THE QUANTUM THEORY OF THE ELECTRICAL CONDUCTIVITY OF METALS IN STRONG MAGNETIC FIELDS

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Submitted to JETP editor April 8, 1960

We consider quantum mechanically galvanomagnetic phenomena in strong magnetic fields at very low temperatures in the limit where the lifetime of an electron is much larger than the period of its revolution in the magnetic field. We investigate metals with a quadratic dispersion law. We obtain formulae for the scattering of an electron by an impurity when a magnetic field is present.

I. M. Lifshitz and co-workers[1,2] have recently constructed in a number of papers a semi-classical theory of galvanomagnetic phenomena in metals in strong magnetic fields, taking the complicated character of the dispersion law for the elementary excitations into account. Also, a number of authors[3-5] obtained the quantum corrections to the resistivity tensor (the Shubnikov—de Haas effect). The results of different papers are, however, not in agreement with one another. A clarification of this problem is essentially connected with the paper by Adams and Holstein,[6] in which the transverse part of the conductivity tensor $\sigma_{\alpha\alpha}$ ($\alpha = x, y$; H is parallel to the z axis) was evaluated for a dispersion law $\epsilon = p^2/2m$ and in which the calculations of other authors were analyzed.

We obtain in the present paper expressions for σ_{ik} for metals with a small number of carriers, the dispersion law of which we know with assurance to be very close to quadratic. The energy surface can then be split up into several mutually nonintersecting ellipsoids. Bismuth is a typical example of such a metal.

One of the basic problems which arise also in the quantum case is that of taking into account the specific character of the scattering of an electron by impurities when a strong magnetic field is present. It will be shown in the following that in several cases an account of this fact determines in an essential way how the different quantities depend on the magnetic field.

1. FREE ELECTRON IN A MAGNETIC FIELD

We consider the motion of an electron with an arbitrary quadratic dispersion law

$$\varepsilon = \tfrac{1}{2} \mu_{ik} p_i p_k \tag{1}$$

in a strong magnetic field. We find the wave functions and energy eigenvalues from the Schrödinger equation (here and henceforth $\hbar = c = 1$)

$$\hat{H}\psi_n = \tfrac{1}{2}\mu_{ik}(\hat{p}_i - eA_i)(\hat{p}_k - eA_k)\psi_n = E_n\psi_n, \tag{2}$$

where μ_{ik} is the symmetrical inverse mass tensor and A_i the components of the vector potential of the magnetic field.

It is well known that the state of an electron in a magnetic field is characterized by the following quantities: the momentum p_z along the z axis, the momentum p_y which is connected with the x component x_0 of the center of the orbit along the x axis by the relation

$$x_0 = p_y/eH$$

and the magnetic quantum number M. In the following the index n denotes the set of all these quantities.

The energy eigenvalue of the n-th state is

$$E_n = \omega(M + \tfrac{1}{2}) + p_z^2/2m_{zz},$$

where $\omega = eH\sqrt{m_{zz}/|m|}$, m_{ik} are the components of the mass tensor ($m_{ik} = \mu_{ik}^{-1}$) and $|m|$ is the determinant of the mass tensor.

We need in this paper the quantity

$$\int (x - x_0)^2 |\psi_n(x)|^2 dx.$$

If we use the well-known solutions of Eq. (2) we get easily

$$\int (x - x_0)^2 |\psi_n(x)|^2 dx = (M + \tfrac{1}{2})\frac{\mu_{xx}}{\omega}. \tag{3}$$

2. SCATTERING OF AN ELECTRON IN A MAGNETIC FIELD BY AN IMPURITY

We need to know in the following the scattering amplitude for the scattering of an electron in a strong magnetic field by an impurity. Finding this amplitude is made much easier by the fact that for the metals with a small number of carriers, which we are considering, the electron wavelength is large compared with the range of the potential. It is well known that in that case we can use a δ-function potential to evaluate the transition amplitude

$$U(r) = f\delta(r), \qquad (4)$$

where f is the scattering amplitude for a zero-energy electron, when there is no magnetic field and where we have assumed for the sake of simplicity that the impurity is at the origin. We have then for the amplitude for the transition from the state n to the state m:

$$F_{mn} = \int \psi_m^*(r) U(r) \psi_n(r) dr = f\psi_m^*(0)\psi_n(0). \qquad (5)$$

Using this expression for the transition amplitude we can obtain the total probability for a transition from the state n to any state m ($E_m = E_n$):

$$W_n = 2\pi f^2 \sum_m |\psi_m(0)|^2 |\psi_n(0)|^2 \delta(E_n - E_m)$$

$$= \sqrt{2}\pi^{-1}f^2 |\psi_n(0)|^2 \omega |m|^{1/2} \sum_M [E_n - \omega(M+1/2)]^{-1/2}. \qquad (6)$$

The summation is over those values of M for which the expression under the radical sign is positive. It is clear from the expression given here for W_n that one can choose a value of the magnetic field in such a way that $E_n = \omega(N + 1/2) + \Delta$, $|\Delta| \ll \omega$. If $\Delta > 0$ and sufficiently small,

$$W_n = f^2 |\psi_n(0)|^2 \frac{\sqrt{2}\omega |m|^{1/2}}{\pi \sqrt{\Delta}}, \qquad (7)$$

i.e., when $\Delta \to 0$ the total transition probability tends to infinity. The result obtained indicates that if one takes the influence of the magnetic field on the scattering into account only through Eq. (5), this will, as is well known, be insufficient in the neighborhood of some values of the magnetic field.

We try to find those corrections to F_{mn} in the higher approximations in U which are due only to the presence of the magnetic field. Generally speaking, one can only use the potential in the form (4) when looking for the transition amplitude in the first Born approximation. We retain (4), however, also when looking for the next approxi-

mations in the scattering amplitude, but keep in the different terms only expressions which are essentially connected with the magnetic field.

