Relations between the Hall and dissipative parts of the electric conductivity of a metal in a magnetic field

G. T. Avanesyan and M. I. Kaganov

Institute of Radiophysics and Electronics, Armenian Academy of Sciences and Institute of Physics Problems, USSR Academy of Sciences
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By starting with classical Boltzmann equation, inequalities are derived connecting the Hall and dissipative parts of the conductivity tensor in a magnetic field. If the isotropic carriers are all of the same sign (electrons or holes), the inequalities go over into equations of the Kramers-Kronig type, where the role of the frequency is assumed by the magnetic field.

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1. The theory of kinetic properties of metals in a magnetic field has been developed quite fully. I. M. Lifshitz and his students (see [1] and the literature cited there) have established a connection between the structure of the electronic energy spectrum and the asymptotic galvanomagnetic characteristics in a strong magnetic field. The conclusions drawn in the cited papers were based on an investigation of the classical Boltzmann equation for electrons as charged fermions with a complicated dispersion law $\epsilon = \epsilon(\mathbf{p})$. The applicability of the classical equation can be justified by the smallness of the ratio $\hbar\omega_c/\epsilon_F$ in comparison with unity (ω_c is the characteristic cyclotron frequency and ϵ_F is the Fermi energy). The scattering of the electrons is described by a collision operator whose structure depends on the concrete mechanism of the scattering (by phonons, by impurities, etc.). One of the most important results of the work by I. M. Lifshitz et al. [1] is the conclusion that the form of the asymptotic characteristics is independent of the collision integral. To be sure, it must be borne in mind that the coefficients in the obtained asymptotic expressions are functionals that depend on the collision operator and on the dispersion law. When describing this stage of the construction of the theory of galvanomagnetic phenomena, it must be emphasized that a very important role in the development of the theory was the conviction that the electronic spectrum is insensitive to the magnetic field in a wide range of magnetic fields, and that the role of the magnetic field reduces only to a bending of the electron trajectories.

It became clear in recent years that the electronic spectrum of many metals becomes restructured under the influence of a relatively-weak magnetic field[1)]—magnetic breakdown sets in ([1], Sec. 10) and leads to a number of observable effects, particularly to a change of the asymptotic relations. For many metals (Cu, Au, Ag, etc.), however, and at arbitrary directions of the magnetic fields for most metals, there is a wide range of magnetic fields in which the spectrum of the metals and the collision operator can be regarded as independent of the magnetic field, and this region covers also the so-called strong fields ($\omega_c\tau \gg 1$, where τ is the average relaxation time).

As already mentioned, the asymptotic values of the galvanomagnetic characteristics contain as a rule coefficients that cannot be calculated without a detailed knowledge of the collision operator. In [2,3], however, it is shown that by using only the hermiticity and the positiveness of the collision operator it is possible to establish definite nontrivial relations between the coefficients that enter in the asymptotic expressions (see also [4]).

The hermiticity and positiveness of the collision operator, furthermore, suffice (see [1], Secs. 24 and 26 and [5] Sec. 88) to ensure satisfaction of the Onsager relations $\sigma_{ij}(\mathbf{H}) = \sigma_{ji}(-\mathbf{H})$ and the requirement $\sigma_{xx}, \sigma_{yy}, \sigma_{zz} > 0$ that the entropy increase ($\hat{\sigma}(\mathbf{H})$ is the tensor of the conductance in a magnetic field $\mathbf{H}$). It will be shown below (see the Appendix) that to satisfy the Kramers-Kronig relations ([5], Sec. 62) between the real and imaginary parts $\mathrm{Re}\,\hat{\sigma}(\omega)$ and $\mathrm{Im}\,\hat{\sigma}(\omega)$ of the tensor $\hat{\sigma}(\omega)$ (ω is the frequency of the electromagnetic wave) it is also sufficient that the collision operator be Hermitian and positive.

