RELATION BETWEEN THE KINETIC COEFFICIENTS DUE TO ELECTRON SCATTERING BY IMPURITIES

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Formulas relating thermomagnetic and galvanomagnetic kinetic coefficients are deduced from the general expressions for the kinetic coefficients. The quantum oscillations of the thermomagnetic kinetic coefficients can be determined from the formulas, provided the expression for electric conductivity is known.

As is well known, the densities of the electric current **I** and of the heat flux $\mathbf{q} - \zeta e^{-1}\mathbf{I}$ in the presence of temperature gradients ∇T and an electrochemical potential $\mathbf{E} - e^{-1}\nabla\zeta$, are equal to

$$\mathbf{I} = \hat{\sigma}\left(\mathbf{E} - \frac{1}{e}\nabla\zeta\right) - \hat{\alpha}\nabla T,$$

$$\mathbf{q} - \frac{\zeta}{e}\mathbf{I} = \hat{\beta}\left(\mathbf{E} - \frac{1}{e}\nabla\zeta\right) - \hat{\gamma}\nabla T.$$

If the electrons are scattered mainly by impurities,1) then the kinetic coefficients $\hat{\sigma}$, $\hat{\alpha}$, $\hat{\beta}$, $\hat{\gamma}$ in the absence of a magnetic field are determined by relations

$$\sigma_{ik} = e^2 \int_{-\infty}^{\infty} dE \frac{\partial f}{\partial E} G_{ik}(E), \tag{1}$$

$$\alpha_{ik} = \frac{1}{T}\beta_{ik} = \frac{e}{T}\int_{-\infty}^{\infty} dE \frac{\partial f}{\partial E}(E-\zeta)G_{ik}(E), \tag{2}$$

$$\gamma_{ik} = \frac{1}{T}\int_{-\infty}^{\infty} dE \frac{\partial f}{\partial E}(E-\zeta)^2 G_{ik}(E), \tag{3}$$

$$G_{ik}(E) = -\frac{\pi}{V}\langle \mathrm{Sp}\{\delta(E-\hat{H})\,\hat{v}_i\delta(E-\hat{H})\,\hat{v}_k\}\rangle,$$

where $f = [\exp\{(E-\zeta)/T\} + 1]^{-1}$ is the Fermi distribution function, V the volume of the system, $\hat{H}$ the Hamiltonian of the electron in the impurity field, and $\hat{\mathbf{v}}$ is the electron velocity operator.2) The angle brackets denote averaging over the random distribution of the impurities.

These formulas can be readily obtained by starting from the general expressions for the kinetic coefficients in terms of the correlators of the electric-current and energy-flux operators,[1] if the main interaction mechanism is scattering of the electrons by impurities. As shown earlier,[1] in the presence of a strong magnetic field analogous expressions hold also for the diagonal components of kinetic tensors.

We shall henceforth omit the tensors of the kinetic coefficients, remembering, however, that all the relations obtained are valid in the presence of an external magnetic field only for the diagonal components of the kinetic tensors, and that in absence of the magnetic field they are valid for all components, both diagonal and non-diagonal.

1. Using the general formulas (1)–(3), we can obtain certain relations, independent of the concrete form of the function G(E), between the kinetic coefficients. To this end we note that an arbitrary function $f((E-\zeta)/T)$, which tends rapidly to zero for large positive values of the argument, satisfies the following relations

$$(E-\zeta)f'\left(\frac{E-\zeta}{T}\right) = T^2\frac{\partial}{\partial T}\frac{1}{T}\int_{-\infty}^{\zeta} f'\left(\frac{E-\zeta'}{T}\right)d\zeta',$$

$$(E-\zeta)^2 f'\left(\frac{E-\zeta}{T}\right) = T^2\frac{\partial}{\partial T}T^2\frac{\partial}{\partial T}\frac{1}{T^2}\int_{-\infty}^{\zeta}(\zeta-\zeta')f'\left(\frac{E-\zeta'}{T}\right)d\zeta'$$

(f' is the derivative of the function f with respect to the argument). Multiplying these expressions by G(E) and integrating with respect to E, we obtain in accordance with (2) and (3)

$$\alpha(T,\zeta) = \frac{1}{e}\frac{\partial}{\partial T}\int_{-\infty}^{\zeta}\sigma(T,\zeta')d\zeta',$$

$$\gamma(T,\zeta) = \frac{1}{e^2}T\frac{\partial^2}{\partial T^2}\int_{-\infty}^{\zeta}(\zeta-\zeta')\sigma(T,\zeta')d\zeta'. \tag{4}$$

1)We note that this interaction mechanism is fundamental in the low-temperature region.

2)We use a system of units in which $\hbar = c = 1$.

