ON THE QUANTUM THEORY OF TRANSPORT PHENOMENA IN STRONG MAGNETIC FIELDS

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Noncollisional particle and heat flows in an electron system due to temperature and chemical-potential gradients orthogonal to a quantized magnetic field are calculated.

1. In developing the quantum theory of thermomagnetic and galvanomagnetic phenomena emphasis is often placed upon the complexities resulting from the need for considering the gradients of temperature and carrier density. In some calculations attempts have been made to disregard these gradients by using as a perturbation only the external electric field; the kinetic coefficients are then determined by means of Onsager symmetry. This was the procedure of Ansel'm and Askerov in their theory of thermomagnetic phenomena in semiconductors.[1] We note here that the expression for the thermoelectric power obtained in [1] contains a term $\sim \hbar\Omega/eT$ which increases without limit as the temperature is reduced. This term appeared because, in addition to Onsager's relations, use was made in [1] of Einstein's relation between the diffusion coefficient and electric conductivity. The latter relation does not actually apply to the nondiagonal elements (the antisymmetric part) of the conductivity and diffusion tensors.

In the present work we consider expressions for the electric and heat currents due to electrons in a magnetic field strong enough to require that we take into account the quantization of particle levels in the field.[1)] We confine ourselves to deriving expressions not depending on collisions between electrons and scatterers,[2)] thus obtaining the aforementioned result of Ansel'm and Askerov. [1] Another purpose of the limitation is that we wish to elucidate the procedure for obtaining collisionless flows using kinetic equations such as those in [2]. The understanding of the method is hindered by the absence of such clarification in the literature.

2. In the linear transport theory currents induced by the gradients of temperature, the chemical potential ζ, and the electric potential φ are additive. We can therefore first calculate the currents produced by statistical forces proportional to ∇T and $\nabla \zeta$, to which we shall then add the currents induced by the electric field.

Since the statistical forces cannot be included in the Hamiltonian, we first calculate the mean quantum-mechanical densities of charge and energy currents for stationary states. The averaging of these currents using the state distribution of particles enables us to obtain the observed macroscopic flows.

Let us consider a system of noninteracting electrons in a strong magnetic field B parallel to the z axis. We write for an electron the Hamiltonian

$$\frac{1}{2\mu}\left(\hat{p}_x^2 + \hat{p}_z^2 + \left(\hat{p}_y - \frac{e}{c}Bx\right)^2\right).$$

The eigenvalues and eigenfunctions of this Hamiltonian are

$$E(n, p_z) = \hbar\Omega\left(n + \tfrac{1}{2}\right) + p_z^2/2\mu,$$

$$|n, p_z, x_0\rangle = (L_y L_z \alpha)^{-1/2}\exp\left(\left[ip_y y + ip_z z\right]/\hbar\right)\Phi_n\left(\frac{x - x_0}{\alpha}\right),$$

where

$$\alpha^2 = c\hbar/|e|B, \quad \Omega = |e|B/\mu c, \quad x_0 = cp_y/eB;$$

L_y and L_z characterize the normalization volume, and $\Phi_n(x)$ is a normalized oscillator eigenfunction.

The foregoing equations enable us to obtain the mean quantum-mechanical densities of the electric and energy currents in a state $|n, p_z, x_0\rangle$. We have

$$j_y(n, p_z, x_0) = \frac{e\Omega}{L_y L_z \alpha}(x - x_0)\Phi_n^2\left(\frac{x - x_0}{\alpha}\right), \quad (1)$$

$$Q_y(n, p_z, x_0) = \frac{\Omega}{L_y L_z \alpha}(x - x_0)E(n, p_z)\Phi_n^2\left(\frac{x - x_0}{\alpha}\right). \quad (2)$$

These are still not the desired results, but must be

[1)]Practical conditions requiring consideration of such quantization exist, for example, in semiconductors at very low temperatures[1] and, of course in semimetals.

[2)]We thus limit ourselves to fields for which the electronic Larmor frequency Ω considerably exceeds the collision frequency τ^{-1}.

averaged using the distribution function $f(n, p_z, x_0)$ describing the electron level populations.