It is convenient in what follows to start with an examination of an example. We shall describe the properties of a metal hydrodynamically, disregarding the electron dispersion. Then

$$\sigma(\omega)=\frac{\sigma_0}{1-i\omega\tau}=\frac{\sigma_0}{1+\omega^2\tau^2}+i\frac{\sigma_0\omega\tau}{1+\omega^2\tau^2}, \tag{1}$$

where $\sigma_0 \equiv \sigma(\omega = 0)$. The Kramers-Kronig relations

$$\mathrm{Re}\,\sigma(\omega)=\frac{1}{\pi}\mathrm{P}\int_{-\infty}^{+\infty}\frac{\mathrm{Im}\,\sigma(\omega')}{\omega'-\omega}d\omega',$$
$$\mathrm{Im}\,\sigma(\omega)=-\frac{1}{\pi}\mathrm{P}\int_{-\infty}^{+\infty}\frac{\mathrm{Re}\,\sigma(\omega')}{\omega'-\omega}d\omega', \tag{2}$$

can be verified directly and are, of course, the consequence of the fact that the poles of $\sigma(\omega)$ (one pole in this case) are in the lower half of the complex ω plane.

The static properties of the metal in the magnetic field are described in this case by the tensor $\hat{\sigma}(\mathbf{H})$:

$$\hat{\sigma}=\begin{pmatrix} s & -a & 0\\ a & s & 0\\ 0 & 0 & \sigma_0\end{pmatrix},\quad s=\frac{\sigma_0}{1+\omega_c^2\tau^2},\quad a=\frac{\sigma_0\omega_c\tau}{1+\omega_c^2\tau^2};\quad \omega_c=\frac{|e|H}{m^*c} \tag{3}$$

(m^* is the effective mass of the electron). It is seen from (3) that it is possible to introduce a complex transverse conductivity

$$\sigma(H)=\sigma_0/(1-i\omega_c\tau), \tag{4}$$

whose real and imaginary parts describe the dissipative and Hall parts of $\sigma(H)$, respectively ($s = \mathrm{Re}\,\sigma$, $a = \mathrm{Im}\,\sigma$). Just as in the preceding case, formulas (3) and (4) lead directly to relations of the Kramers-Kronig type, in which the integration is over the magnetic field[2)]:

$$s(H)=\left|\frac{1}{\pi}\mathrm{P}\int\limits_{-\infty}^{+\infty}\frac{a(H')}{H'-H}dH'\right|,\quad |a(H)|=\left|\frac{1}{\pi}\int\limits_{-\infty}^{+\infty}\frac{s(H')}{H'-H}dH'\right|. \quad (5)$$

Direct generalization of relations (5) to an arbitrary case (it is only in this sense that relations (2) are of interest) is impossible. This is seen from two complicating examples. If the carriers are electrons and holes ($m^* < 0$), then while remaining in the framework of the hydrodynamic approximation, we have (the subscripts 1 and 2 label the electron and hole bands)

$$\sigma(\omega)=\frac{\sigma_{01}}{1-i\omega\tau_1}+\frac{\sigma_{02}}{1-i\omega\tau_2}, \quad (6)$$

$$\sigma(H)=\frac{\sigma_{01}}{1-i\omega_{c1}\tau_2}+\frac{\sigma_{02}}{1-i\omega_{c2}\tau_2}. \quad (7)$$

In spite of the outward similarity of (6) and (7), we see that the two differ significantly: both poles of $\sigma(\omega)$ are in the lower half-plane ($\mathrm{Im}\,\omega < 0$), while one pole of $\sigma(H)$ is in the lower and the other in the upper half-plane (we have in mind the complex H plane). This makes it impossible to establish relations of the Kramers-Kronig type for $\mathrm{Re}\,\sigma(H)$ and $\mathrm{Im}\,\sigma(H)$.