The exact transition amplitude is in the form of a series

$$F_{mn} = U_{mn} - \sum_k \frac{U_{mk}U_{kn}}{E_k - E - i\delta} + \sum_{k,l} \frac{U_{mk}U_{kl}U_{ln}}{(E_k - E - i\delta)(E_l - E - i\delta)}. \qquad (8)$$

We consider the second term in that series in more detail

$$-\sum_k \frac{U_{mk}U_{kn}}{E_k - E - i\delta} = -f^2\psi_m^*(0)\psi_n(0) \sum_k \frac{|\psi_k(0)|^2}{E_k - E - i\delta}$$

$$= -f^2\psi_m^*(0)\psi_n(0)\frac{\omega|m|^{1/2}}{2^{3/2}\pi}\left\{i\sum_M [E - \omega(M+1/2)]^{-1/2}\right.$$

$$\left. +\sum_M [\omega(M+1/2) - E]^{-1/2}\right\}. \qquad (9)$$

Here and henceforth the summation over M is only over those values of M for which the respective expressions under the square root sign are positive. The second sum within the curly brackets diverges. This divergence is caused by the fact that we have used a δ-function potential. If we take f to mean the total amplitude for E = 0 when there is no magnetic field, we must simply drop the divergent terms. The correction to the scattering amplitude in the second Born approximation will be small except when the energy is very near a odd-half-integral multiple of ω, i.e., $\Delta \to 0$. If the absolute magnitude of Δ is sufficiently small the expression within the braces is equal to

$$\frac{i}{\sqrt{\Delta}} = \begin{cases} \dfrac{i}{\sqrt{\Delta}}, & \Delta > 0 \\ \dfrac{1}{\sqrt{|\Delta|}}, & \Delta < 0 \end{cases}$$

and we get for (9) as $\Delta \to 0$

$$-f^2\psi_m^*(0)\psi_n(0)\frac{i\omega|m|^{1/2}}{2^{3/2}\pi\sqrt{\Delta}}.$$

We note easily that if we retain only the terms that tend to infinity in the series (8) near $\Delta = 0$, we get the simple geometric series

$$F_{mn} = f\psi_m^*(0)\psi_n(0)\{1 - fG_1 + f^2G_1^2 - \ldots\}$$

$$= f\psi_m^*(0)\psi_n(0)(1 + fG_1)^{-1},$$

$$G_1 = \frac{\omega|m|^{1/2}}{2^{3/2}\pi\sqrt{\Delta}}. \qquad (10)$$

From the relation just obtained it is clear that as $\Delta \to 0$

$$|F_{mn}|^2 = |\psi_m(0)|^2 |\psi_n(0)|^2 8\pi^2 |\Delta|/\omega^2 |m|.$$

In some cases the amplitude has still another singularity. Let $\Delta < 0$. Then

$$F_{mn} = f\psi_m^*(0)\,\psi_n(0)\left\{1 + \frac{f\omega\,|m|^{1/2}}{2^{3/2}\pi\,\sqrt{|\Delta|}}\right\}^{-1}.$$

If $f < 0$ then for some value of $|\Delta_0|$ such that

$$|\Delta_0|^{1/2} = -f\omega\,|m|^{1/2}/2^{3/2}\pi \ll \omega,$$

F_{mn} will tend formally to infinity. It is clear that when $\Delta = -|\Delta_0|$ and $\Delta = 0$ Eq. (10) for the transition amplitude becomes incorrect, for in fact the amplitude will tend neither to zero nor to infinity.

It is easiest to correct Eq. (10) near $\Delta = -|\Delta_0|$. Near this point it is no longer possible to discard the finite imaginary part in Eq. (9). Taking this fact into account, we get the following expression for the amplitude near the resonance*

$$F_{mn} = f\psi_m^*(0)\,\psi_n(0)\,\left\{1 + \frac{f\omega\,|m|^{1/2}}{2^{3/2}\pi\,\sqrt{|\Delta|}}\right.$$

$$\left. + i\frac{f\omega\,|m|^{1/2}}{2^{3/2}\pi}\sum_M [E - \omega(M + 1/2)]^{-1/2}\right\}^{-1}. \qquad (11)$$

We note here that the resonance width $(\Delta E)_{\text{res}}$ is much smaller than the width of the interval ΔE in which the amplitude is less than its classical value, namely

$$(\Delta E)_{\text{res}} \sim \Delta E\,\sqrt{\sigma}/\lambda,$$

where σ is the scattering cross section for $H = 0$, and $1/\lambda \sim \sqrt{mE}$. The presence of such a resonance is connected with the existence of a bound state of the electron in the attractive potential when a magnetic field is present. To find the energy and the wave function of this bound state we turn to the integral equation for the wave function

$$\psi(r) = -\int G(r,\ r';\ E)\,U(r')\,\psi(r')\,dr', \qquad (12)$$

where

$$G(r,\ r';\ E) = \sum_n \frac{\psi_n(r)\,\psi_n^*(r')}{E_n - E - i\delta} \qquad (\delta \to 0), \qquad (13)$$

is the electron Green function. It is necessary for us to find the wave function in the region where the attractive force is acting, i.e., for very small values of r and r'. In that region, however,

$$G(r,\ r';\ E) = G_0(r,\ r') + G_1(E),$$

where $G_0(r,\ r')$ is the electron Green function for $E = 0$ when there is no magnetic field. To obtain $G_1(E)$ we take it into account that when there is

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no impurity the electron is in the ground state with $M = 0$. The attraction of the impurity causes the energy to become equal to

$$E = \omega/2 - \delta_1, \qquad 0 < \delta_1 \ll \omega.$$

There is then in the sum (13) a large term corresponding to $M = 0$, which is equal to

$$G_1(E) = \frac{\omega\,|m|^{1/2}}{2^{1/2}\pi\sqrt{\omega/2 - E}},$$

so that

$$\psi(r) = -\int [G_0(r,\ r') + G_1(E)]\,U(r')\,\psi(r')\,dr'$$

$$= G_1(E)\,\alpha - \int G_0(r,\ r')\,U(r')\,\psi(r')\,dr',$$

$$\alpha = -\int U(r')\,\psi(r')\,dr'.$$

One obtains easily from this equation the fact that $\psi(r) = G_1(E)\,\alpha\psi_0(r)$, where $\psi_0(r)$ is the electron wave function for $E = 0$ in the field of the impurity when there is no magnetic field. It is clear that

$$f = \int U(r)\,\psi_0(r)\,dr,$$

from which one obtains easily a condition for finding the energy

$$1 = -fG_1(E) = -f\omega\,|m|^{1/2}/2^{1/2}\pi\sqrt{\omega/2 - E},$$

$$E = \omega/2 - f^2\omega^2\,|m|/8\pi^2. \qquad (14)$$

This is indeed the energy of the bound state.

