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On the Use of Variational Methods for Solving Boltzmann Equations Involving Non-Hermitian Operators

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Variational principles yielding upper and lower bounds on transport coefficients can readily be applied to the Boltzmann equation, provided it has the form of a linear, inhomogeneous integrodifferential equation with a Hermitian operator acting on the deviation from equilibrium of the distribution function. In transport problems involving a magnetic field or an alternating electric field, this operator is non-Hermitian. By suitably transforming the transport equation, we show how variational principles may still give upper and lower bounds. The bounds are used for considering the frequency-dependent conductivity associated with a general scattering operator, and the longitudinal magnetoresistivity in the relaxation time approximation for the scattering operator. Explicit results are presented for (1) the frequency-dependent conductivity of a charged Fermi liquid and (2) the longitudinal magnetoresistivity for a weakly anisotropic Fermi surface.

KEY WORDS: Boltzmann equation; variational principles; upper and lower bounds; transport coefficient; Fermi liquid; frequency-dependent conductivity; magnetoresistivity; Fermi surface.

1. INTRODUCTION

It is well known that the Boltzmann equation in general is a complicated integrodifferential equation which cannot be solved directly for the distribution function. One frequently resorts to the use of a variational principle first introduced in transport theory by Kohler (see Ziman[1]). If the operator acting on the deviation from equilibrium is Hermitian and positive, this principle yields a lower bound on such transport coefficients as electrical and thermal conductivity.

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Recently, Jensen *et al.*[2] discussed various other bounds on such transport coefficients and demonstrated how a variety of lower and upper bounds may be generated starting from Kohler's lower bound. The operator in the Boltzmann equation was there also assumed to be Hermitian and positive.

In the present work, we devote our attention to the existence and use of upper and lower bounds in situations where the operator in the Boltzmann equation is *not* Hermitian. Such situations cover a range of physically interesting problems, like transport in the presence of a magnetic field or an alternating electric field.

It has been shown by several authors[1,3–6] that Kohler's variational principle can be generalized to such cases, but although the variational functional is stationary at the exact solution, it has in general neither a minimum nor a maximum, and therefore the method does not provide bounds on the transport coefficient. Bailyn[6] studied the case with a magnetic field present and obtained a variational principle giving a lower bound on that part of the conductivity tensor that is even in the magnetic field.

In the present paper, we consider a quite general Boltzmann equation with a non-Hermitian operator and show that it is possible to obtain variational principles giving both lower *and* upper bounds on certain quantities related to the transport coefficients of interest (Section 2).

Various choices of trial functions give upper and lower bounds on the frequency-dependent conductivity associated with a general scattering operator. The bounds can also be used for calculating the (longitudinal) magnetoresistivity of a metal, in which the scattering of electrons can be described by a relaxation time (Section 3). The frequency-dependent conductivity of a charged Fermi liquid, in which collisions between the quasiparticles themselves determine the scattering operator, is considered in Section 4, and it is shown that the upper and lower bounds determine the exact conductivity very well. Finally, bounds are calculated for the longitudinal magnetoresistivity of a metal with a weakly anisotropic Fermi surface (Section 5). Here, the upper and lower bounds turn out to be identical at all values of the magnetic field to second order in the anisotropy parameters.

2. THE VARIATIONAL PRINCIPLES

Our concern in the present paper is with the solution of linear, inhomogeneous integrodifferential equations which we symbolically write as

$$HQ = X \tag{1}$$

Here, Q is an unknown function of a variable vector $\mathbf{k}$, X is the inhomogeneous term, and H a linear integrodifferential operator. The physical application we shall have in mind is the calculation of transport coefficients from a linearized Boltzmann equation. Rather than seeking the exact solution Q of (1), we are therefore interested in a certain scalar product of Q and X denoted by

$$T = (Q^*, X) \tag{2}$$

In the application to the Boltzmann equation, the scalar product is the transport coefficient associated with the driving term X.

The convention we use for a scalar product of two functions $U(\mathbf{k})$ and $V(\mathbf{k})$ is

$$(U^*, V) = \int d\mathbf{k}\, U^*(\mathbf{k})\, V(\mathbf{k})\, w(\mathbf{k}) \tag{3}$$

where $w(\mathbf{k})$ is a real, positive weight factor to be specified in each case.

It is well known (see Ziman[1]) that if H is Hermitian, that is, if $(U^*, HV) = (V^*, HU)^*$, and also positive in the sense of having only nonnegative eigenvalues, then T may be bounded from below according to

$$T = (Q^*, X) \geqslant [\mathrm{Re}(U^*, X)]^2/(U^*, HU) \tag{4}$$

Here, U is an arbitrary trial function.

If was shown by Jensen *et al.*[3] that if H can be separated into two positive Hermitian operators J and L, i.e.,

$$H = J + L \tag{5}$$

then T may be bounded from above as well, provided either J or L has an inverse. If, say, J^{-1} exists, this upper bound is

$$T = (Q^*, X) \leqslant (X^*, J^{-1}X) - \frac{\{\mathrm{Re}[U^*, (HJ^{-1} - 1)X]\}^2}{(U^*, (HJ^{-1} - 1)\, HU)} \tag{6}$$

In the work of Jensen *et al.*,[2] the attention was confined to real and symmetrical operators H as well as real X, but the extension to (4) and (6) is straightforward.

We shall now show how we may obtain bounds on the scalar product T if H is non-Hermitian. We first observe that the linear operator H can always be written as the sum of a Hermitian part G and an anti-Hermitian part A. The fundamental equation (1) becomes therefore

$$(G + A)Q = X \tag{7}$$

We now define Q^+ by the equation

$$(G - A)Q^+ = X \tag{8}$$

and introduce the functions

$$f = (1/2)(Q + Q^+), \qquad g = (1/2i)(Q - Q^+) \tag{9}$$

By adding and subtracting (7) and (8), we get two equations for f and g, from which we can eliminate g if G^{-1} exists. The result is a single equation for f,[2]

$$(G + iAG^{-1}iA)f = X \tag{10}$$

[2] Such an equation has previously been derived by Bailyn.[6] See his Eq. (3.1b).