3. For the considered case of strong magnetic fields, where the Larmor frequency considerably exceeds the collision frequency, collisions may be neglected in zeroth approximation. The density matrix is then obviously diagonal in the energy representation. We can therefore speak of a distribution function which can be regarded as a function of eigenvalues of the Hamiltonian and other operators commuting with the Hamiltonian and forming a complete set. Specifically, the distribution function can be written as

$$f_0\left(\frac{E(n, p_z) - \zeta(x_0)}{T(x_0)}\right), \qquad (3)$$

where f_0 is the Fermi function.

Equation (3) can be used to determine such quantities as the temperature T and chemical potential ζ, which are taken to be dependent on x_0. This dependence represents the nonuniformity of the particle distribution across the magnetic field.

We shall say that (3) describes the local equilibrium distribution. However, the meaning of this statement differs very considerably from its meaning in conventional kinetic theory based on an equation containing the Boltzmann collision integral. Equation (3) does not make the collision integral vanish. Indeed, in the case of elastic scattering on disordered heavy scatterers the collision integral in the $|n, p_z, x_0\rangle$ representation becomes

$$\sum_{n',q} \frac{2\pi}{\hbar} |C_q|^2 F_{n'n}(\alpha^2 q_\perp^2/2)\, \delta\,(E(n', p_z + \hbar q_z) - E(n, p_z))$$
$$\times [f(n', p_z + \hbar q_z, x_0 + \alpha^2 q_y) - f(n, p_z, x_0)], \qquad (4)$$

where $q_\perp^2 = q_x^2 + q_y^2$, C_q is a Fourier component of the electron-scatterer interaction potential, and

$$F_{n', n} = |\langle n', x_0 + \alpha^2 q_y | \exp(iq_x x) | n, x_0 \rangle|^2.$$

It is obvious that the Fermi (or Boltzmann) distribution (3) makes the collision integral (4) vanish only for a temperature and chemical potential that are independent of x_0. On the other hand, for a spatially nonuniform distribution of temperature and the chemical potential the collision integral does not vanish. This fact was known previously, and was even employed in developing a theory of diffusion. [2] Weak nonuniformity is an essential assumption so that an expansion in powers of $\alpha^2 q_y$ can be used in the argument of the distribution function in (4). The expansion is actually carried out in powers of $\alpha^2 q_y/L$, where L is the characteristic dimension of the distribution nonuniformity. From (4) we then have up to second-order terms [3]

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[3] First order terms in $\alpha^2 q_y$ vanish by symmetry.

$$\sum_{n',q} \frac{2\pi}{\hbar} |C_q|^2 F_{n',n}\,(\alpha^2 q_\perp^2/2)\,\Big\{\delta\,[E(n', p_z + \hbar q_z) - E(n, p_z)]$$
$$\times [f(n', p_z + \hbar q_z, x_0) - f(n, p_z, x_0)]$$
$$+ \frac{1}{2}(\alpha^2 q_y)^2\,\delta[E(n', p_z + \hbar q_z)$$
$$- E(n, p_z)]\frac{\partial^2}{\partial x_0^2} f(n', p_z + \hbar q_z, x_0) + \ldots\Big\}. \qquad (5)$$

This collision integral can be used to determine flows due to collisions; but this is not our present subject. It is important that except for small quantities which are neglected in calculating collisionless flows, the local distribution (3) causes the collision integral (5) to vanish.

4. In accordance with the foregoing, the desired expressions for the electric and energy currents are determined from

$$j_y = 2 \sum_{n, p_z, x_0} f(n, p_z, x_0)\, j_y(n, p_z, x_0), \qquad (6)$$

$$Q_y = 2 \sum_{n, p_z, x_0} f(n, p_z, x_0)\, Q_y(n, p_z, x_0), \qquad (7)$$

where the distribution function has the form of (3).

