Quantum Theory of the Electrical Conductivity of Metals in a Magnetic Field

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A consistent quantum mechanical theory of the electrical conductivity of metals in a magnetic field is constructed. The kinetic equation for the density matrix is derived on the basis of some general assumptions regarding the electron energy spectrum, and the transition to the classical limit is analyzed. The asymptotic values of the kinetic coefficients in a strong magnetic field are analyzed. On the basis of the relations established between the solutions to the quantum and classical equations quantum corrections, including oscillations of the conductivity, are found for the kinetic coefficients.

AS IS WELL KNOWN, the correct description of metallic conductivity is essentially quantum mechanical. Nevertheless, since the wavelength of the electron is small compared with its mean free path and, in the presence of a magnetic field, also compared with the radius of curvature of its trajectory, it is usually sufficient to treat the problem semiclassically. This means that the electron may be treated classically, as a quasi-particle satisfying Fermi statistics and a certain dispersion law

$$\varepsilon = \varepsilon_j(p_x, p_y, p_z) \tag{1}$$

($\varepsilon_j(\mathbf{p})$ is a periodic function with the period of the reciprocal lattice, and j is the band number). It was on this basis that the semiclassical theory of the galvanomagnetic effects in metals[1] was developed.

Such a treatment, however, fails to show up certain specific quantum effects (for instance the oscillation of the resistance with the magnetic field) related to the quantum levels. These effects are experimentally observed,[2] but their theoretical study[3] does not seem to us to be sufficiently consistent or satisfactory.

The present work is an attempt to construct a consistent quantum theory of metallic conduction in a magnetic field. The theory makes it possible to study the above-mentioned oscillatory quantum effects and the transition to the classical limit.

As has been shown,[4] the energy levels ε_n for a particle with the dispersion law of Eq. (1) and in a magnetic field H directed along the z axis are given in the quasi-classical approximation by the condition

$$S(\varepsilon_n, p_z) = (eh/c)H(n+\gamma), \quad n \gg 1, \quad 0 < \gamma < 1, \tag{2}$$

where $S(\varepsilon, p_z)$ is the area of the intersection between the surface of Eq. (1) and the plane p_z = const in quasi-momentum space.

According to Eq. (2), the separation between levels will be

$$\Delta\varepsilon_n = \varepsilon_{n+1} - \varepsilon_n = \hbar\omega^* = \mu^* H; \quad \mu^* = e\hbar/m^* c; \tag{3}$$

$$\omega^* = eH/m^* c; \quad m^* = (1/2\pi)\partial S/\partial\varepsilon; \quad m^* = m^*(\varepsilon, p_z). \tag{4}$$

Thus significant effects may be expected when $\hbar\omega^* \gtrsim kT$. On the other hand, in order for the quasi-classical approximation to be valid and the dispersion law of Eq. (1) to be applicable, it is necessary that $\hbar\omega \ll \zeta$ (where ζ is the chemical potential). In what follows, we shall assume this condition to be fulfilled.

1. THE KINETIC EQUATION FOR THE DENSITY MATRIX

Assuming the electron to be in a homogeneous magnetic field **H** and a weak electric field **E**, let us write its Hamiltonian in the form

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{U}; \quad \hat{U} = -e\mathbf{E}\hat{\mathbf{r}}, \tag{5}$$

where $\hat{\mathcal{H}}_0$ is the kinetic energy operator of the electron in the magnetic field. This operator, at least in the quasi-classical approximation, is obtained from $\varepsilon(\mathbf{p})$ by replacing the components of the momentum $\mathbf{p}$ by the components of the kinetic momentum operator $\hat{\mathbf{p}}$, and by suitable symmetrization whose exact meaning will not be of importance for us.

Since the kinetic momentum operators $\hat{p}_x$, $\hat{p}_y$, $\hat{p}_z$

with a magnetic field $H_z = H$ do not commute $\{\hat{p}_x, \hat{p}_y\} = eH/c$) we shall describe the states of the electron gas by a density matrix $\hat{f}$, rather than by a distribution function.