Similarly, if A^{-1} exists, we can obtain an equation for g:

$$[iA + G(iA)^{-1}G]g = X \tag{11}$$

From (10), we can get lower and upper bounds on the real quantity $(f^*, X) = \mathrm{Re}(Q^*, X)$, provided G is positive. The positiveness of G and the existence of G^{-1} ensures that the operator acting on f is the sum of two Hermitian, positive operators, in which case (4) and (6) apply. (In order to prove that $iAG^{-1}iA$ is positive, we only use that A is anti-Hermitian together with the fact that G^{-1} is positive when G is).

In the same manner, we can obtain lower and upper bounds on the real quantity $(g^*, X) = \mathrm{Im}(Q^*, X)$, provided iA is positive and possesses an inverse.

3. APPLICATION OF THE VARIATIONAL PRINCIPLES

The general variational principles discussed in the previous section are now applied to the calculation of transport coefficients arising from a linearized Boltzmann equation. We shall identify the Hermitian and positive collision operator with the Hermitian part G of the total operator that acts on the deviation from equilibrium Q. The anti-Hermitian part A is due to a magnetic field or an alternating electric field in the examples below. The usefulness of the bounds (4) and (6) obviously depends upon whether G or A (or both) may be inverted in practice.

We have studied two types of problems with the aid of the variational methods. In the present section, we discuss these in a general framework, whereas the next two sections contain specific applications.

3.1. Frequency-Dependent Conductivity

The first type of transport coefficient is the frequency-dependent conductivity in the region where the photon energy $\hbar\omega$ is much less than kT, i.e., Boltzmann's constant times the temperature. The Boltzmann equation is

$$(G + i\omega)Q = X \tag{12}$$

Here, G is the collision operator, Q the deviation from equilibrium of the distribution function, and X is the driving term, which is proportional to the component of the velocity of a charge carrier along the direction of the electric field. The $i\omega$ term in (12) comes from the partial time derivative $\partial/\partial t$ in the Boltzmann equation.

The form of the Boltzmann equation (12) is restricted in two respects: (a) The collision integral is assumed not to depend explicitly on the frequency of the electric field. This is correct if the photon energy is much less than a typical energy transfer in a collision, i.e., $\hbar\omega \ll kT$. In the case $\hbar\omega \gtrsim kT$, the collision integral should be modified[7] in order to account for energy conservation in emission and absorption of photons during a collision. (b) Spatial homogeneity is assumed throughout. For electrons in a metal, this requires that we consider only long-wavelength disturbances satisfying $q \ll \omega/v_F$, where q is a characteristic wave vector and v_F is the

Fermi velocity. In that case, we may neglect the term in the Boltzmann equation that takes into account spatial variation.

For simplicity, we assume in the following that G and X are real.

From (7) and (8), we then deduce that $Q^+ = Q^*$, which according to (9) means that

$$f = \operatorname{Re} Q, \qquad g = \operatorname{Im} Q \tag{13}$$

The conductivity can be written as

$$\sigma = (Q^*, X) = \sigma_R + i\sigma_I \tag{14}$$

with the real part

$$\sigma_R = (f, X) \tag{15}$$

and the imaginary part

$$\sigma_I = -(g, X) \tag{16}$$

From (10) and (11) with $A = i\omega$, we obtain bounds on σ_R and σ_I by using (4) and (6). The separation (5) may be done in two different ways. To get upper bounds on σ_R from (10) and (6), we may either identify J with G or with $\omega^2 G^{-1}$, whereas upper bounds on σ_I are obtained from (11) and (6) with the choice $J = \omega$ or $J = \omega^{-1}G^2$.

If we choose our trial functions U among the set of functions $G^n X$ obtained from X by operating with G a total of n times, then the bounds are determined by the matrix elements a_n defined by

$$a_n = (X, G^n X) \tag{17}$$

These matrix elements satisfy a Schwarz inequality

$$a_m a_n \geqslant a^2_{(m+n)/2} \tag{18}$$

since G is positive.

It is advantageous to use trial functions which are variable linear combinations of two functions from the set $G^n X$. For convenience, we write these in the form

$$U = pG^m X + c(1 - p)\, G^n X \tag{19}$$

where p is the variational parameter, while c is a constant introduced in order to facilitate the calculations. In fact, without loss of generality, c can be chosen such that the numerators in (4) and (6) become independent of the variational parameter p. Then, the dependence of (4) and (6) on p is contained solely in the denominators, which become quadratic forms in p and are readily minimized with respect to variation of p to give the maximum lower and minimum upper bounds.

For future use, we state below such upper and lower bounds on σ_R and σ_I together with the trial functions in question. It is convenient to write the lower (upper) bound on σ_R as an upper (lower) bound on $1/\sigma_R$. In order to get the correct asymptotic behaviour of the bounds at high frequencies, we have in all cases used GX as one of

the functions in the linear combination (19), since $f = \omega^{-2}GX$ is the asymptotic solution of (10), when $A = i\omega$. The bounds listed below are not the simplest we can obtain, but they turn out to be the best ones for determining the frequency-dependent conductivity of a Fermi liquid (Section 4). We get, after straightforward algebraic manipulations,

$$\frac{1}{\sigma_R} \leqslant \frac{\omega^2}{a_1} + \frac{a_3}{a_1^2} \frac{\omega^2 + (a_1 b_{21}/a_3 b_{01})}{\omega^2 + [(a_1^3 + a_0^2 a_3 - 2a_0 a_1 a_2)/a_1 b_{01}]} \tag{20}$$

[from (4) with $U = pX + c(1-p)\,GX$ and $c = a_0/a_1$] and

$$\frac{1}{\sigma_R} \geqslant \frac{\omega^2}{a_1} + \frac{a_3}{a_1^2} \frac{\omega^2 + (a_1 b_{32}/a_3 b_{12})}{\omega^2 + (a_{-1} b_{32}/a_1 b_{12})} \tag{21}$$

[from (6) with $U = pG^{-1}X + c(1-p)\,GX$ and $c = a_1/a_3$; we have chosen $J = \omega^2 G^{-1}$).

Here, b_{nm} is defined as

$$b_{nm} = a_{n+m} a_{n-m} - a_n^2 \tag{22}$$

Note that $b_{nm} \geqslant 0$ due to the Schwarz inequality (18). Upon comparison of (10) and (11), it follows that similar bounds on ω/σ_I may be obtained with trial functions constructed from those above by operating with G^{-1}. The prescription for deriving these bounds from (20) and (21) is in fact simply to change a_n to a_{n-1} everywhere (thus, $a_1 \to a_0$ and $b_{21} \to b_{11}$) and replace $1/\sigma_R$ by ω/σ_I .

