Thermal Conductivity and Thermoelectric Phenomena in Metals in a Magnetic Field

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Asymptotic expressions for the tensors of the thermal conductivity and Thomson coefficients in a strong magnetic field have been found. No special assumptions on the dispersion law or collision integral are made in the derivations.

IT IS KNOWN that the magnetic field changes not only the resistivity of a metal but also the heat conduction, the Thomson and Peltier coefficients, *etc.*[1] Using the techniques developed earlier[2], the dependence of the kinetic coefficients on a strong magnetic field can be determined. As in Ref. 2, we will not take into account quantization of the electron motion in the magnetic field. The limits of the applicability of such a classical analysis are indicated in the reference cited.

To find the kinetic coefficients, it is necessary to calculate the current density j_i and the energy flow w_i due to the electric field E_i, and the temperature gradient $\partial T/\partial x_i$. If the addition to the equilibrium Fermi distribution function $f_0 = (e^{(\varepsilon-\zeta)/T}+1)^{-1}$ [$\varepsilon = \varepsilon(\mathbf{p})$ is the electron energy, $\mathbf{p}$ the quasi-momentum; $\zeta = \zeta(T)$ the chemical potential of the electron gas, and $\zeta(0) = \zeta_0$ the limiting Fermi energy] is denoted by f_1, then

$$j_i = 2e\,(2\pi\hbar)^{-3}\int v_i f_1\,(d\mathbf{p});\qquad w_i = 2\,(2\pi\hbar)^{-3}\int \varepsilon v_i f_1\,(d\mathbf{p}). \tag{1}$$

The function f_1 satisfies the linearized kinetic equation which we write schematically

$$\left(\frac{\partial f_1}{\partial t}\right)_{\text{field}} + \left(\frac{\partial f_1}{\partial t}\right)_{\text{st}} = -\frac{\partial f_0}{\partial \varepsilon} e v_i \left\{E_i + \frac{T}{e}\frac{\partial}{\partial T}\left(\frac{\varepsilon-\zeta}{T}\right)\frac{\partial T}{\partial x_i}\right\}. \tag{2}$$

Here, the first term on the left describes the change in the distribution function in a constant and homogeneous magnetic field. In the notation of Ref. 2,

$$(\partial f_1/\partial t)_{\text{field}} = t_0^{-1}\partial f_1/\partial\tau.$$

However, this form will not need suit us later. One need merely bear in mind that if φ is a function of the energy only then $(\partial\varphi/\partial t)_{\text{field}} \equiv 0$.

Now, let us put

$$f_1 = -\frac{\partial f_0}{\partial\varepsilon}\left\{eE_k\psi_k + T\frac{\partial}{\partial T}\left(\frac{\varepsilon-\zeta}{T}\right)\frac{\partial T}{\partial x_k}\varphi_k\right\}. \tag{3}$$

Then

$$j_i = \sigma_{ik}^{(0)}E_k + s_{ik}^{(0)}\partial T/\partial x_k;\qquad w_i = \sigma_{ik}^{(1)}E_k + s_{ik}^{(1)}\partial T/\partial x_k, \tag{4}$$

where

$$\sigma_{ik}^{(n)} = -e^2\int_0^\infty \varepsilon^n \frac{\partial f_0}{\partial\varepsilon}A_{ik}(\varepsilon)\,d\varepsilon;$$

$$es_{ik}^{(n)} = -Te^2\int_0^\infty \varepsilon^n\frac{\partial}{\partial T}\left(\frac{\varepsilon-\zeta}{T}\right)\frac{\partial f_0}{\partial\varepsilon}B_{ik}(\varepsilon)\,d\varepsilon = -e^2\int_0^\infty \varepsilon^n\frac{\partial f_0}{\partial T}B_{ik}(\varepsilon)\,d\varepsilon, \tag{5}$$

and

$$A_{ik}(\varepsilon) = \frac{2}{(2\pi\hbar)^3}\int_{\varepsilon(\mathbf{p})=\varepsilon}\frac{v_i\psi_k}{v}dS,\qquad B_{ik}(\varepsilon) = \frac{2}{(2\pi k)^3}\int_{\varepsilon(\mathbf{p})=\varepsilon}\frac{v_i\varphi_k}{v}dS. \tag{6}$$