When there is no electric field ($\hat{U} = 0$), the operator $\hat{f} = \hat{f}^0$ is the equilibrium Fermi function

$$\hat{f}^0 = \hat{f}^0(\hat{\mathcal{H}}_0); \quad f^0(\varepsilon) = [1 + e^{(\varepsilon-\zeta)/\Theta}]^{-1}, \quad \Theta = kT \tag{6}$$

(where ζ is the chemical potential). In the presence of an electric field, we shall set

$$\hat{f} = \hat{f}^0 + \hat{f}^1. \tag{7}$$

In what follows we shall treat the operator $\hat{\mathcal{H}}_0$ in the representation in which n and p_z are diagonal, and then as will be seen, in the quasi-classical approximation we may consider $\hat{f}^1$ a matrix with respect to n and a number with respect to p_z (this is related to the fact that the momentum p_z is not quantized).

When dealing with several electron bands, the band number j enters into $\hat{f}$ as a parameter. This follows from the fact that in the classical motion of a particle, j remains constant. Therefore in the quasi-classical approximation, the parameter j can change only as a result of collisions, and this can be accounted for in the collision matrix. The situation is exactly similar with respect to the spin states s, whose treatment requires the introduction of an additional parameter s into $\hat{f}$, since the energy levels depend on s according to

$$\varepsilon_{ns} = \varepsilon_n(p_z) + s\mu_0 H; \quad s = \pm 1; \quad \mu_0 = e\hbar/2m_0c.$$

We shall henceforth suppress the indices j, s.

The kinetic equation for $\hat{f}^1$ can be written in the form

$$\{\hat{f}^0, \hat{\mathcal{H}}\} + \{\hat{f}^1, \hat{\mathcal{H}}\} + \hat{W}\hat{f}^1/t_0 = 0. \tag{8}$$

Here $\hat{W}/t_0$ is a certain linear transformation corresponding to the collision integral, t_0 is the characteristic relaxation time, and the curly brackets indicate quantum Poisson brackets. In order to make the analysis that will follow as clear as possible, let us start with the simplest case $\hat{W} = 1$.

Bearing in mind the obvious relation $\{\hat{f}^0, \hat{\mathcal{H}}_0\} = 0$ and neglecting the term $\{\hat{f}^1, \hat{U}\}$, which is quadratic in the electric field, we obtain

$$\{\hat{f}^1, \hat{\mathcal{H}}_0\} + \hat{f}^1/t_0 = -\{\hat{f}^0, \hat{U}\}. \tag{9}$$

Writing out the matrix elements and taking account of the fact that $\hat{\mathcal{H}}_0$ and $\hat{f}^0$ are diagonal, we have

$$i(\varepsilon_{n'} - \varepsilon_n) f^1_{nn'}/\hbar + f^1_{nn'}/t_0 = (f^0_{n'} - f^0_n) \cdot iU_{nn'}/\hbar. \tag{10}$$

From the equations of motion of the electron in a magnetic field, it follows that

$$-\{\hat{\mathcal{H}}_0, \hat{\mathbf{r}}\} = \dot{\hat{\mathbf{r}}} = \hat{\mathbf{v}}, \tag{11}$$

or, from Eq. (5),

$$(i/\hbar)(\varepsilon_n - \varepsilon_{n'}) U_{nn'} = e\mathbf{E}(\hat{\mathbf{v}})_{nn'}, \tag{11a}$$

where $\hat{\mathbf{v}}$ is the velocity operator corresponding to the classical quantity $\mathbf{v} = \partial\varepsilon/\partial\mathbf{p}$. This gives

$$\left\{\frac{i}{\hbar}(\varepsilon_{n'} - \varepsilon_n) + \frac{1}{t_0}\right\} f^1_{nn'} = -\frac{f^0_{n'} - f^0_n}{\varepsilon_{n'} - \varepsilon_n} e\mathbf{E}\mathbf{v}_{nn'}. \tag{12}$$

According to Eq. (3), we have $\varepsilon_n - \varepsilon_n = (n' - n)\hbar\omega^*$. Now setting

$$\hat{f}^1 = -et_0\mathbf{E}\hat{\Psi} \tag{13}$$

and dividing Eq. (12) by ω^*, we obtain

$$[i(n' - n) + \gamma]\hat{\Psi}_{nn'} = \gamma g_{nn'}\hat{\mathbf{v}}_{nn'},$$

$$\gamma = 1/t_0\omega^* = H^*_0/H; \qquad H^*_0 = m^*c/et_0; \tag{14}$$

$$g_{nn'} = (f^0_{n'} - f^0_n)/(\varepsilon_{n'} - \varepsilon_n).$$

Setting $n' - n = k$, we finally arrive at

$$(ik + \gamma)\Psi_k = \gamma g_k \mathbf{v}_k. \tag{15}$$

Here we have introduced the notation

$$\Psi_{n,\,n+k} = \Psi_k(\varepsilon_n, p_z); \quad \mathbf{v}_{n,\,n+k} = \mathbf{v}_k(\varepsilon_n, p_z), \tag{16}$$