We consider now the simplest anisotropic model of a metal: the carriers are n electrons per unit volume with a dispersion law $\epsilon = p_\perp^2/(2m_\perp) + p_3^2/(2m_\parallel)$ ($p_\perp^2 = p_1^2 + p_2^2$), the magnetic field is inclined at an angle ϑ to the symmetry axis. If we put $m_c^2 = m_\perp m^*$ and $1/m^* = \cos^2\vartheta/m_\perp + \sin^2\vartheta/m_\parallel$, then the components of the transverse (relative to H) conductivity matrix are

$$\sigma_{xx}=\frac{ne^2\tau}{m_\perp}\frac{1}{1+\omega_c^2\tau^2},\quad \sigma_{yy}=\frac{ne^2\tau}{m^*}\frac{1}{1+\omega_c^2\tau^2},$$
$$\sigma_{yx}=-\sigma_{xy}=\frac{ne^2\tau}{m_c}\frac{\omega_c\tau}{1+\omega_c^2\tau^2},\quad \omega_c=\frac{|e|H}{m_c c}. \quad (8)$$

It is seen that we have used the τ approximation. The directions of the axes X and Y are clear from the figure, and the Z axis is directed as always along the magnetic field. Since $\sigma_{xx} \neq \sigma_{yy}$, the question arises of constructing the analytic function $\sigma = s + ia$ (cf. (4)). It is natural to replace s by the arithmetic mean of the symmetrical part of the tensor $\sigma_{\alpha\beta}(\alpha, \beta = x, y)$

$$s(H)={}^1/_2[\sigma_{xx}(H)+\sigma_{yy}(H)], \quad (9)$$

which is invariant to the choice of the axes X and Y, while the quantity

$$a(H)={}^1/_2[\sigma_{yx}(H)-\sigma_{xy}(H)] \quad (10)$$

is also invariant. We shall henceforth use the definitions (9) and (10) also in the general case. Thus, according to (8)–(10),

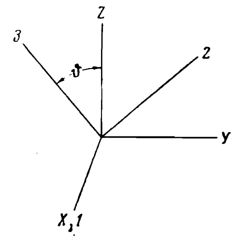
$$s=\frac{s_0}{1+\omega_c^2\tau^2},\quad a=\beta\frac{s_0\omega_c\tau}{1+\omega_c^2\tau^2}. \quad (11)$$

We have introduced

$$s_0=ne^2\tau\frac{1}{2}\left(\frac{1}{m_\perp}+\frac{1}{m^*}\right),\quad \beta=\frac{2\sqrt{m_\perp m^*}}{m_\perp+m^*}, \quad (12)$$

β is a parameter that does not depend on H, $\beta = 1$ in the isotropic case ($m_\perp = m_\parallel$). Comparing (11) with (3) and (4) we see that at $\vartheta \neq 0$ the dispersion relations of the type (2) do not hold. Attention must be called, however, to the fact that for any choice of ϑ and for any ratio of the effective masses $\beta \leq 1$ it follows here directly that s(H) and a(H) satisfy in this case the inequalities

$$s(H)\geqslant\left|\frac{1}{\pi}\mathrm{P}\int\limits_{-\infty}^{\infty}\frac{a(H')}{H'-H}dH'\right|,$$
$$|a(H)|\leqslant\left|\frac{1}{\pi}\mathrm{P}\int\limits_{-\infty}^{+\infty}\frac{s(H')}{H'-H}dH'\right|. \quad (13)$$



It is easy to verify that in the approximation of two isotropic bands (see (7)) the inequalities (13) hold likewise ($s = \mathrm{Re}\,\sigma$; $a = \mathrm{Im}\,\sigma$).

The two considered examples suggest that in the general case (arbitrary dispersion law, arbitrary Hermitian and positive collision operator) the inequalities (13) hold for s(H) and a(H) (see (9) and (10)). The proof of this statement is the main content of this article.

2. To calculate the static conductivity in a magnetic field it is necessary to use the kinetic equation for the vector-function $\boldsymbol{\psi}$, which is connected with the nonequilibrium increment $f - n_F$ to the equilibrium Fermi function n_F by the relation

$$f-n_F=-e\frac{\partial n_F}{\partial\varepsilon}\mathbf{E}\boldsymbol{\psi}$$

(**E** is the intensity of the external electric field),[3)]

$$\frac{\partial}{\partial t_H}\boldsymbol{\psi}+W_p\boldsymbol{\psi}=\mathbf{v},\quad \mathbf{v}=\nabla_p\varepsilon(\mathbf{p}), \quad (14)$$