In specific applications, it may not always be possible to calculate all the matrix elements a_{-2} to a_5 which go into these bounds. In such cases, one might use simpler bounds obtained with $U = G^n X$.

The asymptotic ($\omega \to \infty$) value of the bounds (20) and (21) agree to order ω^0, so

$$1/\sigma_R = (\omega^2/a_1) + (a_3/a_1^2) + O(\omega^{-2}) \tag{23}$$

with a similar expression for ω/σ_I .

If X is an eigenvector of G with eigenvalue $1/\tau$, that is,

$$GX = (1/\tau)X \tag{24}$$

the bounds become equal, since $a_n = \tau^{-n} a_0$ and $b_{nm} = 0$. We then get the Drude–Lorentz result

$$\sigma = \sigma_R + i\sigma_I = a_0\,\tau/(1 - i\omega\tau) \tag{25}$$

Generally, the exact σ_R varies between a_{-1} (which is the dc conductivity obtained from the exact $\omega = 0$ solution $f = G^{-1}X$) and the asymptotic form (23) (note, however, that the condition $\hbar\omega \gg kT$ must always be satisfied). We can write the exact σ_R in the form

$$a_0/\sigma_R = \omega^2 \tau_1 + [1/\tau_2(\omega)] \tag{26}$$

where $\tau_1 = a_0/a_1$, $\tau_2(0) = a_{-1}/a_0$, and $\tau_2(\infty) = a_1^2/a_0 a_3$. It follows from repeated application of the Schwarz inequality (18) that $\tau_2(\infty) \leqslant \tau_1 \leqslant \tau_2(0)$. One can easily

prove that the function $1/\tau_2(\omega)$ is monotonically increasing with increasing ω and has downward curvature when plotted versus ω^2. The latter property follows from consideration of the upper bound on $1/\sigma_R$ obtained from (4) with a trial function equal to the exact solution of (10) at some frequency ω_1. In a plot of $1/\sigma_R$ vs. ω^2 such an upper bound is a straight line tangential to the exact $1/\sigma_R$ at $\omega = \omega_1$. It follows that the exact $1/\sigma_R$ curve must everywhere lie below its tangents and hence curve downward. The Drude–Lorentz result (25) can be characterized in this context as the limiting case $\tau_2(\omega) = \tau_1 = \tau$.

3.2. Longitudinal Magnetoresistivity

The second type of transport coefficient we have considered is the longitudinal magnetoresistivity of a closed, but otherwise arbitrary Fermi surface of electrons. In terms of the magnetoconductivity tensor, this quantity is given by $\rho_{zz} = 1/\sigma_{zz}$, if the electric field **E**, the current density **J**, and the magnetic field **B** all point in the z direction. More generally, bounds can be obtained on the symmetrical part of the magnetoconductivity tensor, but not on the antisymmetrical part (see below).

From the outset, we limit ourselves to the relaxation-time approximation for the scattering operator, i.e., $G = 1/\tau$. The form of the Boltzmann equation is then

$$[(1/\tau) + \omega_c(\partial/\partial\tilde{\varphi})]\, Q = X \tag{27}$$

where the magnetic operator has been given in the well-known form (see Ziman[1]) involving the cyclotron frequency $\omega_c(k_z, \epsilon)$ for an orbit specified by the wave vector component k_z and the energy ϵ, and the phase angle $\tilde{\varphi}$ whose time derivative equals ω_c. The standard definitions of $\tilde{\varphi}$ and ω_c have been employed (see Appendix C). The magnetic operator can be shown to be anti-Hermitian, regardless of whether the Fermi surface is closed or not.

As usual, Q is the deviation from equilibrium and X the (real) driving term proportional to the velocity component along the electric field. We consider electrons in a metal with a closed Fermi surface. Although the exact solution of the Boltzmann equation (27) can be written down formally (see Ziman[1]), the variational method may be helpful for the actual evaluation of the magnetoresistivity, as demonstrated for a particular Fermi surface in Section 5.

In contrast to the previously discussed case of frequency-dependent conductivity, we can only get bounds on the real quantity $(f^*, X) = (f, X)$, since $iA = i\omega_c\, \partial/\partial\tilde{\varphi}$ has both positive and negative eigenvalues. Upon comparing (27) with (8), one observes that $Q^+ = Q(-\mathbf{B})$. The function f defined by (9) is therefore the part of Q that is even in **B**. This means that bounds can be obtained for the symmetrical part of the conductivity tensor only.

It is well known (see Ziman[1]) that the asymptotic ($B \to \infty$) solution of (27) is

$$Q_\infty = \tau\overline{X} = \tau\overline{X}(k_z, \epsilon) \tag{28}$$

where $\overline{X}$ means the average of X over the phase angle $\tilde{\varphi}$ around the orbit. In order to obtain bounds that interpolate between the zero-field resistivity and the asymptotic

value, we use as a trial function the variable linear combination [see the discussion following Eq. (19)]

$$U = pX + c(1 - p)\overline{X} \tag{29}$$

The equation (10) and the bounds (4) and (6) with $J = 1/\tau$ in the latter lead to the following bounds on $\sigma = (f, X)$:

$$\sigma \geqslant \sigma_0 - \frac{\sigma_1(\tau B)^2}{1 + [\sigma_1/(\sigma_0 - \sigma_\infty)](\tau B)^2} \tag{30}$$

and

$$\sigma \leqslant \sigma_0 - \frac{\sigma_1(\tau B)^2}{1 + (\sigma_2/\sigma_1)(\tau B)^2} \tag{31}$$

We have introduced the positive quantities

$$\sigma_n = \tau(-1)^n (X, (\omega_c{}^2 \partial^2/\partial\tilde{\varphi}^2)^n X) B^{-2n} \tag{32}$$

and

$$\sigma_\infty = \tau(\overline{X}, X) = \tau(\overline{X}, \overline{X}) \tag{33}$$

The second equality in (33) follows from the fact that the volume element of integration $d\mathbf{k}$ can be transformed to the product of the inverse of the cyclotron frequency $\omega_c(k_z, \epsilon)$ and $dk_z\, d\epsilon\, d\tilde{\varphi}$. Since the low-field expansion of σ is

$$\sigma = \sigma_0 - \sigma_1(\tau B)^2 + \sigma_2(\tau B)^4 - \sigma_3(\tau B)^6 + \cdots \tag{34}$$

we note that the upper bound (31) is exact to order B^4 and the lower one (30) to order B^2. Both bounds tend to a finite limiting value when $B \to \infty$, the lower bound approaching the exact value σ_∞. The upper bound is independent of the coefficient of $\overline{X}$ in (29) and in general is not exact at high fields. In analogy with the discussion below Eq. (26), we can prove that the exact magnetoresistivity $1/\sigma$ is monotonically increasing with B and has downward curvature when plotted versus B^2.