$$g_k(\varepsilon_n) = g_{n,\,n+k} = g_{n+k,\,n}$$

$$= [f^0(\varepsilon_n + k\hbar\omega^*) - f^0(\varepsilon_n)]/k\hbar\omega^*. \tag{17}$$

When $k = 0$, the expression for g_k is indeterminate. Simple calculation† shows that

$$g_0(\varepsilon) = \partial f^0/\partial\varepsilon. \tag{17a}$$

It is easily seen that as $\hbar\omega^* \to 0$ we have

$$g_k(\varepsilon) \to \partial f^0/\partial\varepsilon, \tag{18}$$

and Eq. (15) becomes

$$(ik+\gamma)\psi_k = \gamma\frac{\partial f^0}{\partial\varepsilon}\mathbf{v}_k; \quad \psi_k = \psi_k(\varepsilon, p_z); \quad \mathbf{v}_k = \mathbf{v}_k(\varepsilon, p_z). \tag{19}$$

This is just the classical kinetic equation for the Fourier components of the distribution function $\psi = \psi(\varepsilon, p_z, \varphi)$ (where φ is the angle variable on the particle trajectory in momentum space, and is proportional to the time of rotation), derived previously.[1] Here the $\mathbf{v}_k$ are the Fourier amplitudes of the classical velocity vector, namely

$$\mathbf{v}(\varepsilon, p_z, \varphi) = \sum\mathbf{v}_k e^{ik\varphi}; \quad \mathbf{v} = \partial\varepsilon/\partial\mathbf{p}, \tag{20}$$

$$\mathbf{v}_k = \frac{1}{2\pi}\int_0^{2\pi}\frac{\partial\varepsilon}{\partial\mathbf{p}}e^{-ik\varphi}d\varphi; \quad \varphi = 2\pi\int\frac{dl}{v_\perp}\Big/\oint\frac{dl}{v_\perp}, \quad dl = |d\mathbf{p}|; \quad v_\perp = \sqrt{v_x^2+v_y^2}. \tag{21}$$

Returning to the quantum mechanical equation (15), let us replace the $\mathbf{v}_k(\varepsilon_n, p_z)$ by their limiting values of Eq. (21) (which corresponds to the quasiclassical approximation for the matrix elements $\mathbf{v}_{nn'}$). A similar replacement ($g_k \to \partial f^0/\partial\varepsilon$) cannot be performed for the g_k, since $f^0(\varepsilon)$ varies very rapidly in the neighborhood of the limiting energy ($\varepsilon - \zeta \sim \Theta$), and the whole effect we are attempting to find is related just to this fact.

Thus as a solution to Eq. (15) we obtain

$$\psi_k = \gamma g_k \mathbf{v}_k/(ik+\gamma). \tag{22}$$

Let us now return to the general kinetic equation (8), and set

$$(\widetilde{W}\hat{\psi})_{n,\,n+k} = \hat{W}_{kk'}\psi_{k'}, \tag{23}$$

where $\hat{W}_{kk'}$ is an operator acting on the variables ε_n and p_z and the functions $\psi_k(\varepsilon_n, p_z)$ according to

$$\hat{W}_{kk'}\psi_{k'} = \sum_{\varepsilon'}\int W_{kk'}(\varepsilon, p_z; \varepsilon', p_z')\psi_{k'}(\varepsilon', p_z')\,dp_z\,\Delta\varepsilon' \quad (\varepsilon = \varepsilon_n, \quad \varepsilon' = \varepsilon_{n'}). \tag{24}$$

(In taking account of transitions between different bands, the kernel $W_{kk'}$ also has the indices j and j'.) Then repeating all the previous considerations, we transform the original equation (8) to a form similar to (15), namely

$$ik\psi_k + \gamma\hat{W}_{kk'}\psi_{k'} = \gamma g_k \mathbf{v}_k. \tag{25}$$

Equation (25), just as (15), goes over to the classical equation (31) of Ref. 1 when $g_k(\varepsilon)$ is replaced by its value $\partial f^0/\partial\varepsilon$ in the limit and in going over from summation in Eq. (24) to integration. Then in agreement with the correspondence principle, the $\hat{W}_{kk'}$ of Eq. (25) are the Fourier amplitudes of the collision operator in the classical Eq. (31) of Ref. 1.