where the variable t_H has the meaning of the time of motion of the electron along a classical trajectory in a magnetic field, and W_p is a hermitian collision operator satisfying the positiveness condition ([1], Sec. 23)

$$\langle u,\ W_p u\rangle\geqslant 0. \quad (15)$$

The angle brackets denote integration over **p**-space (this symbol emphasizes the fact that the resultant integrals have the meaning of scalar products):

$$\langle u, v\rangle=-e^2\int\frac{\partial n_F}{\partial\varepsilon}u(\mathbf{p})v(\mathbf{p})d\Gamma,\quad d\Gamma=\frac{2V}{(2\pi\hbar)^3}d\mathbf{p}. \quad (16)$$

The components of the conductivity tensors are scalar products of the type

$$\sigma_{ij}=\langle v_i,\ \psi_j\rangle. \quad (17)$$

Acting on both sides of (15) with the operator W_p^{-1} and carrying out elementary transformations, we obtain

$$(U-i\eta I)\boldsymbol{\psi}=-i\eta\mathbf{w},\quad \mathbf{w}=W_p^{-1}\mathbf{v}, \quad (18)$$

where $\eta = c/H$ and

$$U=-i\frac{c}{H}W_p^{-1}\frac{\partial}{\partial t_H}$$

is an operator that is self-adjoint relative to the "new" scalar product $(u, v) \equiv \langle\bar{u}, W_p v\rangle$; the bar denotes complex conjugation. We emphasize that U does not depend on the magnetic field, since $t_H \sim 1/H$. The self-adjoint character of U follows from the anti-hermiticity of the operator $\partial/\partial t_H$ with respect to the scalar product (16). The components of the conductivity tensor are expressed with the aid of the "new" scalar product in analogy with (17):

$$\sigma_{ij}=(w_i,\ \psi_j). \quad (19)$$

Changing over to complex notation for the vectors $\mathbf{w}_\perp$ and $\boldsymbol{\psi}_\perp$ in the XY plane (H ∥ Z),

$$w_\perp\to w=2^{-1/2}(w_x+iw_y),\quad \psi_\perp\to\psi=2^{-1/2}(\psi_x+i\psi_y),$$

and using (19), we get

$$\sigma=(w,\psi)=\frac{1}{2}[\sigma_{xx}+\sigma_{yy}]+\frac{i}{2}[\sigma_{xy}-\sigma_{yx}]=s+ia.$$

From (18) we have

$$\psi=-i\eta(U-i\eta I)^{-1}\mathbf{w}=-i\eta R_{i\eta}\mathbf{w},$$

where $R_{i\eta}$ is the resolvent of the self-adjoint operator U. For σ we obtain the expression

$$\sigma(\eta)=-i\eta(w, R_{i\eta}w). \tag{20}$$

As follows from the theory of linear operators in Hilbert space ([8], Chap. 6), for the resolvent of any self-adjoint operator the function $\varphi(z) = (w, R_z s)$, where w is an arbitrary vector of Hilbert space, is analytic at Im z $\neq$ 0 and has the following integral representation:

$$\varphi(z)=\int_{-\infty}^{+\infty}\frac{d\omega(u)}{u-z} \tag{21}$$

with a monotonically non-decreasing function of limited variation w(u). We obtain accordingly for σ

$$\sigma(\eta)=-i\eta\int_{-\infty}^{+\infty}\frac{d\omega(u)}{u-i\eta}. \tag{22}$$

As will be shown below, the integral representation (21) leads to the system of inequalities (13).