Upon comparison of the lower and upper bounds (30) and (31), we note that the following inequality must hold:

$$\sigma_2/\sigma_1 \geqslant \sigma_1/(\sigma_0 - \sigma_\infty) \tag{35}$$

Like (18), this is simply a Schwarz inequality which may be derived by considering matrix elements of the form (32) with X replaced by $(X - \overline{X})$. The degree to which (35) is nearly an equality determines how close the bounds (30) and (31) lie to each other and hence to the exact conductivity.

4. FREQUENCY-DEPENDENT CONDUCTIVITY OF A CHARGED FERMI LIQUID

As a specific application of the bounds on the frequency-dependent conductivity discussed in the previous section, we consider here the Boltzmann equation of a charged Fermi liquid at low temperature. The distribution function of the quasi-

particles is assumed to relax toward equilibrium due to collisions between the quasiparticles themselves. The transport equation is given below [Eq. (37)] in reduced form as a one-dimensional integral equation in the (reduced) energy variable

$$s = (\epsilon - \mu)/kT \tag{36}$$

which measures energies from the Fermi energy μ. The essential steps in the reduction of the Boltzmann equation to the form (37) are discussed in Appendix A. The reduced Boltzmann equation is

$$GQ(s) + i\Omega Q(s) = X(s) \tag{37}$$

Here, the unknown $Q(s)$ is related to the deviation from equilibrium of the distribution function by Eq. (A7) of Appendix A. The inhomogeneous term is

$$X(s) = 1/\cosh(s/2) \tag{38}$$

whereas the reduced collision operator G is defined by[2]

$$GQ(s) = (\pi^2 + s^2)\, Q(s) - \alpha \int_{-\infty}^{\infty} \{[(s-u)/2]/\sinh[(s-u)/2]\}\, Q(u)\, du \tag{39}$$

The dimensionless constant Ω is proportional to the frequency ω of the electric field,

$$\Omega = \omega\tau_e \tag{40}$$

where the constant of proportionality τ_e is a characteristic time for the scattering of quasiparticles (electrons) against one another,

$$1/\tau_e = (1 + \tfrac{1}{3}F_1^s)[m^{*3}(kT)^2/16\pi^4\hbar^6]\langle w(\theta, \varphi)/\cos(\theta/2)\rangle \tag{41}$$

Here, the Fermi liquid parameter F_1^s and the effective mass m^* are defined as by Pines and Nozières.[8] The scattering angles θ and φ and the collision probability $w(\theta, \varphi)$ are those of Abrikosov and Khalatnikov.[9] The bracket denotes an angular average.

The dimensionless parameter α occurring in (39) is a ratio of two weighted angular averages of the collision probability $w(\theta, \varphi)$ (see Appendix A for specific examples).

The solution $Q(s)$ of (37) determines a reduced conductivity Σ given by the scalar product

$$\Sigma = (Q^*, X) = \int_{-\infty}^{\infty} Q^*(s)\, X(s)\, ds \tag{42}$$

The actual conductivity σ is shown in Appendix A to be proportional to the complex conjugate Σ^*. It is

$$\sigma = [(ne^2/m_0)\, \tau_e]\, \tfrac{1}{4}\Sigma^* \tag{43}$$

Here, m_0 denotes the optical mass, defined as

$$m_0 = m^*(1 + \tfrac{1}{3}F_1^s)^{-1} \tag{44}$$

In the static limit ($\Omega = 0$), the solution $Q^0(s)$ of (37) when inserted in (42) gives a dc conductivity Σ^0 equal to

$$\Sigma^0 = \frac{1}{3} + \frac{4}{\pi^2}\alpha \sum_{n=1,3,\ldots} \frac{2n+1}{n^2(n+1)^2} \frac{1}{n(n+1) - \alpha} \tag{45}$$

as shown by Jensen *et al.*[10] (see also Brooker and Sykes[11]).

The dc resistivity of a pure, translationally invariant Fermi liquid is of course zero, since the collisions conserve the total momentum of the electrons. This is consistent with the fact that the parameter occurring in (39) is 2 in this case (cf. Appendix A), which results in an infinite Σ^0 according to (45). When the translational invariance is broken in various ways as discussed in Appendix A, the parameter α may be less than 2 and the dc conductivity finite.

The operator G of (39) is positive, real, and symmetrical for $\alpha < 2$, so the bounds on the conductivity derived in Section 3 apply immediately. The matrix elements a_n defined by (17) can be calculated in a straightforward fashion by Fourier transformation of the kernel in (39). They are listed in Appendix B as functions of α.

The bounds on the real part Σ_R of the reduced conductivity Σ are obtained from (20) and (21) by replacing σ_R and ω with Σ_R and Ω, respectively, and using the expressions in Appendix B for the matrix elements a_n. The bounds on the imaginary part are obtained by the similar replacement $(\sigma_I, \omega) \to (\Sigma_I, \Omega)$ in the bounds on ω/σ_I derived according to the prescription below (22). The resulting bounds on Σ are exhibited in Figs. 1 and 2 for the choice $\alpha = 1$. That the upper and lower bounds lie very close is apparent from the blown-up section of Fig. 1.