The functions Ψ_k and φ_k are the solutions of the following equations

$$\left(\frac{\partial\psi_k}{\partial t}\right)_{\text{field}} + \left(\frac{\partial f_0}{\partial\varepsilon}\right)^{-1}\left(\frac{\partial}{\partial t}\right)_{\text{st}}\left(\frac{\partial f_0}{\partial\varepsilon}\psi_k\right) = v_k,$$
$$\left(\frac{\partial\varphi_k}{\partial t}\right)_{\text{field}} + \left(\frac{\partial f_0}{\partial T}\right)^{-1}\left(\frac{\partial}{\partial t}\right)_{\text{st}}\left(\frac{\partial f_0}{\partial T}\varphi_k\right) = v_k, \tag{7}$$

which differ from each other only in the form of the component describing the change in the distribution function because of collisions.

If the collision operator is an energy δ-function, we see from (6) and (7) that

$$A_{ik}(\varepsilon) \equiv B_{ik}(\varepsilon). \tag{8}$$

This holds in two cases: a) at temperatures high in comparison with the Debye temperature, when the collision integral is f_1/t_0 (t_0 is the relaxation time) and b) for very low temperatures (the criterion depends on the purity of the metal) when elastic collisions between electrons and impurities play a fundamental part.

To express the experimentally-measurable coefficients (resistivity, heat conduction, Thomson coefficient) in terms of $\sigma_{ik}^{(n)}$ and $s_{ik}^{(n)}$, let us write the law of conservation of energy for an electron gas.

If Q denotes the internal energy of the electrons, then evidently

$$(\partial Q / \partial t) + (\partial w_i / \partial x_i) = E_i j_i. \tag{9}$$

We easily obtain from (4) and (9)

$$\frac{\partial Q}{\partial t} = \sigma_{ik}^{(0)-1} j_i j_k - \left\{\sigma_{il}^{(0)-1} s_{lk}^{(0)} + \frac{1}{e}\frac{\partial}{\partial T}\left(\sigma_{kl}^{(1)}\sigma_{li}^{(0)-1}\right)\right\} j_i \frac{\partial T}{\partial x_k} - \frac{1}{e}\frac{\partial}{\partial x_i}\left\{\left[s_{ik}^{(1)} - \sigma_{il}^{(1)}\sigma_{lm}^{(0)-1}s_{mk}^{(0)}\right]\frac{\partial T}{\partial x_k}\right\}.$$

Hence, it is seen that

$$\sigma_{ik}^{(0)-1} = \rho_{ik} \tag{10}$$

is the resistivity tensor, whose asymptotic form in a strong magnetic field was studied in Ref. 2;

$$-e^{-1}\{s_{ik}^{(1)} - \sigma_{ip}^{(1)}\sigma_{pq}^{(0)-1}s_{qk}^{(0)}\} = \varkappa_{ik} \tag{11}$$

is the tensor of the heat conduction coefficient*; and

$$\sigma_{il}^{(0)-1}s_{lk}^{(0)} + \frac{1}{e}\frac{\partial}{\partial T}\left(\sigma_{kp}^{(1)}\sigma_{pi}^{(0)-1}\right) = \mu_{ik} \tag{12}$$

is the Thomson coefficient tensor.

Let us note that relations (10)–(12) are always valid and are not related to the presence or absence of a magnetic field (see for example Ref. 3).

All the kinetic coefficients depend on the temperature for two reasons: First, because the collision integral depends on the temperature; second, because of the temperature dependence of the electron equilibrium distribution function f_0. Since the electron gas is always strongly degenerate ($T \ll \zeta_0$), a calculation of the first non-vanishing terms of the expansion of these coefficients in powers of the small parameter T/ζ_0 is of interest.