Using (12) one obtains easily an expression for the wave function of the bound state far from the impurity (for the sake of simplicity we have written down here the expression for the case $\epsilon = p^2/2m$)

$$\psi(r) = A\exp\left\{-|z|\sqrt{2m\,(\omega/2 - E)} - \frac{1}{4}\,(x^2 + y^2)eH\right\}, \qquad (15)$$

where A is a normalizing factor. It is clear that there can only be a bound state if the magnitude of the reciprocal volume occupied by the electron is much larger than the impurity concentration, i.e., the condition

$$N_{\text{imp}} \ll (eH)^2\,mf$$

must be satisfied.

It is clear that the resonance found in the foregoing for the scattering of electrons when $M > 0$ is caused by the virtual transition to the bound state. In the following we discuss the problem of the possibility to observe this resonance by investigating the behavior of the resistivity in a magnetic field.

We now turn to an investigation of the behavior

of F_{mn} near $\Delta = 0$, i.e., near the point where it tends to zero, according to (10). To do this we turn to the integral equation for the wave function $\psi(\mathbf{r})$

$$\psi_n(\mathbf{r}) = \psi_{n0}(\mathbf{r}) - \int G(\mathbf{r}, \mathbf{r}'; E) U(\mathbf{r}') \psi_n(\mathbf{r}') d\mathbf{r}'. \quad (16)$$

When $\Delta \approx 0$ Eq. (13) for $G(\mathbf{r}, \mathbf{r}'; E)$ can be written as the sum of two terms

$$G(\mathbf{r}, \mathbf{r}'; E) = G'(\mathbf{r}, \mathbf{r}'; E) + \Delta^{-1/2} g_N(\boldsymbol{\rho}, \boldsymbol{\rho}'), \quad \Delta \to 0.$$

In the expression for $G'(\mathbf{r}, \mathbf{r}'; E)$ the summation is over all magnetic quantum numbers $M \neq N$ ($E = \omega(N + \frac{1}{2})$) and we can thus put $\Delta = 0$ in $G'(\mathbf{r}, \mathbf{r}'; E)$ and $g_N(\boldsymbol{\rho}, \boldsymbol{\rho}')$. It is clear that $g_N(\boldsymbol{\rho}, \boldsymbol{\rho}')$ is independent of z and z', i.e., the z component of the vector $\boldsymbol{\rho}$ is equal to zero.

The function $\psi_n(\mathbf{r})$ satisfies in the point $\Delta = 0$ two equations

$$\int g_N(\boldsymbol{\rho}, \boldsymbol{\rho}') U(\mathbf{r}') \psi_n(\mathbf{r}') d\mathbf{r}' = 0, \quad (17)$$

$$\psi_n(\mathbf{r}) = \psi_{n0}(\mathbf{r}) + A(\boldsymbol{\rho}) - \int G'(\mathbf{r}, \mathbf{r}'; E) U(\mathbf{r}') \psi_n(\mathbf{r}') d\mathbf{r}', \quad (17')$$

where $A(\rho)$ is some function which is independent of z and which is determined by (17). Because (17) must be satisfied for any ρ, Eq. (17') is equivalent to the condition

$$\int U(\boldsymbol{\rho}, z) \psi_n(\boldsymbol{\rho}, z) dz = 0. \quad (17'')$$

If the potential $U(\mathbf{r})$ is sufficiently weak it is clear from (17') that

$$\frac{\partial \psi_n}{\partial z} = \frac{\partial \psi_{n0}}{\partial z} = ip_z^n \psi_{n0}, \qquad \frac{\partial^2 \psi_n}{\partial z^2} = \frac{\partial^2 \psi_{n0}}{\partial z^2} = -(p_z^n)^2 \psi_{n0},$$

$$p_z^n \neq 0.$$

We put $\psi_{n0}(\mathbf{r}) = \exp(ip_z^n z) \varphi_n(\boldsymbol{\rho})$. We have then from (17'')

$$\psi_n(\boldsymbol{\rho}, 0) \int U(\boldsymbol{\rho}, z) \, dz + ip_z^n \varphi_n(\boldsymbol{\rho}) \int z U(\boldsymbol{\rho}, z) \, dz$$

$$- \frac{(p_z^n)^2}{2} \varphi_n(\boldsymbol{\rho}) \int z^2 U(\boldsymbol{\rho}, z) \, dz = 0,$$

$$\psi_n(\boldsymbol{\rho}, 0) = -ip_z^n \varphi_n(\boldsymbol{\rho}) \frac{\int z U(\boldsymbol{\rho}, z) \, dz}{\int U(\boldsymbol{\rho}, z) \, dz}$$

$$+ \frac{(p_z^n)^2}{2} \varphi_n(\boldsymbol{\rho}) \frac{\int z^2 U(\boldsymbol{\rho}, z) \, dz}{\int U(\boldsymbol{\rho}, z) \, dz}.$$

We now get easily the amplitude for the transition from the state n to the state m

$$F_{mn} = \int \psi_{m0}^*(\mathbf{r}) U(\mathbf{r}) \psi_n(\mathbf{r}) d\mathbf{r} = p_z^n p_z^m \int d\boldsymbol{\rho} \varphi_m^*(\boldsymbol{\rho}) \varphi_n(\boldsymbol{\rho})$$

$$\times \left\{ \int z^2 U(\boldsymbol{\rho}, z) dz - \left[\int U(\boldsymbol{\rho}, z) z dz\right]^2 \Big/ \int U(\boldsymbol{\rho}, z) dz \right\},$$

$$p_z^n \neq 0, \quad p_z^m \neq 0, \quad (18)$$

i.e., we get for $\Delta = 0$ a transition amplitude which though very small is different from zero.

We considered the case where there was one group of electrons. In practice, however, the energy surface in metals splits up into several ellipsoids and to each of these there corresponds a well defined group of electrons. In the scattering field of the impurity there are now possible not only transitions within a given group, but also a transition from one group into another one. In the following we shall give a qualitative analysis of this case.