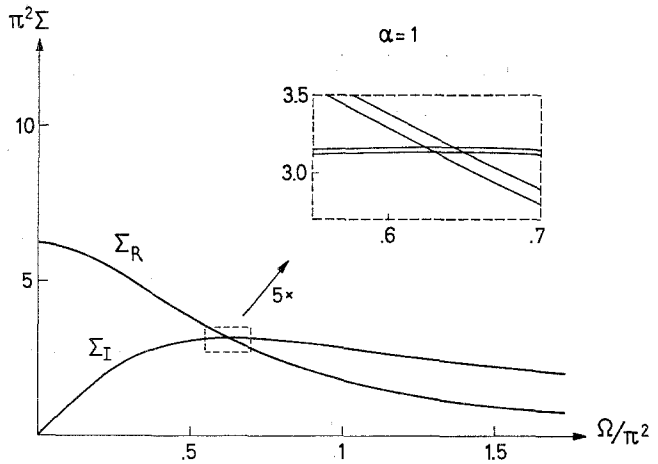

Fig. 1. Each of the curves Σ_R and Σ_I has two close-lying curves, which are our best upper and lower bounds on the real and imaginary parts of the reduced conductivity Σ plotted versus the reduced frequency Ω defined by (40). The parameter α is chosen as 1. To exhibit the bounds, we have blown up a section, which is in the region of maximum relative difference between the upper and lower bounds.

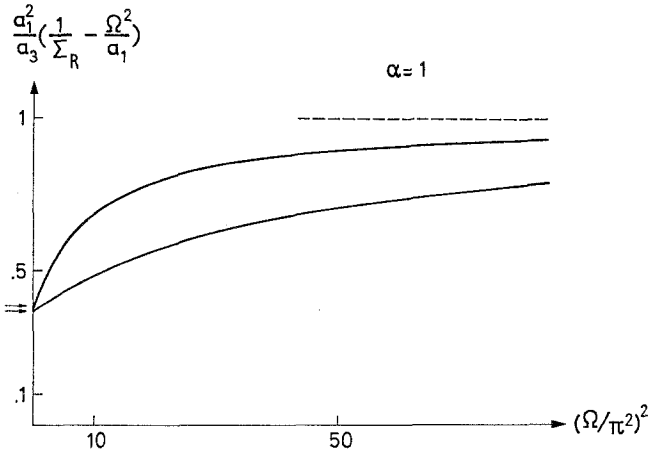

Fig. 2. Upper and lower bounds on the inverse real part after subtraction of the term proportional to Ω^2 [cf. (20) and (21)]. The bounds are normalized so that they tend toward 1 in the limit $\Omega \to \infty$. The Drude–Lorentz form (25) would correspond to a straight horizontal line at the top arrow to the left. The bottom arrow is the exact zero-frequency result. Note that the scale on the abscissa is different in Figs. 1 and 2.

Our final results for the actual conductivity $\sigma = \sigma_R + i\sigma_I$ are given below in a form analogous to (26):

$$\sigma_R = (ne^2/m_0)\{\omega^2\tau_1 + [1/\tau_2(\omega)]\}^{-1} \tag{46}$$

where

$$\begin{aligned} \tau_1 &= \tau_e(3/4\pi^2)[1 - (\alpha/2)]^{-1} \\ \tau_2(0) &= \tau_e(a_{-1})/a_0 \simeq \tau_e\{(1/12) + (3/4\pi^2)[\alpha/(2-\alpha)]\} \\ \tau_2(\infty) &= \tau_e(35/12\pi^2)(8 - 3\alpha)^{-1} \end{aligned} \tag{47}$$

Note that τ_1 and $\tau_2(0)$ become infinite at $\alpha = 2$, whereas $\tau_2(\infty)$ stays finite. The bounds on the variation of $1/\tau_2(\omega)$ with frequency are essentially those exhibited in Fig. 2, since $1/\tau_2(\omega)$ as a function of ω is proportional to the ordinate in Fig. 2, when use is made of (40) in the latter.

Similarly, we get for the imaginary part

$$\sigma_I = -(ne^2/m_0)\{\omega + [1/\omega\tau_e\tau_3(\omega)]\}^{-1} \tag{48}$$

where expressions for the exact values $\tau_3(0)$ and $\tau_3(\infty)$ can be obtained in terms of the a_n of Appendix B. However, in this case, the variation of $\tau_3(\omega)$ with frequency is much less dramatic. When $\alpha \to 2$, both $\tau_3(0)$ and $\tau_3(\infty)$ become infinite. At high frequencies, (48) gives the well-known result $\sigma_I = -ne^2/m_0\omega$ (see Pines and Nozières[8]).

5. LONGITUDINAL MAGNETORESISTIVITY FOR A WEAKLY ANISOTROPIC FERMI SURFACE

Upper and lower bounds on the magnetoresistivity have been derived in Section 3 and are given by (30) and (31). To examine these bounds, we evaluate σ_0, σ_1, σ_2, and σ_∞ defined in (32) and (33) for a metal in which the departure of the Fermi surface from sphericity is not too great. For this purpose, we consider a model Fermi surface in which the modulus of the **k** vector is expanded in terms of spherical harmonics of cubic symmetry as

$$k(\epsilon, \theta, \varphi) = \alpha_0(\epsilon) + \alpha_1(\epsilon)\, Y_4(\cos\theta, \varphi) \tag{49}$$

where α_0 and α_1 are energy-dependent coefficients. Here,

$$Y_4(x, \varphi) = P_4(x) + P_4{}^4(x)(\cos 4\varphi)/168$$

where the P's are Legendre functions, $P_4 = (35x^4 - 30x^2 + 3)/8$, $P_4{}^4 = 105(1 - x^2)^2$. We have included only the two lowest-order harmonics. Note that the maximum value of Y_4 is 1, so that $|\alpha_1(\epsilon)|$ is the maximum perturbation of the sphere $k = \alpha_0(\epsilon)$.

Both σ_0 and σ_1 have been calculated for this case by Davis[12] and our calculation confirms his results. Garcia-Moliner[13] has made use of Davis's calculations to discuss the magnetoresistance of alkali metals. σ_2 has not, to our knowledge, been given for this model. It is only slightly more laborious to obtain. In Appendix C, we indicate how σ_∞ is evaluated, as this does not appear to have been calculated before for this particular model.

