phi\sin\theta+b_\alpha\sin\phi\sin\theta+h_\alpha\cos\theta)^n d\phi$$
$$=\sum_{r=0}^{n/2}\frac{n!}{(n-2r)!2^{2r}(r!)^2}\times h_\alpha^{n-2r}(1-h_\alpha^2)^r\cos^{n-2r}\theta\sin^{2r}\theta\,, \tag{C4}$$

where $[\frac{1}{2}n]$ denotes the integral part of $\frac{1}{2}n$. We obtain

$$\bar{\kappa}_h=\cos\theta\,, \tag{C5}$$

$$\bar{u}_h=\tfrac{3}{2}\cos\theta(1-s_4)-\cos^3\theta(\tfrac{3}{2}-\tfrac{5}{2}s_4)\,, \tag{C6}$$

$$\bar{P}_0=\frac{4\pi mk_0}{\hbar^2}L\left[1+\mu\left\{\frac{3}{8}(1+s_4)+\cos^2\theta\left(\frac{9}{4}-\frac{15}{4}s_4\right)-\cos^4\theta\left(\frac{21}{8}-\frac{35}{8}s_4\right)\right\}\right], \tag{C7}$$

where

$$s_4=\sum_\alpha h_\alpha^4. \tag{C8}$$

Hence, from (2.14), (2.21), (B6), and (C1),

$$s_\infty=r_\infty^{-1}=\frac{e^2v_0^2}{4\pi^3L}I_1(\mu,s_4)\,, \tag{C9}$$

$$S_\infty=\frac{e^2}{4\pi^3}W_\infty=\frac{e^2v_0}{4\pi^3L}I_2(\mu,s_4)\,, \tag{C10}$$

$$A_\infty=(1/L)I_3(\mu,s_4)\,, \tag{C11}$$

where $v_0 = \hbar k_0/m$, and

$$I_1 = \int_0^1 \frac{x^2 dx}{1+\mu\{\frac{3}{8}(1+s_4)+x^2(9/4-(15/4)s_4)-x^4(21/8-(35/8)s_4)\}}, \quad \text{(C12)}$$

$$I_2 = \int_0^1 \frac{\frac{3}{2}x^2(1-s_4)-x^4(\frac{3}{2}-\frac{5}{2}s_4)}{1+\mu\{\frac{3}{8}(1+s_4)+x^2(9/4-(15/4)s_4)-x^4(21/8-(35/8)s_4)\}}dx, \quad \text{(C13)}$$

$$I_3 = \int_0^1 \frac{(9/4)x^2(1-s_4)^2-3x^4(1-s_4)(\frac{3}{2}-\frac{5}{2}s_4)+x^6(\frac{3}{2}-\frac{5}{2}s_4)^2}{1+\mu\{\frac{3}{8}(1+s_4)+x^2(9/4-(15/4)s_4)-x^4(21/8-(35/8)s_4)\}}dx. \quad \text{(C14)}$$

These integrals can be evaluated explicitly in terms of elementary functions, but for general values of μ and s_4 the resulting expressions are cumbersome and in practice it is simpler to evaluate the integrals by direct numerical integration.

APPENDIX D: SOME RESTRICTIONS ON THE COEFFICIENTS IN $p(\mathbf{k},\mathbf{k}')$

The transition probability (3.4) must be non-negative for all values of the variables κ_α and κ_α'. Consider the special cases

$$(\kappa_x,\kappa_y,\kappa_z)=(1,0,0,), \quad (\kappa_x',\kappa_y',\kappa_z')=\pm(1,0,0), \quad \text{(D1)}$$

$$(\kappa_x,\kappa_y,\kappa_z)=(1,0,0), \quad (\kappa_x',\kappa_y',\kappa_z')=(0,1,0), \quad \text{(D2)}$$