We can now write the wave function in the following form

$$\psi(\mathbf{r}) = \psi_n^l(\mathbf{r}) e^{ip_l \mathbf{r}},$$

where $\psi_n^l(\mathbf{r})$ is the solution of Eq. (2) with the inverse mass tensor μ_{ik}^l corresponding to the ellipsoid with index 1, while the phase factor $e^{ip_l \mathbf{r}}$ is due to the fact that the center of the ellipsoid in quasi-momentum space is not the same as the origin.

It is now no longer possible to assume the potential to have a δ-function shape, since when an electron goes from one group to another there occurs an appreciable transfer of quasi-momentum. At the same time, we shall assume that when H $=0$ the potential is a Born potential. We have then in first approximation

$$F_{mn}^{l'l} = \int e^{-p_{l'} \mathbf{r}} \psi_m^{*l'}(\mathbf{r}) U(\mathbf{r}) e^{ip_l \mathbf{r}} \psi_n^l(\mathbf{r}) d\mathbf{r}$$

$$\approx \psi_m^{l'*}(0) \psi_n^l(0) \int e^{-i(p_{l'}-p_l)\mathbf{r}} U(\mathbf{r}) d\mathbf{r}$$

$$= f_{l'l} \psi_m^{l'*}(0) \psi_n^l(0) = U_{mn}^{l'l}.$$

We assume now that in the group l_0 there is for given H a state with $v_z \sim 0$, i.e., $\Delta l_0 \sim 0$. It is now no longer possible to restrict ourselves to the first Born approximation, so that

$$F_{mn}^{l'l} = U_{mn}^{l'l} - \sum_{l_i, k} \frac{U_{mk}^{l'l_i} U_{kn}^{l_i l}}{E_k - E - i\delta} + \cdots$$

It is clear that in the sum over intermediate states we must retain only the term with $l_i = l_0$. The term in the second order in U is then of the form

$$- f_{l'l_0} f_{l_0 l} \psi_m^{l'*}(0) \psi_n^l(0) G_{l_0}(E), \quad (19)$$

where

$$G_{l_0}(E) = i\omega_{l_0} |m^{l_0}|^{1/2}/2^{1/2} \pi \sqrt{\Delta_{l_0}}. \quad (19')$$

When we consider the terms in the next approximations in U we find easily that near $\Delta_{l_0} = 0$

$$F_{mn}^{l'l} = \psi_m^{l'*}(0) \psi_n^l(0) \left[f_{l'l} - \frac{f_{l'l_0} f_{l_0 l} G_{l_0}}{1 + G_{l_0} f_{l_0 l_0}} \right]$$

and that as

$$\Delta_{l_0} \to 0, \quad G_{l_0} \to \infty$$

we have

$$F_{mn}^{l'l} = \psi_m^{l'*}(0)\,\psi_n^l(0)\,[f_{l'l} - f_{l'l_0}f_{l_0l}/f_{l_0l_0}]. \tag{20}$$

From this formula it is clear that if either l or l' is equal to l_0 the corresponding amplitude tends to zero. When $l \neq l_0$, $l' \neq l_0$ it is always different from zero.

It is easy to investigate the case when for two or more electrons there occur states with $v_z = 0$. To do this we turn to the integral equation for $\psi(r)$

$$\psi_n(r) = \psi_{n0}^l(r)\,e^{ip_l r} - \int G(r, r'; E)\,U(r')\,\psi_n(r')\,dr'. \tag{21}$$

One can write the function $G(r, r'; E)$ in the form

$$G(r, r'; E) = \sum_j e^{ip_j(r-r')}\,G_j(E) + G_0(r, r'),$$

where G_j is described by Eq. (19') and where $G_0(r, r')$ is the Green function when there is no magnetic field.

As we assume the potential to be a Born one, we can neglect on the right hand side of (21) the term with G_0. We have then

$$\psi_n(r) = \psi_{n0}^l(r)\,e^{ip_l r} - \sum_j e^{ip_j r}\,G_j(E)\int e^{-ip_j r'}\,U(r')\,\psi_n(r')\,dr'. \tag{22}$$

Here $\psi_{n_0}^l(r)$ is the electron wave function when there are no impurities. By definition the ampli-

tude of the transition from a state described by the wave function $\psi_{n_0}^l(r)$ to a state $\psi_{m_0}^{l'}(r)$ is

$$F_{mn}^{l'l} = \int e^{-ip_{l'}\cdot r}\,\psi_{m0}^{l'*}(r)\,U(r)\,\psi_n(r)\,dr,$$

where $\psi_n(r)$ is a solution of Eq. (22). It is thus necessary to know $\psi_n(r)$ within the range of the potential. Assuming as before that the potential is a short-range one we can put in (22) $\psi_{n_0}^l(r)$ constant within the range of the impurity field.

It is, however, not possible to replace the exponential by unity since when we go from a state corresponding to the group l to a state corresponding to the group l', a large momentum transfer takes place. If we take this fact into account we can write the solution of (22) in the form

$$\psi_n(r) = \psi_{n0}^l(0)\,\{e^{ip_l r} - \sum_j e^{ip_j r}\,G_j(E)\,\alpha_j\}.$$

It is clear from Eq. (22) that the quantities α_j can be found from the equation

$$\alpha_j = f_{jl} - \sum_k G_k\,\alpha_k\,f_{jk}. \tag{23}$$

The final expression for the amplitude $F_{mn}^{l'l}$ will be of the form

$$F_{mn}^{l'l} = \psi_{m0}^{l'*}(0)\,\psi_{n0}^l(0)\,[f_{l'l} - \sum_k G_k\,f_{l'k}\,\alpha_k]. \tag{24}$$