We define a scalar product as

$$(f, g) = (1/4\pi^3) \int d\mathbf{k}(-\partial n_0/\partial\epsilon)^{-1} f(\mathbf{k})\, g(\mathbf{k}) \tag{50}$$

where n_0 is the Fermi distribution function. We furthermore define four parameters

$$\begin{aligned} k_F &= \alpha_0(\mu) & 1/\hbar v_F &= \alpha_0'(\mu), \\ R &= \alpha_1(\mu)/\alpha_0(\mu), & S &= \alpha_1'(\mu)/\alpha_0'(\mu), \end{aligned} \tag{51}$$

with prime denoting differentiation with respect to ϵ. Here, μ is the Fermi energy. In terms of these four parameters, we obtain the following results, to quadratic order in R and S:

$$\begin{aligned} \sigma_0 &= (ne^2\tau/m^*)[1 + (4/21)(21R^2 - 2RS + S^2)] \\ \sigma_\infty &= (ne^2\tau/m^*)[1 + (1/231)(879R^2 - 58RS + 39S^2)] \\ \sigma_1(B\tau)^2 &= (ne^2\tau/m^*)(\omega_0\tau)^2\,(80/231)(S - 3R)^2 \\ \sigma_2(B\tau)^4 &= (ne^2\tau/m^*)(\omega_0\tau)^4 16(80/231)(S - 3R)^2 \end{aligned} \tag{52}$$

where $n = k_F{}^3/3\pi^2$, $m^* = \hbar k_F/v_F$, and $\omega_0 = eB/m^*$.

In evaluating the integrals, we have, following Davis, assumed complete degeneracy for the integral over the energy and have neglected third and higher powers of R and S in the binomial expansions. We have found the magnitude of the coefficient of S^3 in σ_0 to be approximately half of that of S^2. Therefore, we believe that the contribution from the higher-order terms are negligible if R and S are of the order of 0.1 or less. This value of R corresponds to a maximum deviation of 10% from sphericity.

We now proceed to discuss the results given in (52). The absence of terms linear in R and S are in accord with the requirement that the magnetoresistivity should always be positive. As a further check on our results, we observe that σ_1 vanishes when $S = 3R$. From (30) and (31), it follows that when σ_1 is zero then $\sigma = \sigma_0$ at all fields, so that $\sigma_0 - \sigma_\infty$ is identically zero. Consequently, $\sigma_0 - \sigma_\infty$ must contain the factor $(S - 3R)$, and furthermore be proportional to $(S - 3R)^2$ to satisfy the requirement of a positive magnetoresistivity. For similar reasons, σ_2 has to be proportional to $(S - 3R)^2$.

With the values (52) put into the inequality (35), the latter turns out to be an equality. This shows that our upper and lower bounds are identical. The reason for this rather surprising result is that the Fourier expansion of the inhomogeneous term X in the phase-angle variable $\tilde{\varphi}$ contains, apart from the constant term $\bar{X}$, only a single Fourier component (to quadratic order in R and S).

From (30), we derive an expression for the relative change in resistivity $(\rho - \rho_0)/\rho_0$, where ρ_0 is the zero-field resistivity, since this is the quantity usually measured in practice. Using (52), we obtain

$$(\rho - \rho_0)/\rho_0 = (5/231)(S - 3R)^2 \{16(\omega_0\tau)^2/[1 + 16(\omega_0\tau)^2]\} \tag{53}$$

We note that the magnetoresistivity saturates when $\omega_0\tau \gtrsim 1$. The saturation value is $\sim 10^{-3}$ when R and S are $\sim 10^{-1}$. Furthermore, it vanishes when $S = 3R$. This ratio of R/S follows if in (49) we have, for example, $\alpha_0(\epsilon) \propto \epsilon^{1/2}$ and $\alpha_1(\epsilon) \propto \epsilon^{3/2}$.

Since the deviations from sphericity in, for example, potassium are known[14] to be $\sim 10^{-3}$, the saturation value from (53) would thus be $\sim 10^{-7}$. This is several orders of magnitude less than the experimentally observed magnetoresistivity in potassium,[15] which clearly demonstrates the need for a mechanism other than ordinary impurity scattering to explain these results.

APPENDIX A

The reduction of the Boltzmann equation of a charged Fermi liquid to a one-dimensional integral equation is briefly described in the following. It was performed in detail for the case of the (static) thermal conductivity in Appendix B of Jensen *et al.*[2] Since the case of electrical conductivity is closely related, we limit ourselves to pointing out the differences.

As mentioned in Section 3.1, we neglect any spatial dependence of the distribution function. The oscillating field $\mathbf{E} = \mathbf{E}_0 e^{i\omega t}$ causes the distribution function n to depend

explicitly on time. The kinetic equation for quasiparticles with momentum $\mathbf{p}$ and energy ϵ is then

$$(\partial n/\partial t) + (-\partial\epsilon/\partial\mathbf{x}) \cdot \partial n/\partial\mathbf{p} = I(n) \tag{A1}$$

where I is the collision integral arising from scattering between the quasiparticles. Since we assume "classical" conditions $\hbar\omega \ll kT$, the collision integral is independent of ω (cf. Section 3.1 and Gurzhi).[7]

To linear order in $\mathbf{E}$, the driving term of the Boltzmann equation (A1) is

$$-\partial\epsilon/\partial\mathbf{x} \cdot \partial n/\partial\mathbf{p} = -[1/4 \cosh^2(s/2)](1/kT)\, e\mathbf{E} \cdot \mathbf{v} \tag{A2}$$

upon introduction of the velocity $\mathbf{v} = \partial\epsilon/\partial\mathbf{p}$ and the reduced energy variable

$$s = (\epsilon - \mu)/kT \tag{A3}$$

As usual in Fermi liquid theory, one expands in the collision integral the distribution function about *local* equilibrium $n_0(\epsilon)$ according to

$$n = n_0(\epsilon) + (\partial n_0/\partial\epsilon)\, \psi_{\mathbf{p}} e^{i\omega t} \tag{A4}$$

where n_0 is the Fermi distribution function.

However, the $\partial/\partial t$ operator of (A1) acts on the deviation from *true* equilibrium $n_0(\epsilon_0)$ given by

$$n - n_0(\epsilon_0) = (\partial n_0/\partial\epsilon)\, \phi_{\mathbf{p}} e^{i\omega t} \tag{A5}$$

In (A5), ϵ_0 is the quasiparticle energy in the absence of any disturbance of the system ($\delta n = 0$).