Differentiating these relations with respect to ζ, we obtain

$$\frac{\partial\alpha}{\partial\zeta}=\frac{1}{e}\frac{\partial\sigma}{\partial T},\quad \frac{\partial\gamma}{\partial\zeta}=\frac{1}{e}T\frac{\partial\alpha}{\partial T}. \tag{5}$$

In the low-temperature region, $T \ll \zeta$, we have in accord with formula (1)[4]

$$\sigma(T,\zeta)=-e^2G(\zeta)-\frac{\pi^2e^2}{6}G''(\zeta)T^2-\frac{7\pi^4e^2}{24\cdot 15}G''''(\zeta)T^4+\ldots$$

Substituting this expression in (4), we get

$$\alpha(T,\zeta)=\frac{\pi^2}{3e}\frac{\partial\sigma(0,\zeta)}{\partial\zeta}T+\frac{7\pi^4}{90e}\frac{\partial^3\sigma(0,\zeta)}{\partial\zeta^3}T^3+\ldots,$$
$$\gamma(T,\zeta)=\frac{\pi^2}{3e^2}\sigma(0,\zeta)T+\frac{7\pi^4}{30e^2}\frac{\partial^2\sigma(0,\zeta)}{\partial\zeta^2}T^3+\ldots$$

The second term in the last formula is a correction to the Wiedemann–Franz law.

2. Formulas (4) and (5) allow us to find the quantum oscillations of the thermomagnetic kinetic coefficients in a strong magnetic field, if the quantum oscillations of the electric conductivity are known.

In [1-3] we obtained the following formula for the electric conductivity in the region $T \le \omega_H$ (ω_H is the Larmor frequency of the electron) in the case of electron scattering by the short-range potential of the impurity:[4]

$$\sigma_{xx}(T,\zeta)=\frac{8}{3\pi}n_ie^2a^2\left(\frac{\zeta}{\omega_H}\right)^2\left\{1+\frac{\pi^2}{3}\frac{T^2}{\zeta^2}+\frac{5}{2}\left(\frac{\omega_H}{\zeta}\right)^{1/2}\sum_{r=1}\frac{(-1)^r}{\sqrt{2r}}\Psi(\alpha_r)\cos\left(\frac{2\pi r\zeta}{\omega_H}-\frac{\pi}{4}\right)+\Delta_\sigma\right\}, \tag{6}$$

where n_i is the concentration of the impurities, a the amplitude for scattering of an electron with zero energy by the impurity in the absence of a magnetic field, $\Psi(x) = x/\sinh x$, $\alpha_r = 2\pi^2 rT/\omega_H$, and Δ_σ is defined by the formula

$$\Delta_\sigma=-\frac{3}{8}\frac{\omega_H}{\zeta}\int_0^\infty\frac{\partial f}{\partial E}\frac{E}{\zeta}\frac{dE}{(\sqrt{\eta}+a\sqrt{eH/2})^2+a^2eH/2}.$$

η is defined by

$$E=\omega_H(N+1/2)+\eta\omega_H,\quad 0\leqslant\eta<1,$$

where N is a large positive integer, (∇T, $\nabla\zeta$, and the electric field **E** are directed along the x axis, and the external magnetic field **H** along the z axis). Substituting (6) in (4), we obtain for the kinetic coefficients α_{xx} and γ_{xx}

$$\alpha_{xx}(T,\zeta)=\frac{16\pi}{9}n_iea^2\frac{T\zeta}{\omega_H^2}\left\{1-\frac{3}{2\pi}\frac{5}{2}\frac{\zeta}{T}\left(\frac{\omega_H}{\zeta}\right)^{1/2}\times\sum_{r=1}^\infty\frac{(-1)^r}{\sqrt{2r}}\Psi'(\alpha_r)\cos\left(\frac{2\pi r\zeta}{\omega_H}+\frac{\pi}{4}\right)+\Delta_\alpha\right\},$$

$$\gamma_{xx}(T,\zeta)=\frac{8\pi}{9}n_ia^2\left(\frac{\zeta}{\omega_H}\right)^2T\left\{1-\frac{15}{2}\left(\frac{\omega_H}{\zeta}\right)^{1/2}\times\sum_{r=1}^\infty\frac{(-1)^r}{\sqrt{2r}}\Psi''(\alpha_r)\cos\left(\frac{2\pi r\zeta}{\omega_H}-\frac{\pi}{4}\right)+\Delta_\gamma\right\}, \tag{7}$$

where

$$\Delta_\alpha=-\frac{9}{16\pi^2}\frac{\omega_H\zeta}{T^2}\int_0^\infty\frac{\partial f}{\partial E}\frac{E}{\zeta}\left(\frac{E}{\zeta}-1\right)\times\frac{dE}{(\sqrt{\eta}+a\sqrt{eH/2})^2+a^2eH/2}$$

$$\Delta_\gamma=-\frac{9}{8\pi^2}\frac{\omega_H\zeta}{T^2}\int_0^\infty\frac{\partial f}{\partial E}\frac{E}{\zeta}\left(\frac{E}{\zeta}-1\right)^2\times\frac{dE}{(\sqrt{\eta}+a\sqrt{eH/2})^2+a^2eH/2}.$$

We note that an error crept in in the derivation given in [1] for the expressions for α_{xx} and γ_{xx} (in the substitution of (46) in (24)). The correct expressions for α_{xx} and γ_{xx} are given by formulas (7) of the present paper.