We easily get from Eqs. (23) and (24), for instance, the expression for $F_{mn}^{l'l}$ when G_α and $G_\beta \to \infty$. In that case

$$F_{mn}^{l'l} = \psi_{m0}^{l'*}(0)\,\psi_{n0}^l(0)\left[f_{l'l} - \frac{f_{l'\alpha}\,G_\alpha\,f_{\alpha l}\,(1 + G_\beta\,f_{\beta\beta}) + f_{l'\beta}\,G_\beta\,f_{\beta l}\,(1 + G_\alpha\,f_{\alpha\alpha}) - f_{l'\alpha}\,G_\alpha\,f_{\alpha\beta}\,G_\beta\,f_{\beta l}}{(1 + f_{\alpha\alpha}\,G_\alpha)(1 + f_{\beta\beta}\,G_\beta) - G_\alpha\,f_{\alpha\beta}\,G_\beta\,f_{\beta\alpha}}\right.$$

$$\left. - \frac{f_{l'\beta}\,G_\beta\,f_{\beta\alpha}\,G_\alpha\,f_{\alpha l}}{(1 + f_{\alpha\alpha}\,G_\alpha)(1 + f_{\beta\beta}\,G_\beta) - G_\alpha\,f_{\alpha\beta}\,G_\beta\,f_{\beta\alpha}}\right],$$

and as $G_\alpha = G_\beta = \infty$ we get

$$F_{mn}^{l'l} = \psi_{m0}^{l'*}(0)\,\psi_{n0}^l(0)\left[f_{l'l} - \frac{f_{l'\alpha}\,f_{\alpha l}\,f_{\beta\beta} + f_{l'\beta}\,f_{\beta l}\,f_{\alpha\alpha} - f_{l'\alpha}\,f_{\alpha\beta}\,f_{\beta l} - f_{l'\beta}\,f_{\beta\alpha}f_{\alpha l}}{f_{\alpha\alpha}\,f_{\beta\beta} - f_{\alpha\beta}\,f_{\beta\alpha}}\right]. \tag{25}$$

From this formula it is at once clear that if either l or l' is equal to α or β, the corresponding amplitude tends to zero. If, however, $l \neq \alpha$, β; $l' \neq \alpha$, β the amplitude differs from zero. This result has a general character and can be formulated as follows: If $l^{(1)}$, $l^{(2)}$, ... are the numbers of the groups of electrons which possess for a given H a state with $v_z = 0$, then $F_{mn}^{l'l} = 0$ if either l or l' is equal to $l^{(1)}$, $l^{(2)}$, ..., and $F_{mn}^{l'l}$ is different from zero if $l \neq l^{(1)}$, $l^{(2)}$, ..., $l' \neq l^{(1)}$, $l^{(2)}$, ...

3. GALVANOMAGNETIC PHENOMENA

We turn to a direct investigation of the dependence of the electrical conductivity on the magnetic field. We shall in the following be interested only in the case where the period of revolution of the electron in the magnetic field is appreciably less than the time of mean free flight, i.e., where the relation $1/\omega\tau \ll 1$ is satisfied. Since the scattering is elastic the total current of the system of electrons is simply the sum of the currents caused by the different electrons. It is also necessary to

take into account the fact that the scattering is by a random distribution of impurities the average distance between which is larger than the electron wave length and the scattering amplitude. The waves scattered by different impurities do therefore not interfere with one another.

It is well known that the conductivity σ in a magnetic field is a tensor quantity whose components σ_{ik} satisfy the symmetry relations[8] $\sigma_{ik}(H)$ = $\sigma_{ki}(-H)$. It is convenient to write σ_{ik} as a sum of two terms

$$\sigma_{ik} = s_{ik} + a_{ik},$$
$$s_{ik}(H) = s_{ki}(H), \quad a_{ik}(H) = -a_{ki}(H).$$

When we change over from the components of the conductivity tensor to the components of the resistivity tensor, we must take it into account that in pure metals with a quadratic dispersion law the condition that there be as many electrons as holes must be satisfied. Applied to a real metal this means that a_{xy} though different from zero is appreciably less than s_{xy} in spite of the fact that the first one is proportional to H^{-1} and the second one to H^{-2}. Account of this leads to the following equations expressing the resistivity tensor in terms of the conductivity tensor

$$\sigma_{ik}^{-1} = \rho_{ik} + b_{ik}, \quad \rho_{ik}(H) = \rho_{ki}(H),$$

$$b_{ik}(H) = -b_{ki}(H).$$

If we now introduce a vector $\mathbf{a}$ which is the dual of the tensor a_{ik} and a vector $\mathbf{b}$ which is dual to b_{ik} we get for the most important components of the tensor σ_{ik}^{-1}[8]

$$\rho_{xx} = |\sigma|^{-1}(a_x^2 + s_{yy} s_{zz}), \quad \rho_{xy} = |\sigma|^{-1}(a_x a_y - s_{xy} s_{zz}),$$

$$\rho_{yy} = |\sigma|^{-1}(a_y^2 + s_{xx} s_{zz}), \quad \rho_{zz} = |\sigma|^{-1}(s_{xx} s_{yy} - s_{xy}^2) \quad (26)$$

for the symmetric part and

$$b_x = -|\sigma|^{-1}(a_x s_{xx} + a_y s_{xy}), \quad b_y = -|\sigma|^{-1}(a_x s_{xy} + a_y s_{yy}),$$

$$b_z = -|\sigma|^{-1}(a_x s_{xz} + a_y s_{yz} + a_z s_{zz}) \quad (27)$$

for the antisymmetric part of the resistivity tensor. Here $|\sigma|$ is the determinant of the tensor σ_{ik}:

$$|\sigma| = (s_{xx} s_{yy} - s_{xy}^2) s_{zz} + \sum_{\alpha, \beta} a_\alpha a_\beta s_{\alpha\beta} \quad (\alpha, \beta = x, y).$$

We must find the tensor s_{ik} and the vector $\mathbf{a}$. The simplest to find are the components a_x and a_y, and we now proceed to evaluate these.

In the approximation considered ($1/\omega\tau \ll 1$) these components are independent of τ and can thus be found using the classical equations of motion for an electron when there are no impurities

$$\frac{d\mathbf{p}}{dt} = e\mathbf{E} + e[\mathbf{v} \times \mathbf{H}].$$

We take the magnetic field strength vector $\mathbf{H}$ in the direction of the z axis and the electrical field strength vector in the direction of the x axis.

Then

$$\frac{dp_x}{dt} = eE + ev_y H, \quad \frac{dp_y}{dt} = -ev_x H, \quad \frac{dp_z}{dt} = 0.$$

Using these equations for quantities averaged over a period of the motion in the magnetic field, we get

$$\bar{v}_y = -E/H, \quad \bar{v}_x = 0, \quad p_z = \text{const.} \quad (28)$$

From the relation $\epsilon = \tfrac{1}{2}\mu_{ik} p_i p_k$ we get $\bar{p}_i$ = $m_{ik}\bar{v}_k$.