Since the g_k, and therefore also the ψ_k, are rapidly varying functions of ε_n and slowly varying functions of p_z (for fixed $\varepsilon_n = \varepsilon$), it is convenient to go over to integration over ε and summation over p_{zn} (*i.e.*, to the independent variables ε and n) in Eqs. (25) and (24). Solving Eq. (2) $n = n(\varepsilon, p_z)$ for p_z, we have

$$\sum_n\int F(\varepsilon_n, p_z)\,dp_z\,\Delta\varepsilon_n = \int\Big\{\sum_{p_{zn}} F(\varepsilon, p_{zn})\,\Delta p_{zn}\Big\}d\varepsilon; \quad p_{zn} = p_z(n, \varepsilon); \quad \Delta p_{zn} = \frac{\partial P_z}{\partial n} = \frac{ehH}{c}\Big/\frac{\partial S}{\partial p_z} \tag{26}$$

(the limits of summation over n now depend on ε!).

Thus, for instance, for elastic scattering impurities, we have

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† From the fact that $\dot{\hat{\mathscr{H}}}_0 = e\mathbf{E}\hat{\mathbf{v}}$, we have

$$\{\hat{f}^0, \hat{U}\} = \dot{\hat{f}}^0 = \lim\frac{f^0(\hat{\mathscr{H}}_0 + e\mathbf{E}\hat{\mathbf{v}}\delta t) - f^0(\hat{\mathscr{H}}_0)}{\delta t}.$$

Since $\hat{\mathscr{H}}_0$ is diagonal,

$$\{(\hat{\mathscr{H}}_0 + e\mathbf{E}\hat{\mathbf{v}}\delta t)^m - \hat{\mathscr{H}}_0^m\}/\delta t\,|_{nn} = e\mathbf{E}\mathbf{v}_{nn}\varepsilon_n^{m-1}m,$$

for all m, and for an arbitrary function $f^0(\hat{\mathscr{H}}_0)$ we have

$$\{\hat{f}^0, \hat{U}\}_{nn} = e\mathbf{E}\mathbf{v}_{nn}\partial f^0/\partial\varepsilon,$$

which corresponds to (17a).

$$\hat{W}_{kk'}\psi_{k'} = \sum_{\varepsilon'}\int w_{kp_z,\,k'p_z'}(\varepsilon)\,\delta(\varepsilon-\varepsilon')\,[\psi_k(\varepsilon,p_z)-\psi_{k'}(\varepsilon',p_z')]\,dp_z'\,\Delta\varepsilon' = \sum_{p_z'} w_{kp_z,k'p_z'}(\varepsilon)\,[\psi_k(\varepsilon,p_z)-\psi_{k'}(\varepsilon,p_z')]\,\Delta p_z'. \tag{27}$$

Correspondingly, now the quantities $\boldsymbol{\psi}_k$, $\mathbf{v}_k$ and g_k in Eqs. (25) and (27) are considered functions of the continuous variable ε and the discrete variable $p_{zn} = p_z(n, \varepsilon)$:

$$\psi_k = \psi_k(\varepsilon, p_{zn}); \quad \mathbf{v}_k = \mathbf{v}_k(\varepsilon, p_{zn});$$
$$g_k = g_k(\varepsilon, p_{zn}) = [f^0(\varepsilon + k\hbar\omega^*) - f^0(\varepsilon)]/k\hbar\omega^*;$$
$$g_0 = \partial f^0/\partial\varepsilon. \tag{28}$$

For scattering by impurities, the parameter $\hbar\omega^*/kT$ does not enter into the kernel of the collision operator of Eq. (27), and therefore the kernel w can be replaced by its classical expression. For inelastic scattering by phonons, such a replacement would seem to be invalid.

As in the classical case, it is impossible to obtain an explicit solution of Eq. (25) for arbitrary fields and without any specific assumptions with regard to the collision integral. Thus our problem is first to study the asymptotic behavior of the conductivity σ_{ik} for strong fields ($\gamma \ll 1$), and second to clarify the connection between the quantum mechanical and classical expressions for σ_{ik} for arbitrary values of γ. In this second case we shall consider the classical problem solved, and shall describe the quantum effects in terms of the classical solution.