We will use the well known formula[4]:

$$\int_0^\infty \varphi(\varepsilon) f_0(\varepsilon)\, d\varepsilon = \int_0^\zeta \varphi(\varepsilon)\, d\varepsilon + \frac{\pi^2}{6} T^2 \frac{\partial \varphi}{\partial \varepsilon}\Big|_{\varepsilon=\zeta} + \dots \tag{13}$$

[$\varphi(\varepsilon)$ is an arbitrary function of the energy]. This expression can be considered as an expansion in powers of the temperature if it is recognized that the chemical potential of the electrons ζ is constant. However, the number of electrons n is constant. Consequently, the ζ-function of the temperature, which can be found from the normalization condition

$$2(2\pi\hbar)^{-3}\int f_0(\varepsilon)\,(d\mathbf{p}) = 2(2\pi\hbar)^{-3}\int_0^\infty f_0(\varepsilon)\, g(\varepsilon)\, d\varepsilon = n$$

(n is the electron density), where

$$g(\varepsilon) = \oint_{\varepsilon(\mathbf{p})=\varepsilon} dS / v$$

is the density of the levels in the energy interval $d\varepsilon$. Denoting $\zeta(T) - \zeta_0$ by Δ, we obtain, using (13)

$$\Delta = -(\pi^2 T^2 / 6)\, g'(\zeta_0) / g(\zeta_0). \tag{14}$$

We have from (13) and (14)

$$\int_0^\infty \varphi(\varepsilon) f_0(\varepsilon)\, d\varepsilon = \int_0^{\zeta_0} \varphi(\varepsilon)\, d\varepsilon + \frac{\pi^2 T^2}{6}\left[\varphi' - \varphi \frac{g'(\varepsilon)}{g(\varepsilon)}\right]_{\varepsilon=\zeta_0} + \dots$$

Using the expressions obtained, we easily find

$$\sigma_{ik}^{(0)} = e^2\left\{A_{ik}(\zeta_0) - \frac{\pi^2 T^2}{6}\left[A'_{ik}(\zeta_0)\frac{g'(\zeta_0)}{g(\zeta_0)} - A''(\zeta_0)\right]\right\};$$

$$\sigma_{ik}^{(1)} = e^2\left\{A_{ik}(\zeta_0)\zeta_0 - \left[\frac{\partial}{\partial \zeta_0}(\zeta_0 A_{ik}(\zeta_0))\left(\frac{g'(\zeta_0)}{g(\zeta_0)} - \frac{\partial^2}{\partial \zeta_0^2}(\zeta_0 A_{ik}(\zeta_0))\right)\right]\frac{\pi^2 T^2}{6}\right\}.$$

$$s_{ik}^{(0)} = e\left\{\frac{\partial}{\partial T}\int_0^{\zeta_0} B_{ik}(\varepsilon)\, d\varepsilon - \frac{\pi^2 T}{3}\left[B'_{ik}(\zeta_0) - B_{ik}(\zeta_0)\frac{g'(\zeta_0)}{g(\zeta_0)}\right]\right\}. \tag{15}$$

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* As is known, the heat conduction of a metal is determined not only by electrons but also by other "quasi-particles" in the metal (phonons, spin waves, etc.). Hereinafter we shall understand $\varkappa_{ik}$ to mean only the electron part of the heat conduction.

In obtaining the last formulas, we used the fact that $A_{ik}(\varepsilon)$ and $B_{ik}(\varepsilon)$ are smooth functions of ε. The latter follows from (6) and (7). It can be shown that this is not so because Eqs. (7) contain derivatives of the Fermi function. However, if the general form of the linearized collision integral is taken into account [see for example (8.18) of Ref. 1], it is easy to show that ψ_k and φ_k do not have singularities at $\varepsilon = \varepsilon_0$ (as $T \to 0$).