The connection between ϕ and ψ is made in the usual manner (see, e.g., Pines and Nozières[8]) by observing that the angular dependence of the solution to (A1) is set by $\mathbf{v} \cdot \mathbf{E}$. Then, ϕ and ψ are simply related by the Landau parameter F_1^s according to

$$\phi_{\mathbf{p}} = \psi_{\mathbf{p}}(1 + \tfrac{1}{3}F_1^s)^{-1} \tag{A6}$$

and the linearized equation (A1) may be written as an equation for the energy dependence of $\psi_{\mathbf{p}}$ only. To achieve this, we follow the same steps as in Appendix B of Jensen *et al.*[2] after writing

$$\psi_{\mathbf{p}} = -2\tau_0[\cosh(s/2)]\, Q(s)\, \mathbf{v} \cdot \mathbf{E}_0 e \tag{A7}$$

The Boltzmann equation then finally becomes

$$\{i\omega[2\tau_0/(1 + \tfrac{1}{3}F_1^s)] + G\}\, Q = X \tag{A8}$$

where G is the operator (39) and X is given by (38). The definition of τ_0 in (A7) is that used by Jensen *et al.*,[2] so the product $2\tau_0(1 + \tfrac{1}{3}F_1^s)^{-1}$ is the characteristic time τ_e defined by (41), which completes the identification of (A8) with (37).

We still need to comment on the meaning of the parameter α in the integral operator (39). In a translationally invariant Fermi liquid, α is 2, and the dc conductivity

(45) is infinite. However, if the translational invariance is broken by the existence of Umklapp processes, an equation like (37) may still be obtained[16,17] with α less than 2.

The translational invariance is also broken in the two-band model used by Bennett and Rice[18] for the dc conductivity. There (light) s electrons are assumed to scatter against (heavy) d electrons taken to be in equilibrium. The Boltzmann equation (37) is then obtained with $\Omega = 0$ and α given by

$$\alpha = 2 \int_0^1 w(u)(1 - 2u^2)\, du \Big/ \int_0^1 w(u)\, du \tag{A9}$$

Here, the collision probability $w(u)$ is expressed as a function of $u = q/2k_s$, i.e., the ratio of the wave vector transfer q to twice the Fermi wave vector k_s for the s electrons. The result (A9) holds when the Fermi wave vector k_d of the d electrons is greater than k_s. When this is not the case, the upper limits on the integrals are replaced by the ratio k_d/k_s.

Finally, we must relate the conductivity σ to the solution Q of (A8). The current density $\mathbf{J}$ is generally

$$\mathbf{J} = \sum_{\mathbf{p}\sigma} e(\partial\epsilon_0/\partial\mathbf{p})\, \delta n \tag{A10}$$

with $\delta n = (\partial n_0/\partial\epsilon)\, \psi_{\mathbf{p}} e^{i\omega t}$ being the deviation from local equilibrium [see (A4)]. The index σ denotes a spin sum.

With the expression (A7) for $\psi_{\mathbf{p}}$ the conductivity obtained from (A10) becomes

$$\sigma = e^2(m^* k_F/\pi^2\hbar^2) \times \int_{-\infty}^{\infty} ds\, \tfrac{1}{3} v_F^2(\tau_0/2)[1/\cosh(s/2)]\, Q(s) \tag{A11}$$

in terms of the density of states $m^* k_F/\pi^2\hbar^2$ and the Fermi velocity v_F. Defining $X(s) = 1/\cosh(s/2)$ in agreement with (38) and using $v_F = \hbar k_F/m^*$ and the number of electrons per unit volume $n = k_F^3/3\pi^2$, we obtain

$$\sigma = (ne^2/m^*)(\tau_0/2) \int_{-\infty}^{\infty} ds\, Q(s)\, X(s) \tag{A12}$$

The integral in (A12) is simply the complex conjugate of the reduced conductivity Σ defined by (42). In terms of the time τ_e defined by (41) and the optical mass m_0 defined by (44), the result (A12) is seen to be identical to (43).

APPENDIX B

Below we list the matrix elements

$$a_n = (X, G^n X) = \int_{-\infty}^{\infty} ds\, X(s)\, G^n X(s)$$

with X given by (38) and G by (39):

$$\begin{aligned}
a_{-2} &= \pi^{-4}\{2.847 + 2.250[\alpha^2/(2-\alpha)^2] + 4.935[\alpha/(2-\alpha)] \\
&\quad + 0.461[\alpha/(12-\alpha)] + 0.292[\alpha^2/(2-\alpha)(12-\alpha)] \\
&\quad + 0.057[\alpha^2/(12-\alpha)^2] + \cdots\} \\
a_{-1} &= \Sigma^0 \quad \text{given by (45)} \\
a_0 &= 4 \\
a_1 &= \pi^2(16/3)[1-(\alpha/2)] \\
a_2 &= \pi^4(128/15)[1-(\alpha/2)]^2 \\
a_3 &= \pi^6(256/105)[1-(\alpha/2)]^2(8-3\alpha) \\
a_4 &= \pi^8(2048/315)[1-(\alpha/2)]^2\,(12-6\alpha+\alpha^2) \\
a_5 &= \pi^{10}(4096/3465)[1-(\alpha/2)]^2\,(480-228\alpha+50\alpha^2-5\alpha^3)
\end{aligned}$$

The matrix elements a_{-2} and a_{-1} are given in terms of rapidly converging series. The matrix element $a_{-2} = (G^{-1}X, G^{-1}X)$ is calculated by means of the solution Q^0 of (37) with $\Omega = 0$, since $Q^0 = G^{-1}X$. The solution Q^0 is in turn readily obtained from Jensen *et al.*[10] as a rapidly converging series of functions.