2. HIGH-FIELD ($\gamma \ll 1$) LIMIT OF THE CONDUCTIVITY

As has been previously mentioned,[1] the high-field limit of the conductivity is determined essentially by the topology of the Fermi surface. Since the equations are quantized only for the case of closed orbits (finite motion), all our quantum mechanical considerations pertain indeed to this case.

This means, in particular, that in view of the equation of motion in a magnetic field, we have

$$\{\hat{\mathbf{p}}, \hat{\mathscr{H}}_0\} = \frac{e}{c}[\mathbf{vH}], \tag{29}$$

which, in terms of matrix elements, can be written in the form

$$ik\mathbf{p}_k = m^*[\mathbf{v}_k\mathbf{n}]; \quad \mathbf{H} = H\mathbf{n}. \tag{30}$$

The diagonal matrix elements of the velocity in the xy plane, perpendicular to the direction $\mathbf{n}$ of the magnetic field, vanish, so that

$$[\mathbf{v}_{nn}\mathbf{n}] = [\mathbf{v}_0\mathbf{n}] = 0. \tag{31}$$

Let us introduce the components of the operator $\hat{\boldsymbol{\psi}}$ according to

$$[\hat{\psi}\mathbf{n}] = \hat{\boldsymbol{\varphi}}; \quad (\hat{\psi}\mathbf{n}) = \hat{\vartheta}. \tag{32}$$

From (13) we have

$$\hat{f}^1 = et_0\{(\hat{\boldsymbol{\varphi}}[\mathbf{En}]) + \hat{\vartheta}(\mathbf{En})\}. \tag{33}$$

Bearing (30) in mind, Eq. (25) leads to

$$ik\varphi_k + \gamma\hat{W}_{kk'}\varphi_{k'} = ik\gamma g_k\mathbf{p}_k/m^*. \tag{34}$$

In order to expand φ_k in powers of γ, we must first eliminate φ_0 from (34). Setting $k = 0$ in (34), we have

$$\varphi_0 = -\hat{W}_{00}^{-1}\hat{W}_{0k'}\varphi_{k'}; \quad k' \neq 0. \tag{35}$$

From this we obtain

$$\varphi_k - \gamma\hat{L}_{kk'}\varphi_{k'} = \gamma g_k\mathbf{p}_k/m^*; \quad k, k' \neq 0, \tag{36}$$

$$\hat{L}_{kk'} = (i/k)\{\hat{W}_{kk'} - \hat{W}_{k0}\hat{W}_{00}^{-1}\hat{W}_{0k'}\}; \quad k, k' \neq 0, \tag{37}$$

and the solution is easily written in the form of a power series in γ, namely

$$\varphi_k = (1-\gamma\hat{L})^{-1}_{kk'}\gamma\frac{g_{k'}\mathbf{p}_{k'}}{m^*} = \gamma\frac{g_k\mathbf{p}_k}{m^*} + \gamma\hat{L}_{kk'}\gamma\frac{g_{k'}\mathbf{p}_{k'}}{m^*} + \cdots \tag{38}$$

Similarly,

$$\vartheta_0 = \hat{W}_{00}^{-1}\{v_0^z\partial f^0/\partial\varepsilon - \hat{W}_{0k'}\vartheta_{k'}\}, \tag{39}$$

whence

$$\vartheta_k - \gamma\hat{L}_{kk'}\vartheta_{k'} = \gamma h_k;$$
$$\frac{\gamma}{ik}\left\{g_k v_k^z - \hat{W}_{k0}\hat{W}_{00}^{-1}\frac{\partial f^0}{\partial\varepsilon}v_0^z\right\} = \gamma h_k, \tag{40}$$

and therefore

$$\vartheta_k = \gamma h_k + \gamma \hat{L}_{kk'} \gamma h_{k'} = \cdots, \quad (k \neq 0), \tag{41}$$

$$\vartheta_0 = \hat{W}_{00}^{-1} \frac{\partial f^0}{\partial \varepsilon} v_0^z - \hat{W}_{00}^{-1} \hat{W}_{0k'} \gamma h_{k'} + \cdots \tag{41a}$$

We thus see that as in the classical case all the φ_k and ϑ_k, except ϑ_0, start with the first power of γ (of the order of $1/H$). Furthermore, the terms linear in γ in the expression for φ_k (with $k \neq 0$) do not depend on the collision integral.