$$(\kappa_x,\kappa_y,\kappa_z)=\left(\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}},0\right), \quad (\kappa_x',\kappa_y',\kappa_z')=\pm\left(\frac{1}{\sqrt{2}},0,\frac{1}{\sqrt{2}}\right), \quad \text{(D3)}$$

$$(\kappa_x,\kappa_y,\kappa_z)=\left(\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}},0\right), \quad (\kappa_x',\kappa_y',\kappa_z')=\pm\left(\frac{1}{\sqrt{2}},-\frac{1}{\sqrt{2}},0\right), \quad \text{(D4)}$$

$$(\kappa_x,\kappa_y,\kappa_z)=\left(\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}}\right), \quad (\kappa_x',\kappa_y',\kappa_z')=\pm\left(\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}}\right), \quad \text{(D5)}$$

$$(\kappa_x,\kappa_y,\kappa_z)=\left(\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}}\right), \quad (\kappa_x',\kappa_y',\kappa_z')=\pm\left(\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}},-\frac{1}{\sqrt{3}}\right). \quad \text{(D6)}$$

Substituting these values into (3.4), we obtain the conditions

$$a_0+2a_4+b_4\pm(c_2+2c_4)\geqslant 0, \quad \text{(D7)}$$

$$a_0+2a_4\geqslant 0, \quad \text{(D8)}$$

$$a_0+a_4+\tfrac{1}{4}b_4\pm\tfrac{1}{2}(c_2+c_4)\geqslant 0, \quad \text{(D9)}$$

$$a_0+a_4+\tfrac{1}{2}b_4-\tfrac{1}{4}e_4\geqslant 0, \quad \text{(D10)}$$

$$a_0+\tfrac{2}{3}a_4+\tfrac{1}{3}b_4+\tfrac{1}{3}e_4\pm\tfrac{1}{3}(3c_2+2c_4)\geqslant 0, \quad \text{(D11)}$$

$$a_0+\tfrac{2}{3}a_4+\tfrac{1}{3}b_4-\tfrac{1}{9}e_4\pm\tfrac{1}{9}(3c_2+2c_4)\geqslant 0, \quad \text{(D12)}$$

or, with $L=a_0+\frac{3}{5}a_4+\frac{1}{3}b_4$,

$$L\{1+(7/5)\mu+\tfrac{2}{3}\sigma\pm(\lambda+2\nu)\}\geqslant 0, \quad \text{(D13)}$$

$$L\{1+(7/5)\mu-\tfrac{1}{3}\sigma\}\geqslant 0, \quad \text{(D14)}$$

$$L\{1+\tfrac{2}{5}\mu-\tfrac{1}{12}\sigma\pm\tfrac{1}{2}(\lambda+\nu)\}\geqslant 0, \quad \text{(D15)}$$

$$L\{1+\tfrac{2}{5}\mu+\tfrac{1}{6}\sigma-\tfrac{1}{4}\tau\}\geqslant 0, \quad \text{(D16)}$$

$$L\{1+(1/15)\mu+\tfrac{1}{3}\tau\pm\tfrac{1}{3}(3\lambda+2\nu)\}\geqslant 0, \quad \text{(D17)}$$

$$L\{1+(1/15)\mu-\tfrac{1}{9}\tau\pm\tfrac{1}{9}(3\lambda+2\nu)\}\geqslant 0, \quad \text{(D18)}$$

where λ, ν, μ are given by (3.10) and

$$\sigma=b_4/L, \quad \tau=e_4/L. \quad \text{(D19)}$$

Equation (D13) implies that

$$L(1+(7/5)\mu+\tfrac{2}{3}\sigma)\geqslant 0,$$

and this, together with (D14), gives

$$L(1+(7/5)\mu)\geqslant 0. \quad \text{(D20)}$$

Also, if (D17) and (D18) are to be simultaneously satisfied,

$$L(1+(1/15)\mu)\geqslant 0. \quad \text{(D21)}$$

It follows from (D20) and (D21) that μ cannot lie in the interval $(-15, -5/7)$.