It is clear that the average drift velocity along the z axis is independent of p_z when the dispersion law is quadratic. For $p_z = 0$ we have thus

$$0 = m_{zx}\bar{v}_x + m_{zy}\bar{v}_y + m_{zz}\bar{v}_z,$$

or, if we take (28) into account

$$\bar{v}_z = Em_{zy}/Hm_{zz}.$$

For the components a_i we get, however, at once

$$a_l = \frac{E}{H}\sum_l \frac{m_{lz}^l}{m_{zz}^l} n_l. \quad (29)$$

The summation over l is here over all ellipsoids and for the groups corresponding to electrons $n_l > 0$ and for holes $n_l < 0$. In practice only the components a_x and a_y are different from zero since

$$a_z = (E/H)(n_e - n_h) = 0$$

in the approximation considered.

We find now the symmetric part s_{ik} (except the component s_{zz}). We use the Einstein relation according to which the current along the x axis (H is parallel to the z axis and E parallel to the x axis) is connected with the mean square displacement of the center of the electron orbit per unit time due to collisions:

$$\overline{(\Delta x)^2} = 2D, \quad (30)$$

where D is the diffusion coefficient. Then

$$j_x = -e^2 E \int d\varepsilon \frac{\partial f_0}{\partial \varepsilon} \sum_l D_l(\varepsilon) \frac{dn_l}{d\varepsilon}. \quad (31)$$

Here f_0 is the electron Fermi distribution function

$$f_0 = \left\{1 + \exp\left(\frac{\varepsilon - \zeta}{kT}\right)\right\}^{-1}$$

(ζ has clearly different values for the electrons and the holes) $dn_l/d\varepsilon$ is the density of states with the given energy which is well known to be equal to

$$\frac{dn_l}{d\varepsilon} = \frac{\omega_l \cdot m_l^{1/2}}{\sqrt{2}\,\pi^2}\sum_M \frac{1}{\sqrt{\varepsilon - \omega_l(M + 1/2)}} \quad (32)$$

in a magnetic field.

The problem of evaluating $s_{xx} = j_x/E$ is reduced to calculating the average value $\langle \Delta x \rangle^2$.

It is clear that

$$\langle (\Delta x)^2 \rangle = \langle \sum_{l', m} (x_m - x_n)^2 \, 2\pi \, | F_{mn}^{l'l} |^2 \, \delta \, (E_m - E_n) \rangle.$$

The symbol $\langle \ldots \rangle$ indicates averaging over all initial states n with energy ε; x_n and x_m are the centers of the electron orbits in the initial and final states.

If we now take it into account that according to the results obtained in Sec. 2

$$| F_{mn}^{l'l} |^2 = | f_{l'l} |^2 \, | \psi_m''(0) |^2 \, | \psi_n^l (0) |^2,$$

then

$$\langle (\Delta x)^2 \rangle = 4\pi \sum_{l,'m} x_m^2 \, | \psi_m''(0) |^2 \delta \, (E_m - \varepsilon) \, | f_{l'l} |^2 \, N_{\text{imp}}$$

$$= \frac{\sqrt{2}}{\pi^2} \sum_{l'} | m^{l'} |^{1/2} \mu_{xx}^{l'} \sum_M \frac{M + 1/2}{\sqrt{\varepsilon - \omega_{l'}(M + 1/2)}} 2\pi N_{\text{imp}} | f_{l'l} |^2. \tag{33}$$

We used Eq. (3) in deriving (33).

Substituting the expression obtained for $\langle (\Delta x)^2 \rangle$ into (31) we get finally*

$$s_{xx} = - \frac{\sqrt{2} \, e^2 \, N_{\text{imp}}}{\pi} \int d\varepsilon \frac{\partial f_0}{\partial \varepsilon} \sum_{l', l} | m^{l'} |^{1/4} \mu_{xx}^{l'} | f_{l'l} |^2 \frac{dn_l}{d\varepsilon}$$

$$\times \sum_M \frac{M + 1/2}{\sqrt{\varepsilon - \omega_{l'} (M + 1/2)}}. \tag{34}$$

Expressions for the other components of S_{ik} (except S_{zz}) are obtained from Eq. (34) by substituting there μ_{ik} for μ_{xx}.

We consider now the component s_{zz}. To evaluate this we can use a transport equation which in this special case has a very simple form (we write the distribution function f as $f = f_0 + f^1$)

$$- eE \frac{p_z}{m_{zz}^l} \frac{\partial f_0}{\partial E_n} + \sum_{l', m} 2\pi | F_{mn}^{l'l} |^2 (f_m^1 - f_n^1) \, \delta \, (E_m - E_n) = 0. \tag{35}$$

It is clear from (35) that $f^1 \sim p_z$ so that the term with f_m^1 drops out as f_m^1 is an odd function of p_z while $| F_{mn}^{l'l} |^2$ is an even one. Taking this into account we get

$$f_n^1 \sum_{l', m} 2\pi | \psi_m''(0) |^2 \, | \psi_n^l (0) |^2 | f_{l'l} |^2 | \, \delta \, (E_m - E_n)$$

$$= - eE \frac{p_z}{l_{zz}} \frac{\partial f_0}{\partial E_n}.$$

Summing over all m and l' and averaging over the position of the center of the electron orbit in the initial state we find

$$f_n^1 \, N_{\text{imp}} \sum_{l'} \frac{dn_{l'}}{d\varepsilon} \, 2\pi | f_{l'l} |^2 = - eE \frac{p_z}{m_{zz}^l} \frac{\partial f_0}{\partial \varepsilon},$$

$$s_{zz} = - \frac{e^2 \pi}{\sqrt{2}} \int \frac{\partial f_0}{\partial \varepsilon} d\varepsilon \sum_l n_l \left\{ N_{\text{imp}} \sum_{l'} | f_{l'l} |^2 m_{zz}^l \, \omega_{l'} \, | m^{l'} |^{1/2} \right.$$

$$\left. \times \sum_M \frac{1}{\sqrt{\varepsilon - \omega_{l'} \, (M + 1/2)}} \right\}^{-1}. \tag{36}$$

It is clear from the equations obtained for σ_{ik} that $a, a_y \sim H^{-1}$; $a_z \sim H^{-3}$; s_{ik} ($i \neq z$, $k \neq z$) $\sim H^{-2}$; $s_{zz} \sim 1$. As far as σ_{ik}^{-1} is concerned, the components $\sigma_{\alpha\beta}^{-1}$ ($\alpha, \beta = x, y$) and ρ_{zz} are the most important ones.