Using formulas (15), the first non-vanishing terms of the expansion in powers of T/ζ_0 can be obtained for the quantities of interest to us:

$$\sigma_{ik} = e^2 A_{ik}(\zeta_0), \quad \varkappa_{ik} = {}^1/_3 \pi^2 k^2 T B_{ik}(\zeta_0),$$
$$\mu_{ik} = \frac{\pi^2 k^2 T}{3e}\Big\{(2A_{li}^{-1}A'_{kl} - A_{il}^{-1}B'_{lk}) - (\delta_{ik} - A_{il}^{-1}B_{lk})\frac{g'(\zeta_0)}{g(\zeta_0)}\Big\} + \frac{1}{e}A_{il}^{-1}\frac{\partial}{\partial T}\int_0^{\zeta_0} B_{lk}(\varepsilon)\,d\varepsilon. \tag{16}$$

The last term in the expression for μ_{ik} can be omitted, as a rule, since electron scattering by impurities, which is practically independent of the temperature, plays a fundamental part at low temperatures (which are of greatest interest).

When condition (8) is satisfied, the expressions obtained are simplified considerably

$$\sigma_{ik} = e^2 A_{ik}(\zeta_0), \quad \varkappa_{ik} = {}^1/_3 \pi^2 k^2 T A_{ik}(\zeta_0),$$
$$\mu_{ik} = (\pi^2 k^2 T / 3e)(2A_{li}^{-1}A'_{kl} - A_{il}^{-1}A'_{lk}). \tag{17}$$

As is seen, the Wiedemann-Franz law, independent of the magnitude and direction of the magnetic field (see Ref. 3), holds here for each of the components of the conductivity and heat conduction tensors.

The asymptotic form of the conductivity tensor σ_{ik} [*i.e.*, $A_{ik}(\zeta_0)$] was analyzed in Ref. 2 in a strong magnetic field, where it was shown that this asymptotic form is independent of the kind of collision integral and is determined only by the topology of the equal-energy surfaces. Since the equations for φ_k and Ψ_k differ only in the kind of collision integral, evidently the asymptotic expression for the tensor $B_{ik}(\zeta_0)$ differs from that for the tensor $A_{ik}(\zeta_0)$ only by those factors of the corresponding powers of the magnetic field which depend on the kind of collision integral (see Sec. 3 of Ref. 2). Hence, the asymptotic form of the heat conduction tensor $\varkappa_{ik}(H)$ is similar to that of the tensor $\sigma_{ik}(H)$. If the z axis is directed along the magnetic field, then

$$\varkappa_{ik}(H) \sim \begin{pmatrix} \dfrac{a_{xx}}{H^2} & \dfrac{1}{3}\left(\dfrac{\pi k}{e}\right)^2 T\,\dfrac{ec(n_1-n_2)}{H} & \dfrac{a_{xz}}{H} \\ -\dfrac{1}{3}\left(\dfrac{\pi k}{e}\right)^2 T\,\dfrac{ec(n_1-n_2)}{H} & \dfrac{a_{yy}}{H^2} & \dfrac{a_{yz}}{H} \\ \dfrac{a_{zx}}{H} & \dfrac{a_{zy}}{H} & a_{zz} \end{pmatrix}.$$

Here n_1 (or n_2) is the number of electrons (or "holes")[2]. The expansion of the matrices a_{ik} in powers of $1/H$ starts with the zero term. If $n_1 = n_2$, then $\varkappa_{xy} \sim 1/H^2$.

Let us note that the *Wiedemann-Franz law* is always satisfied [independently of condition (8)] *for asymptotic values* of the $\varkappa_{xy}$ and σ_{xy} components independent of the kind of collision integral *for unequal numbers* of electrons and "holes." A comparison of the results of the present analysis concerning heat conduction with experiment is difficult. This is because of the scantiness of experimental data on simultaneous measurements of resistivity and heat conduction in strong magnetic fields and because the total heat conduction (which does not equal the electron heat conduction) is always measured. However, the latter difficulty is automatically avoided if the following quantity is measured

$$[\varkappa_{xy}(H) - \varkappa_{xy}(-H)] / [\sigma_{xy}(H) - \sigma_{xy}(-H)]\,T,$$

which must be asymptotically equal to the Lorentz number $\frac{1}{3}(\pi k/e)^2$ for $n_1 \neq n_2$. Here, the phonon part of the heat conduction (which evidently is independent of the magnetic field) drops out.