Assuming weak nonuniformity, we use

$$\zeta(x_0) = \zeta + x_0 \nabla_x \zeta, \quad T(x_0) = T + x_0 \nabla_x T,$$

where $\nabla_x T$ and $\nabla_x \zeta$ are small. We then have, up to linear terms in $\nabla_x \zeta$ and $\nabla_x T$,

$$f(n, p_z, x_0) = f_0\left(\frac{E(n, p_z) - \zeta}{T}\right)$$
$$+ f_0(1 - f_0)\left[\nabla_x \zeta + \frac{E(n, p_z) - \zeta}{T}\nabla_x T\right]\frac{x_0}{T}.$$

Using this expression for the distribution function, we obtain

$$j_y = \frac{c}{BT}\frac{2}{(2\pi\alpha)^2 \hbar}\sum_n \hbar\Omega\left(n + \frac{1}{2}\right)\int dp_z f_0(1 - f_0)$$
$$\times \left[\nabla_x \zeta + \frac{E(n, p_z) - \zeta}{T}\nabla_x T\right], \qquad (8a)$$

with

$$N = \frac{2}{(2\pi\alpha)^2 \hbar}\sum_n \int dp_z f_0$$

representing the number of electrons per unit volume.

For heat flow we have similarly

$$w_y = \frac{c}{eBT}\frac{2}{(2\pi\alpha)^2 \hbar}\sum_n \hbar\Omega\left(n + \frac{1}{2}\right)\int dp_z f_0(1 - f_0)$$
$$\times [E(n, p_z) - \zeta]\left[\nabla_x \zeta + \frac{E(n, p_z) - \zeta}{T}\nabla_x T\right]. \qquad (9a)$$

To these currents we must add the corresponding currents due to the electric field with the potential $\varphi = -\mathcal{E}_x x$, given in [3,1]:

$$j_y = -\frac{ceN}{B}\mathcal{E}_x, \qquad (8b)$$

$$w_y = -\frac{cN}{B}(\bar{E} + \bar{E}_\perp - \zeta)\mathscr{E}_x, \qquad (9b)$$

where

$$(\bar{E} + \bar{E}_\perp)N = \frac{2}{(2\pi\alpha)^2\hbar}\sum_n \int dp_z\left[E(n, p_z) + \hbar\Omega\left(n + \frac{1}{2}\right)\right]f_0.$$

These equations of the approximation that is linear in $\mathscr{E}_x$ can also be derived by averaging (1) and (2) using a distribution function for a spatially uniform particle density (independent of x_0) $f_0[E(n, p_z) - \zeta)/T]$. In (1) and (2) we must first make the substitutions $x_0 \to x_0 - \mu c\mathscr{E}_x/eB$, and

$$E(n, p_z) \to E(n, p_z) - e\mathscr{E}_x x_0 + \mu c^2\mathscr{E}_x^2/2B^2,$$

because to the Hamiltonian we are now adding the potential energy $e\varphi$, thus shifting the energy eigenvalues by the amount $(-e\mathscr{E}_x x_0 + \mu c^2\mathscr{E}_x^2/2B^2)$ and x_0 by the amount $(-\mu c\mathscr{E}_x/eB)$. The eigenfunctions remain unchanged.

Adding (8a) and (8b), and (9a) and (9b), we have as the final equations for the currents:

$$j_y = -\frac{ceN}{B}\mathscr{E}_x + \frac{c}{BT}\frac{2}{(2\pi\alpha)^2\hbar}\sum_n\hbar\Omega\left(n + \frac{1}{2}\right)$$
$$\times \int dp_z f_0(1 - f_0)\left[\nabla_x\zeta + \frac{E(n, p_z) - \zeta}{T}\nabla_x T\right], \qquad (8)$$

$$w_y = -\frac{cN}{B}(\bar{E} + \bar{E}_\perp - \zeta)\mathscr{E}_x + \frac{c}{eBT}\frac{2}{(2\pi\alpha)^2\hbar}$$
$$\times \sum_n\hbar\Omega\left(n + \frac{1}{2}\right)\int dp_z f_0(1 - f_0)[E(n, p_z)$$
$$- \zeta]\left[\nabla_x\zeta + \frac{E(n, p_z) - \zeta}{T}\nabla_x T\right]. \qquad (9)$$

A comparison of these equations reveals the symmetry of the kinetic coefficients characterizing the currents due to the spatial nonuniformity of the electron distribution. In other words, the coefficient of the temperature gradient in (8) when multiplied by T/e coincides with the coefficient of the chemical potential gradient in (9). It is very important, however, that the electric field strength and the chemical potential gradient are included entirely differently in (8) and (9). In this sense Einstein's relation between conductivity and the diffusion coefficient is violated. It should be noted that the possibility of this violation had been noted previously by Kasuya[4].