It follows from (25) and (26) that

$$\rho_{\alpha\beta} \sim H^2, \qquad b_z \sim H,$$

so that we shall only be interested in the following in $\rho_{\alpha\beta}$ and ρ_{zz}.

We start our investigation of the conductivity with the semi-classical region where the relation $\omega/\zeta \ll 1$ is satisfied. We can then represent the sums over the magnetic quantum number occurring within the braces in Eqs. (34) and (36), with sufficient accuracy, as follows

$$\sum_M \frac{1}{\sqrt{\varepsilon - \omega \, (M + 1/2)}} \approx 2 \frac{\varepsilon^{1/2}}{\omega} + \frac{1}{\sqrt{\Delta}},$$

$$\sum_M \frac{M + 1/2}{\sqrt{\varepsilon - \omega \, (M + 1/2)}} \approx \frac{4}{3} \frac{\varepsilon^{1/2}}{\omega^2} + \frac{\varepsilon}{\omega \sqrt{\Delta}}, \tag{37}$$

where Δ is defined as before by the equation

$$\varepsilon = \omega \, (N + 1/2) + \Delta, \quad \Delta \ll \omega.$$

In (37), $\Delta > 0$.

For the range of values of the magnetic field considered it is convenient to introduce quantities $s_{\alpha\beta}^{l'l}$ (cl) defined by means of the relations

$$s_{\alpha\beta} \, (\text{cl}) = \sum_{l', l} s_{\alpha\beta}^{l'l} \, (\text{cl}).$$

Then

$$s_{\alpha\beta}^{l'l} \, (\text{cl}) = N_{\text{imp}} \frac{4e^2}{3\pi^4} | m^{l'} | \, \mu_{\alpha\beta}^{l'} \frac{\zeta^2}{\omega_{l'}^2} 2\pi | f_{l'l} |^2. \tag{38}$$

If we use the results obtained we shall get for $s_{\alpha\beta}$ and s_{zz}

$$s_{\alpha\beta} = s_{\alpha\beta}(\text{cl})$$

$$- \sum_{l', l} s_{\alpha\beta}^{l'l} \, (\text{cl}) \int \frac{\partial f_0}{\partial \varepsilon} d\varepsilon \left[\frac{3\omega_{l'}}{4\zeta^{1/2} \sqrt{\Delta_{l'}}} + \frac{\omega_l}{2\zeta^{1/2} \sqrt{\Delta_l}} + \frac{3\omega_l \omega_{l'}}{8\zeta \sqrt{\Delta_l \Delta_{l'}}} \right]$$

$$s_{zz} = - \frac{e^2 \pi}{2^{1/2} N_{\text{imp}}}$$

$$\times \int \frac{\partial f_0}{\partial \varepsilon} d\varepsilon \sum_l n_l \left\{ \sum_{l'} | f_{l'l} |^2 \, m_{zz} | m^{l'} |^{1/2} \zeta \left(1 + \frac{\omega_{l'}}{2\zeta^{1/2} \sqrt{\Delta_{l'}}} \right) \right\}^{-1} \tag{39}$$

It is necessary to emphasize here that the $f_{l'l}$ are different from zero only when the indices l' and l

refer either only to electron or only to hole states, i.e., when the electrons do not go over into holes, or vice versa, in the scattering by the impurity.

The terms containing $\Delta^{-1/2}$ in the expressions which we have written down describe the usual semi-classical oscillations of the conductivity in a magnetic field.

If we substitute the quantities $s_{\alpha\beta}$ and s_{zz} which we have found into (26) we obtain the final equations for the ρ_{ik}. These formulae are very cumbersome, for when the magnetic field has an arbitrary orientation with respect to the crystallo- graphic directions, all the electron groups connect- ed with the various ellipsoids will give contribu- tions of the same order. We note that the formulae for the conductivity for the case when the magnetic field is perpendicular to the three-fold axis of bis- muth were investigated in detail by I. Pomeranchuk and B. Davydov.[4] We shall therefore in the follow- ing investigate $\rho_{\alpha\beta}$ and ρ_{zz} only in the region where their behavior is anomalous.

1. By changing the magnitude of the magnetic field we can get $\Delta \ll \omega^2 \zeta^{-1}$ for one or several electron groups. In practice this can apparently only be obtained for electrons corresponding to some given ellipsoids, which we denote by l_0. When we change over to the resistivity tensor we note that for sufficiently small Δ_{l_0}

$$\rho_{xx} = s_{yy}(s_{xx}s_{yy} - s_{xy}^2)^{-1}, \qquad \rho_{yy} = s_{xx}(s_{xx}s_{yy} - s_{xy}^2)^{-1},$$

$$\rho_{xy} = - s_{xy}(s_{xx}s_{yy} - s_{xy}^2)^{-1}, \qquad \rho_{zz} = s_{zz}^{-1}. \quad (40)$$

As far as s_{zz} is concerned in terms of which ρ_{zz} in (40) is expressed, if the group l_0 refers to electrons, only the term corresponding to holes remains in Eq. (39) for s_{zz}.

If Δ_{l_0} is so small that we can retain in (39) just the term with Δ, then

$$s_{\alpha\beta} = -\frac{3}{8} s_{\alpha\beta}^{l_0 l_0}(\mathrm{cl}) \;\frac{\omega_{l_0}^2}{\zeta} \int \frac{\partial f_0}{\partial \varepsilon}\frac{d\varepsilon}{\Delta_{l_0}}, \qquad (41)$$

$$\rho_{xx} = -\frac{8}{3}\rho_{xx}^{l_0 l_0}(\mathrm{cl})\;\frac{\zeta}{\omega_{l_0}^2}\left[\int \frac{\partial f_0}{\partial \varepsilon}\frac{d\varepsilon}{\Delta_{l_0}}\right]^{-1}$$

$$= -\frac{\pi^3 \mu_{yy}^{l_0}}{e^2 \zeta N_{\mathrm{imp}}|f_{l_0 l_0}|^2 m_{zz}^{l_0}}\left[\int \frac{\partial f_0}{\partial \varepsilon}\frac{d\varepsilon}{\Delta_{l_0}}\right]^{-1}. \quad (42)$$

One obtains similar expressions for ρ_{xy} and ρ_{yy}.