3. In order to recast formulas (5) in a form having an intuitive physical meaning, we change from the variables T, ζ, to the variables T, V. Regarding the chemical potential ζ as a function of these variables, we obtain from (5)

$$\left(\frac{\partial\alpha}{\partial V}\right)_T=\frac{1}{e}\left\{\left(\frac{\partial\sigma}{\partial T}\right)_V\left(\frac{\partial\zeta}{\partial V}\right)_T-\left(\frac{\partial\sigma}{\partial V}\right)_T\left(\frac{\partial\zeta}{\partial T}\right)_V\right\}$$
$$\left(\frac{\partial\gamma}{\partial V}\right)_T=\frac{1}{e}T\left\{\left(\frac{\partial\alpha}{\partial T}\right)_V\left(\frac{\partial\zeta}{\partial V}\right)_T-\left(\frac{\partial\alpha}{\partial V}\right)_T\left(\frac{\partial\zeta}{\partial T}\right)_V\right\} \tag{8}$$

Introducing the coefficient of isothermal compressibility K_T:

$$K_T=-\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T,$$

we can rewrite (8) in the form

$$\left(\frac{\partial\alpha}{\partial P}\right)_T=-\frac{1}{e}\left\{\left(\frac{\partial\sigma}{\partial T}\right)_V\left(\frac{\partial\zeta}{\partial V}\right)_T VK_T+\left(\frac{\partial\sigma}{\partial P}\right)_T\left(\frac{\partial\zeta}{\partial T}\right)_V\right\},$$

$$\left(\frac{\partial\gamma}{\partial P}\right)_T = -\frac{1}{e}T\left\{\left(\frac{\partial\alpha}{\partial T}\right)_V\left(\frac{\partial\zeta}{\partial V}\right)_T VK_T + \left(\frac{\partial\alpha}{\partial P}\right)_T\left(\frac{\partial\zeta}{\partial T}\right)_V\right\}. \quad (9)$$

In these formulas, P is the external pressure. The derivatives $(\partial\zeta/\partial T)_V$ and $(\partial\zeta/\partial V)_T$ must be determined from the equation

$$n\left(\frac{V}{N_0}, T\right) = \int\frac{d\mathbf{p}}{(2\pi)^3}\left(\exp\left\{\frac{1}{T}\left[E\left(\mathbf{p}, \frac{V}{N_0}\right)-\zeta\right]\right\}+1\right)^{-1}, \quad (10)$$

which defines ζ as a function of T and V. Here N_0 is the number of unit cells in the body ($V/N_0 = \Omega$ is the unit-cell volume), $E(\mathbf{p}, V/N_0)$ is the conduction-electron dispersion law, and depends, generally speaking, on Ω, and $n(V/N_0, T)$ is the electron density in the body and depends on the volume of the unit cell and on the temperature.

Differentiating (10) with respect to V, we obtain

$$\left(\frac{\partial\zeta}{\partial V}\right)_T = A^{-1}\left\{\left(\frac{\partial n}{\partial V}\right)_T - \frac{1}{V}\int\frac{d\mathbf{p}}{(2\pi)^3}\frac{\partial f}{\partial E}\lambda(\mathbf{p})\right\}, \quad (11)$$

where

$$A = -\frac{1}{T}\int\frac{d\mathbf{p}}{(2\pi)^3}f'\left(\frac{E-\zeta}{T}\right), \quad \lambda(\mathbf{p}) = \Omega\frac{\partial E}{\partial\Omega}.$$

Similarly, differentiating (10) with respect to T, we obtain

$$\left(\frac{\partial\zeta}{\partial T}\right)_V = A^{-1}\left\{\left(\frac{\partial n}{\partial T}\right)_V + \frac{1}{T^2}\int\frac{d\mathbf{p}}{(2\pi)^3}[E(\mathbf{p})-\zeta]f'\right\}. \quad (12)$$

Formulas (9), (11), and (12) determine the connections between the derivatives of the kinetic coefficients with respect to temperature and pressure. These formulas can serve for the determination of $(\partial n/\partial T)_V$ and $(\partial n/\partial V)_T$, if the derivatives of the kinetic coefficients with respect to pressure and temperature are known.

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