We express the function $\varphi(z)$ having the integral representation (21) in the form

$$\varphi(z)=\tilde{\varphi}(z)-\omega_0/z,$$

where

$$\omega_0=\lim_{\eta\to 0}\eta\,\mathrm{Im}\,\varphi(i\eta)$$

is the discontinuity of the function $\omega(u)$ at the point 0. The function $\tilde{\varphi}(z)$ has a representation analogous to (21):

$$\tilde{\varphi}(z)=\int_{-\infty}^{0}\frac{d\tilde{\omega}(u)}{u-z}+\int_{0}^{+\infty}\frac{d\tilde{\omega}(u)}{u-z}=\varphi^-(z)+\varphi^+(z), \tag{23}$$

but $\tilde{\omega}(u)$ is continuous at the point 0. Each of the functions φ^- and φ^+ corresponding to the first and second integrals in (23) satisfies on the imaginary axis the relations

$$\frac{1}{\pi}\mathrm{P}\int_{-\infty}^{+\infty}\frac{\mathrm{Re}\,\varphi^{\pm}(i\eta')}{\eta'-\eta}d\eta'=\mp\mathrm{Im}\,\varphi^{\pm}(i\eta),$$

$$\frac{1}{\pi}\mathrm{P}\int_{-\infty}^{+\infty}\frac{\mathrm{Im}\,\varphi^{\pm}(i\eta')}{\eta'-\eta}d\eta'=\pm\mathrm{Re}\,\varphi^{\pm}(i\eta). \tag{24}$$

In that and only that special case when one of the functions φ^- or φ^+ vanishes identically, the relations (24) are obviously satisfied also for the function $\tilde{\varphi}$. Then, making the substitution $\varphi(i\eta) = i\sigma(\eta)/\eta$ in (24), we arrive at the equations that lead to relations (5).

In the general case (neither φ^- nor φ^+ equal to zero) it must be recognized that the sign of Im $\varphi^{\pm}(i\eta)$ coincides with the sign of η, while Re $\varphi^-(i\eta) < 0$ and Re $\varphi^+(i\eta) > 0$ for all η. From this we easily get

$$|\mathrm{Im}\,\tilde{\varphi}(i\eta)|\geqslant\left|\frac{1}{\pi}\mathrm{P}\int_{-\infty}^{+\infty}\frac{\mathrm{Re}\,\tilde{\varphi}(i\eta')}{\eta'-\eta}d\eta'\right|,$$

$$|\mathrm{Re}\,\tilde{\varphi}(i\eta)|\leqslant\left|\frac{1}{\pi}\mathrm{P}\int_{-\infty}^{+\infty}\frac{\mathrm{Im}\,\tilde{\varphi}(i\eta')}{\eta'-\eta}d\eta'\right|. \tag{25}$$

Changing over to integration in the direct field and using the connection between $\varphi(i\eta)$ and $\sigma(\eta)$, we obtain immediately inequalities (13). The transition from the function φ to $\tilde{\varphi}$ is connected with the elimination of the singularity at $\eta = 0$ (i.e. as $H \to \infty$). Therefore in formulas (13), s(H) should be taken to mean the difference $\frac{1}{2}[\sigma_{xx}(H) + \sigma_{yy}(H) - \sigma_{xx}(H \to \infty) - \sigma_{yy}(H \to \infty)]$. In the case of a closed Fermi surface we have $\sigma_{xx}(H \to \infty) = 0$ and $\sigma_{yy}(H \to \infty) = 0$. On the other hand in the case of open surfaces the procedure of separating the values at infinity is analogous to the separation of the static conductivity in the Kramers-Kronig relations for the dielectric constant of a conductor ([5], Sec. 62).

Since the here-investigated dependence of the components of the tensor σ_{ik} on the magnetic field[4)] is only insignificantly "perturbed" by quantum effects (by oscillations of the Shubnikov—de Haas type), for most metals, inequalities (13) can apparently always be used for the average values of s(H) and a(H). Of course, it would be desirable to establish relations between the magnetoresistance (in place of s) and the Hall "constant" (in place of a). So far, however, we have not succeeded in doing this. It is possible to use relations (13) by calculating σ_{ik} from the measured values of ρ_{ik} ($\sigma_{ik} = \rho_{ik}^{-1}$). The analogy with the "genuine" Kromers-Kronig relations (with respect to frequency) suggests that the inequalities (13) are more profound than established by us here. They hold possibly also if account is taken of the quantization of electron motion in a magnetic field. This question is not considered in the present article.