APPENDIX C

We evaluate σ_∞ for our model Fermi surface given by (49). From (33) and our definition of a scalar product (50), σ_∞ becomes

$$\sigma_\infty = \tau(-e^2/4\pi^3)\int (\partial n_0/\partial\epsilon)\, v_z \bar{v}_z k^2 \sin\theta\, dk\, d\theta\, d\varphi \tag{C1}$$

where

$$v_z = (\partial k/\partial\epsilon)^{-1}\{\cos\theta + [(\sin\theta)/k]\,\partial k/\partial\theta\} \tag{C2}$$

and $\bar{v}_z$ is the average velocity in the direction of the magnetic field, the average being over an orbit on the Fermi surface with respect to the phase angle $\tilde{\varphi}$,

$$\bar{v}_z = (1/2\pi)\int_0^{2\pi} v_z\, d\tilde{\varphi} = (1/2\pi)\int_0^{2\pi} v_z(d\tilde{\varphi}/d\varphi)\, d\varphi \tag{C3}$$

To evaluate $d\tilde{\varphi}/d\varphi$, we use the definition (see for example, Ziman,[1] pp. 513–515)

$$d\tilde{\varphi} = dl\,(v_x^2 + v_y^2)^{-1/2} \Big/ \Big[(1/2\pi)\oint dl\,(v_x^2 + v_y^2)^{-1/2}\Big] \tag{C4}$$

The line integral is over an orbit on the Fermi surface in a plane of constant k_z and

$$dl = k(\sin\theta)\, d\varphi/\cos\psi \tag{C5}$$

is the element arc on this orbit. Here, ψ is the angle between the components in the plane of the orbit of the velocity and the wave vector. With (C5) in (C4) and the obvious expressions for the velocity and wave vector in spherical polar coordinates, we obtain

$$d\tilde{\varphi}/d\varphi = \Omega \Big/ \Big[(1/2\pi) \int_0^{2\pi} \Omega \, d\varphi\Big] \tag{C6}$$

where

$$\Omega = \Big(\frac{\partial k}{\partial \epsilon}\Big)\Big[\frac{1}{k} - \frac{\cos\theta}{k \sin\theta} \frac{\partial k/\partial\theta}{k}\Big]^{-1}$$

Equation (C3) implies an integration in which k_z and ϵ are constant. In carrying out the integration over φ of functions of k and θ, we have to take into account the fact that k and θ vary on the orbit defined by k_z and ϵ. We need, therefore, to determine the dependence of θ and k on k_z, ϵ, and φ from the two equations

$$\begin{aligned} k_z &= k \cos\theta \\ k &= k_F[1 + RY_4(\cos\theta, \varphi)] \end{aligned} \tag{C7}$$

Equation (C7) is obtained from (49) with $\epsilon = \mu$ using (51). As always, we assume complete degeneracy. We solve for θ and k by iteration starting with $R = 0$, $k = k_F$, and $\cos\theta_0 = k_z/k_F$. To first order, we get

$$\cos\theta_1 = (\cos\theta_0)[1 - RY(\cos\theta_0, \varphi)] \tag{C8}$$

and to second order,

$$\cos\theta_2 = (\cos\theta_0)[1 - RY(\cos\theta_1, \varphi) + R^2Y^2(\cos\theta_0, \varphi)] \tag{C9}$$

(The subscript in Y_4 is hereafter suppressed.) We now expand Y as a Taylor expansion and, using (C8) and (C9), we obtain to second order

$$\cos\theta = (\cos\theta_0)\{1 - RY_0 + R^2[Y_0^2 + (\cos\theta_0)\, Y_0Y_0']\} \tag{C10}$$

$$k = k_F[1 + RY_0 - R^2(\cos\theta_0)\, Y_0Y_0'] \tag{C11}$$

where $Y_0' = \partial Y_0/\partial(\cos\theta_0)$ and for brevity we write $Y_0 = Y(\cos\theta_0, \varphi)$.

To evaluate $d\tilde{\varphi}/d\varphi$ from (C6), we first substitute for k, $k^{-1}\,\partial k/\partial\theta$ from (C7) and $\partial k/\partial\epsilon$ from (49) and (51). We then carry out a binomial expansion in powers of R and neglect third and higher powers. Prior to carrying out the integration over φ, we convert all functions of θ to functions of θ_0 with the use of (C10), (C11), and other relations easily derived from them. The series obtained for $d\tilde{\varphi}/d\varphi$ is then inserted into (C3) to calculate $\bar{v}_z$. The same procedure for expansion and conversion to functions of θ_0, where necessary, is carried out before integration. We can now evaluate σ_∞ from (C1) after inserting the result obtained for $\bar{v}_z$ and carrying out expansions in powers of R and S as before. As a final step before performing the integration over θ and φ, we convert all functions of θ_0 back to functions of θ using (C10). All integrations are carried out analytically. Those involving products of Legendre polynomials can be carried out using the formulas given by Gaunt.[19]

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REFERENCES

1. J. M. Ziman, *Electrons and Phonons*, Oxford University Press, London (1960).
2. H. Højgaard Jensen, H. Smith, and J. W. Wilkins, *Phys. Rev.* **185**:323 (1969).
3. F. Garcia-Moliner and S. Simons, *Proc. Cambridge Phil. Soc.* **53**:848 (1957).
4. N. K. Hindley and F. Garcia-Moliner, *Phys. Rev.* **A140**:343 (1965).
5. E. I. Blount, *Phys. Rev.* **131**:2354 (1963).
6. M. Bailyn, *Phys. Rev.* **126**:2040 (1962).
7. R. Gurzhi, *Soviet Phys.—JETP* **8**:673 (1959).
8. D. Pines and P. Nozières, *Quantum Liquids*, Vol. I, W. A. Benjamin, New York (1966).
9. A. A. Abrikosov and I. M. Khalatnikov, *Rept. Progr. Phys.* **22**:329 (1959).
10. H. Højgaard Jensen, H. Smith, and J. W. Wilkins, *Phys. Letters* **27B**:532 (1968).
11. G. Brooker and J. Sykes, *Phys. Rev. Letters* **21**:279 (1968).
12. L. Davis, Jr., *Phys. Rev.* **56**:93 (1939).
13. F. Garcia-Moliner, *Proc. Roy. Soc.* **A249**:73 (1958).
14. M. J. G. Lee and L. M. Falicov, *Proc. Roy. Soc.* **A304**:319 (1968).
15. P. A. Penz and R. Bowers, *Phys. Rev.* **172**:991 (1968).
16. H. Smith and J. W. Wilkins, *Phys. Rev.* **183**:624 (1969).
17. W. E. Lawrence, Thesis, Cornell University, Ithaca, New York (1970).
18. A. J. Bennett and M. J. Rice, *Phys. Rev.* **185**:968 (1969).
19. J. A. Gaunt, *Trans. Roy. Soc.* **228**:151 (1929).