In the classical limit ($\hbar = 0$) Eqs. (8) and (9) become

$$j_y = -\frac{cNe}{B}\left(\mathscr{E}_x - \frac{1}{e}\nabla_x\zeta\right) + \frac{cN}{BT}(\bar{E} + \bar{E}_\perp - \zeta)\nabla_x T, \qquad (10)$$

$$w_y = -\frac{cN}{B}(\bar{E} + \bar{E}_\perp - \zeta)\left(\mathscr{E}_x - \frac{1}{e}\nabla_x\zeta\right)$$
$$+ \frac{cN}{eBT}\overline{((E - \zeta)(\zeta - E - 2E_\perp))}\nabla_x T. \qquad (11)$$

Here

$$N = \frac{2}{(2\pi\hbar)^3}\int d\mathbf{p}f_0,$$

$$(\bar{E} + \bar{E}_\perp)N = \frac{2}{(2\pi\hbar)^3}\int d\mathbf{p}\left(\frac{\mathbf{p}^2}{2\mu} + \frac{p_x^2 + p_y^2}{2\mu}\right)f_0,$$

$$\overline{((E - \zeta)(E + 2E_\perp - \zeta))}N$$
$$= \frac{2}{(2\pi\hbar)^3}\int d\mathbf{p}\left(\frac{\mathbf{p}^2}{2\mu} - \zeta\right)\left(\frac{\mathbf{p}^2}{2\mu} + \frac{p_x^2 + p_y^2}{\mu} - \zeta\right)f_0.$$

Equations (10) and (11) obviously satisfy the symmetry of kinetic coefficients. Einstein's relation is also satisfied, since the electric field strength and chemical potential appear in the combination $\mathscr{E}_x - \nabla_x\zeta/e$.

It appears from the foregoing that Einstein's relation is violated only when the quantization of orbital electronic motion is essential. This can be accounted for in an elementary way. In a state of thermodynamic equilibrium, as is evident from the distribution function (3) used in the calculations, the electrochemical potential is constant; this results from the entropy maximum. The fact that the expressions for the currents in the quantum case do not vanish for a constant electrochemical potential does not conflict with the principle of maximum entropy, because these flows do not change the entropy. The existence of an electric current in a state of thermodynamic equilibrium is associated in the quantum case with Landau diamagnetism. Indeed, in the presence of an equilibrium concentration gradient of the chemical potential in the x direction perpendicular to B, the diamagnetic susceptibility χ will be a function of x. This means that the magnetization χB will also depend on x. But then $(j_y)_{qu} = c$ curl$_y$ χB (see the Appendix) is a current associated with Landau diamagnetism. In the classical case this current disappears because the diamagnetism of the electron gas disappears.

An expression for the electric current similar to (8) has already been given by Ansel'm and Askerov[5] without a valid derivation. However, these authors did not observe the violation of the Einstein relation in the quantum case, and therefore could not have determined the causes of this violation. Moreover, upon observing the conflict between their results and the Onsager principle, they rejected their results in their following publication.[1] The latter work was based on the so-called "π approach" of Herring,[6] which assumes the fulfillment of both the Einstein relation and Onsager symmetry. It follows from our treatment that Herring's π approach should not be transferred from the classical to the quantum region.

APPENDIX

No detailed discussion can be found anywhere of the violation of Einstein's relation between the nondiagonal antisymmetric parts of the diffusion and electric conductivity tensors in a quantized magnetic field. We therefore considered it advisable to present a different, thermodynamic, derivation of the equation for the current resulting from a spatially nonuniform chemical potential. This derivation leads to a more intuitively clear understanding of the reason for violation of the Einstein relation.