Using inequalities (13), we can of course obtain different corollaries, of the type

$$s(0)\geqslant\left|\frac{2}{\pi}\int_{0}^{\infty}\frac{a(H)}{H}dH\right|. \tag{26}$$

In conclusion, the authors take the opportunity to thank I. M. Lifshitz for interest in the work and for valuable remarks.

APPENDIX

The kinetic equation for the conduction electrons, which we use to calculate the conductivity tensor that depends on the frequency ω and wave vector **k**, is of the form

$$-i\omega\psi+i(\mathbf{kv})\psi+W_p\psi=\mathbf{v}. \tag{A.1}$$

The solution of this equation is

$$\psi=R_{i\omega}\mathbf{v}, \tag{A.2}$$

where $R_{i\omega}$ is the resolvent of the operator $W_p + i(\mathbf{k}\cdot\mathbf{v})$ satisfying the condition

$$\mathrm{Re}(u,\ [W_p+i(\mathbf{kv})]u)=(u,\ W_p u)\geqslant 0, \tag{A.3}$$

that follows from the condition (15), and the requirement that the operator of multiplication by the real function $(\mathbf{k}\cdot\mathbf{v})$ be self-adjoint. The scalar product in (A.3) differs from (16) in that the first of the functions is complex-conjugate: $(u, v) = \langle\bar{u}, v\rangle$.

We shall show that satisfaction of the condition (A.3) ensures the existence of Kramers-Kronig states for the components of the conductivity tensor $\hat{\sigma}(\omega)$. We consider the resolvent $R_z = (A - zI)^{-1}$ of a certain bounded linear operator A satisfying the condition

$$\mathrm{Re}(u,\ Au)\geqslant 0 \tag{A.4}$$

at all u. It is easy to verify that the left half-plane of the complex variable z is contained in the resolvent set of the operator A. According to a known theorem [9], for any linear functional f the function $F(z) = f(R_z)$ is analytic in the resolvent set of the operator A, and $F(z) \to 0$ as $z \to \infty$. From this it follows automatically on the basis of the Cauchy theorem that dispersion relations exist for $F(i\omega)$:

$$\frac{1}{\pi} P \int_{-\infty}^{+\infty} \frac{\operatorname{Im} F(i\omega'-\varepsilon)}{\omega'-\omega} d\omega' = \operatorname{Re} F(i\omega-\varepsilon),$$

$$\frac{1}{\pi} P \int_{-\infty}^{+\infty} \frac{\operatorname{Re} F(i\omega'-\varepsilon)}{\omega'-\omega} d\omega' = -\operatorname{Im} F(i\omega-\varepsilon). \quad (A.5)$$

In the case of the kinetic equation, $\epsilon \to +0$ corresponds to adiabatic switching on of an external field. The role of the functional f is played in our case by the scalar product

$$f(R_z) = (u, R_z v) = F(z). \quad (A.6)$$

It is easily seen that by substituting (A.2) in (17) we can rewrite the components of the conductivity tensor $\sigma_{ij}(\omega)$ in the form (A.6) whence, on the basis of the foregoing, follows the validity of the Kramers-Kronig relations (2) for the conductivity calculated with the aid of Eq. (A.1). The Fermi-liquid interaction between the electrons, under likely assumptions concerning the Landau correlation function, does not change the conclusion presented here.

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1)A measure of the weakness of a magnetic field under magnetic-breakdown conditions is not the inequality $\hbar\omega_c/\epsilon_F \ll 1$, but $\hbar\omega_c \ll \Delta^2/\epsilon_F$, where Δ is the minimal energy barrier that separates the classical trajectories; frequently $\Delta \ll \epsilon_F$, especially at definite magnetic-field directions.

2)The Kramers-Kronig relations "with respect to the magnetic field" were derived, as is well known, only for Re χ and Im χ (χ is the paramagnetic susceptibility), and use was made of the smallness of the nonresonant component of χ (see [6,7]).

3)Fermi-liquid effects are taken into account automatically (see [1], Sec. 23). In the case when several bands take part in the conductivity, Eq. (14) should be regarded as a system of equations, and the integration with respect to $d\Gamma$ includes summation over the bands.

4)Consequence—solutions of Boltzmann's equation.

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