If $T = 0$ we have $\int \frac{\partial f_0}{\partial \varepsilon}\frac{d\varepsilon}{\Delta_{l_0}} = -\frac{1}{\Delta_{l_0}(\zeta)}$. When $T \ll \omega^2 \zeta^{-1}$ (but $T \neq 0$) we must take into account the behavior of $|F_{mn}^{l'l}|^2$ as $\Delta_{l_0} \rightarrow 0$ when integrating. This leads to the following integral

$$\int \frac{\partial f_0}{\partial \varepsilon}\frac{d\varepsilon}{\Delta_{l_0}+a} = -\left[\frac{1}{\Delta_{l_0}(\zeta)} + \frac{\partial f_0(-\Delta_{l_0}(\zeta))}{\partial \zeta}\ln a\right],$$

where

$$a = |f_{l_0 l_0}|^2 \omega_{l_0}^2 |m^{l_0}|/8\pi^2.$$

It is clear from Eq. (42) that $\rho_{\alpha\beta} \sim \Delta_{l_0}$, i.e., that $\rho_{\alpha\beta}$ is appreciably decreased when Δ_{l_0} is sufficiently small. The steep decrease of $\rho_{\alpha\beta}$ which we have obtained when $\Delta_{l_0} \rightarrow 0$ can in practice be observed only when the following con- ditions are satisfied:

$$kT \ll \omega_{l_0}^2 \zeta^{-1}, \qquad (\omega_{l_0}\tau)^{-1} \ll \omega_{l_0}\zeta^{-1}$$

and when the magnetic field is stabilized $\Delta H/H \ll \omega_{l_0}^2 \zeta^{-2}$. We note that this effect takes place not only in the semi-classical region but everywhere, so long as $\zeta = \omega(N + \frac{1}{2}) + \Delta$ and $\Delta \rightarrow 0$.

When the field is sufficiently strong ζ is not equal to its value when there is no field and must be determined from two conditions: the fact that the number of electrons must be equal to the number of holes $n_e = n_h$, and the condition that $\zeta_1 + \zeta_2 = E_0$ where $\zeta_1 \rightarrow \zeta_e$, $\zeta_2 \rightarrow \zeta_h$ and E_0 is a constant which is independent of H_0.

2. The expressions for $\rho_{\alpha\beta}$ and ρ_{zz} which we wrote down in the foregoing are valid for suffi- ciently small, but not too small values of Δ_{l_0}. If Δ_{l_0} is very small it is essential to take into ac- count the dependence of the scattering amplitude $F^{l'l}$ on the magnetic field H. For the sake of sim- plicity we restrict ourselves to the case $T = 0$. We note now immediately that it is apparently practically impossible to observe the anomaly in the resistivity near the resonance for scattering by impurities with an attractive potential because of the too stringent limitations as to the purity of the metal and the temperature. We shall therefore not investigate ρ_{ik} near this resonance.

When $\Delta_{l_0} \rightarrow 0$

$$s_{\alpha\beta} = \pi^{-3}e^2 N_{\mathrm{imp}}|m^{l_0}||\mu_{\alpha\beta}^{l_0}||f_{l_0 l_0}|^2 \zeta$$

$$\times\left[\Delta_{l_0} + \frac{1}{8}\pi^{-2}|f_{l_0 l_0}|^2 \omega_{l_0}^2 m^{l_0}|\right]^{-1} \quad (43)$$

and we have, for instance, for ρ_{xx}

$$\rho_{xx} = \frac{\pi^3 \mu_{yy}^{l_0}}{e^2 N_{\mathrm{imp}}|f_{l_0 l_0}|^2 m_{zz}^{l_0}\zeta}\left[\Delta_{l_0} + \frac{|f_{l_0 l_0}|^2 \omega_{l_0}^2 |m^{l_0}|}{8\pi^2}\right].$$

It is clear from this formula that as $\Delta_{l_0} \rightarrow 0$, $\rho_{\alpha\beta}$ tends to some very small though finite limit.

We investigate now the behavior of ρ_{zz} for very small Δ_{l_0}. As before we have then $\rho_{zz} = s_{zz}^{-1}$. If we take the results of Sec. 2 into account we are led to the conclusion that for $\Delta_{l_0} = 0$ all amplitudes for which either l' or l is equal to l_0 tend to zero and that there remain only terms with $l \neq l_0$ and $l' \neq l_0$. At the same time these amplitudes $F^{l'l}$

are changed according to the results of Sec. 2. Finally, s_{zz} is given by Eq. (36) where $l' \neq l_0$ and $l \neq l_0$ and where we have instead of $|f_{l'l}|^2$

$$|f_{l'l} - f_{l'l_0}f_{l_0l}/f_{l_0l_0}|^2.$$

This result can be summarized as follows: for some values of H the group l_0 does not make any contribution to the conductivity s_{zz}. Up to now we considered the case where Δl_0 tended to zero from the positive side. However, the opposite case is, of course, also possible. The equation for s_{zz} is then not changed. $s_{\alpha\beta}$ will be given by Eq. (34) with $l \neq l_0$ and $l' \neq l_0$ if in that equation we replace

$$f_{l'l} \quad \text{by} \quad f_{l'l} - f_{l'l_0}f_{l_0l} / f_{l_0l_0}.$$

The transition from the s_{ik} to the ρ_{ik} is then performed by means of Eqs. (26).

The final results about the behavior of the tensor ρ_{ik} near $\Delta l_0 = 0$ can be summarized as follows: when $\Delta l_0 \to 0$, $\rho_{\alpha\beta} \sim \Delta l_0$ and tends to a finite though very small limit; in a narrow region near $\Delta l_0 = 0$ $\rho_{\alpha\beta}$ changes quickly and the limits of $\rho_{\alpha\beta}$ when $\Delta l_0 \to + 0$ and when $\Delta l_0 \to - 0$ are essentially different from one another.

In conclusion I express my gratitude to Academician L. D. Landau and to I. M. Khalatnikov for valuable discussions when this research was done.

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