We begin with the thermodynamic equation for the density of the magnetic moment, $M(x_0)$:

$$M_z(x_0) = -\partial F(x_0)/\partial B_z, \qquad (A.1)$$

where $F(x_0)$ is the free-energy density of a Fermi gas;

$$F(x_0) = N(x_0)\,\zeta(x_0) - 2T \sum_{n,\,p_z} \ln\left[1 + \exp\left(-\left[E(n, p_z)\right.\right.\right.$$

$$\left.\left.\left. - \zeta(x_0)\right]/T\right)\right]. \qquad (A.2)$$

From (A.1) and (A.2) we obtain

$$M_z(x_0) = -\frac{2}{B_z} \sum_{n,\,p_z} \hbar\Omega\left(n + \tfrac{1}{2}\right) f_0\left(\frac{E(n, p_z) - \zeta(x_0)}{T}\right), \qquad (A.3)$$

where f_0 is the Fermi function.

In the case of weak spatial nonuniformity, when $\zeta(x_0) = \zeta + \nabla_x\zeta x_0$ we have from (A.3), as a linear approximation in $\nabla_x\zeta$,

$$M_z(x_0) = M_{0z} - \frac{2}{BT} \sum_{n,\,p_z} \hbar\Omega\left(n + \tfrac{1}{2}\right) f_0\,(1 - f_0)\,\nabla_x\zeta x_0, \qquad (A.4)$$

where M_0 is the spatially uniform part of the magnetic moment (independent of x_0).

The spatially nonuniform distribution of the magnetic moment can correspond to a "molecular current" $j = c\,\mathrm{curl}\,M$. In our case

$$j_y = -c\frac{\partial}{\partial x_0} M_z = \frac{c}{BT} 2 \sum_{n,\,p_z} \hbar\Omega\left(n + \tfrac{1}{2}\right) f_0\,(1 - f_0)\,\nabla_x\zeta. \qquad (A.5)$$

Averaging over x_0 and transforming the summation over p_z into an integral, we obtain

$$j_y = \frac{c}{BT}\frac{2}{(2\pi\alpha)^2\hbar} \sum_n \hbar\Omega\left(n + \tfrac{1}{2}\right) \int dp_z f_0\,(1 - f_0)\,\nabla_x\zeta. \qquad (A.6)$$

This agrees with (8a) for $\nabla_x T = 0$. In the presence of an electric field in the x direction, we add to (A.6) the current

$$- \sigma_{xy}\mathscr{E}_x = -\frac{cNe}{B}\mathscr{E}_x = \frac{cNe}{B}\nabla_x\Phi.$$

Adding these currents and writing separately the classical part of (A.6) (the limit at $\hbar = 0$), we obtain

$$j_y = \frac{cN}{B}\nabla_x(e\Phi + \zeta) + (j_y)_{\mathrm{qu}}, \qquad (A.7)$$

where the quantum current $(j_y)_{\mathrm{qu}}$ is

$$(j_y)_{\mathrm{qu}} = (c\,\mathrm{curl}\,\chi\,\mathbf{B})_y$$

$$= \left\{\frac{c}{BT}\frac{2}{(2\pi\alpha)^2\hbar} \sum_n \hbar\Omega\left(n + \tfrac{1}{2}\right)\int dp_z f_0\,(1 - f_0) - \frac{cN}{B}\right\}\nabla_x\zeta. \qquad (A.8)$$

In thermodynamic equilibrium we have the electrochemical potential $(e\Phi + \zeta) = \mathrm{const}$, and $j_y = (j_y)_{\mathrm{qu}}$. It is easily seen from the derivation of (A.6) that this current results from the spatially nonuniform distribution of the Landau diamagnetic moment. In the classical limit the diamagnetism disappears and, according to (A.8), $\lim_{\hbar=0} (j_y)_{\mathrm{qu}} = 0$. It follows from the foregoing that the Einstein relation is violated because of Landau diamagnetism.

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