As we saw, the asymptotic forms of the tensors $\varkappa_{ik}$ and σ_{ik} differ substantially in those cases when $n_1 \neq n_2$ and $n_1 = n_2$. It is seen from (16) that the asymptotic form of the Thomson-coefficient tensor is also related to the topology of the equal-energy surfaces. Generally speaking, its components depend on the kind of the collision integral. However, if $n_1 \neq n_2$, then

$$\mu_{xx} \approx \mu_{yy} \approx (\pi^2 k^2 / 3e)\, T V'(\zeta_0) / V(\zeta_0).$$

Here $V(\zeta_0) = V_1(\zeta_0) - V_2(\zeta_0)$; $V_1(\zeta_0)$ is the volume in momentum space occupied by the electrons; $V_2(\zeta_0)$ is the volume "occupied" by the "holes."

As is seen, μ_{xx} and μ_{yy} depend in this case on the angles between the field and the crystallographic axes and are determined exclusively by the energy spectrum. If the open surfaces are substantial[2], then μ_{xx} and μ_{yy} are functions of the angles. If $n_1 = n_2$ [hence $V(\zeta_0) = V_1(\zeta_0) - V_2(\zeta_0) = 0$ and $V'(\zeta_0) \neq 0$]*, then the asymptotic form of the tensor μ_{ik} is as follows: the $\mu_{\alpha\beta}$ increase linearly with the magnetic field ($\alpha, \beta = x, y$), and the μ_{iz} approach saturation. Hence, a study of the asymptotic form of the Thomson coefficient tensor in a strong magnetic field affords an additional possibility of investigating the topology of the equal-energy surfaces of the conduction electrons.

* There is no foundation for the assumption $V'(\zeta_0) = 0$. For example, in the case of a quadratic isotropic dependence:

$$V'(\zeta_0) = 2\pi (3V_{1,2}/4\pi)^{1/3}[(2m_1)^{1/2} + (2m_2)^{1/2}],$$

$m_1(m_2)$ is the effective mass of the electrons ("holes").

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Quantum States of Particles Coupled to a Harmonically Oscillating Continuum with Arbitrarily Strong Interaction, I. Case of Absence of Translational Symmetry

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The ground-state energy is calculated by a variational method for the system defined by Hamiltonian (1). The trial wave-function is given by Eq. (3). The results are applied to the special cases of F and F'-centers. In the limits of weak and strong coupling, the calculated energy agrees with the exact results of second-order perturbation theory and of the adiabatic treatment respectively. The calculation can be regarded as an interpolation through the intermediate coupling region. It is valid when the effective size of the localized electron state is large, and when the conditions of the continuum model of F and F' centers are fulfilled.

WE CONSIDER systems described by a Hamiltonian of the form

$$H = -\sum_{i=1}^{N} \frac{\hbar^2}{2m_i}\Delta_i + \sum_{\varkappa, t} {}^1/_2\hbar\omega_{\varkappa t}\left(q_{\varkappa t}^2 - \frac{\partial^2}{\partial q_{\varkappa t}^2}\right) + \sum_{\varkappa i t} c_{\varkappa t}^i q_{\varkappa t}\chi_{-\varkappa}(\mathbf{r}_i) + V(\mathbf{r}_1, \ldots, \mathbf{r}_N). \quad (1)$$

Here $\mathbf{r}_i$ is the radius-vector of the ith particle, m_i is its mass, $\omega_{\varkappa t}$ is the vibration frequency of the continuum corresponding to a wave-vector $\varkappa$ and to branch number t of the energy-surface, $q_{\varkappa t}$ is the normal coordinate of the same vibration, $c_{\varkappa t}^i$ is the coupling-constant between this vibration and the ith particle, $V(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ is the potential of the interaction of the particles with each other and with external fields, and

$$\chi_{+\varkappa}(\mathbf{r}_i) = \sqrt{\frac{2}{V}}\sin\left(\varkappa\mathbf{r}_i + \frac{\pi}{4}\right)$$
$$\varkappa_j = \frac{2\pi}{L}\nu_j;\ j = 1, 2, 3; \quad (2)$$
$$\nu_j = 0 \pm 1, \pm 2, \ldots \quad V = L^3$$