The current in which we are interested is given by the expression

$$\mathbf{j} = e \operatorname{Sp} \hat{f}^1 \hat{\mathbf{v}}. \tag{42}$$

In view of the above, the terms linear in $\gamma \sim 1/H$ in the components σ^{xx}, σ^{xy}, and σ^{yy} of the conductivity tensor are not related to the collision integral, and an explicit expression for them is easily obtained. In order to find the components j^x and j^y, let us find the expression $[\mathbf{jn}]$. From (29) and (8) we have

$$\begin{aligned} [\mathbf{jn}] = e \operatorname{Sp} \hat{f}^1 [\hat{\mathbf{v}}\mathbf{n}] &= \frac{c}{H} \operatorname{Sp} \hat{f}^1 \{\hat{\mathbf{p}}, \hat{\mathscr{H}}_0\} \\ &= \frac{c}{H} \operatorname{Sp} \hat{\mathbf{p}} \{\hat{\mathscr{H}}_0, \hat{f}^1\} \\ &= \frac{c}{H} \operatorname{Sp} \hat{\mathbf{p}} \{\hat{f}^0, \hat{U}\} + \frac{c}{Ht_0} \operatorname{Sp} \hat{\mathbf{p}} \tilde{W} \hat{f}^1. \end{aligned} \tag{43}$$

As follows from (33) and (38), retaining terms of order $1/H$, we have

$$(c/Ht_0) \operatorname{Sp} \hat{\mathbf{p}} \tilde{W} \hat{f}^1 = (ec/H) E_z \operatorname{Sp} \hat{\mathbf{p}} \tilde{W} \hat{\vartheta}.$$

Terms proportional to E_x and E_y are given by the first term. Since $\hat{U} = -eE_j x^j$, we have

$$[\mathbf{jn}] = -\frac{ec}{H} E_i \operatorname{Sp} \hat{\mathbf{p}} \{\hat{f}^0, \hat{x}^i\}. \tag{44}$$

Going over to the components j^x and j^y of the current, up to terms of order $1/H^2$ we obtain

$$\sigma_{ik} = \sigma_{ik}^{(1)} + O(H^{-2}),$$

$$\sigma_{xx}^{(1)} = \frac{ec}{H} \operatorname{Sp} \hat{p}_y \{\hat{f}^0, \hat{x}\}, \quad \sigma_{yy}^{(1)} = -\frac{ec}{H} \operatorname{Sp} \hat{p}_x \{\hat{f}^0, \hat{y}\},$$

$$\sigma_{xy}^{(1)} = \frac{ec}{H} \operatorname{Sp} \hat{p}_x \{\hat{f}^0, \hat{x}\}. \tag{45}$$

From the equation

$$\operatorname{Sp} \hat{p}_y \{\hat{f}^0, \hat{x}\} = \operatorname{Sp} \hat{f}_0 \{\hat{x}, \hat{p}_y\} = 0$$

and a similar one for $\sigma_{yy}^{(1)}$, we have

$$\sigma_{xx}^{(1)} = \sigma_{yy}^{(1)} = 0. \tag{46}$$

In view of the relation $\{\hat{p}_x, \hat{x}\} = 1$, the expression for $\sigma_{xy}^{(1)}$ must be dealt with more carefully (it is not correct simply to change the order of the factors in the trace). Detailed calculations show that when all the isoenergetic surfaces of Eq. (1) in the neighborhood $|\varepsilon - \zeta| \sim \Theta$ are closed, we obtain the expressions

$$\begin{aligned} &\operatorname{Sp} \hat{p}_x \{\hat{f}^0, \hat{x}\} = \operatorname{Sp} \hat{f}^0 = N_+ \qquad \text{for } \partial\varepsilon/\partial n > 0, \\ &\operatorname{Sp} \hat{p}_x \{\hat{f}^0, \hat{x}\} = \operatorname{Sp} (\hat{f}^0 - 1) = -N_- \\ &\qquad \text{for } \partial\varepsilon/\partial n < 0, \end{aligned} \tag{47}$$

for each band separately, where N_+ is the number of occupied states with $m^* > 0$ (number of "electrons"), and N_- is the number of occupied states with $m^* < 0$ (number of "holes"). Thus in this case we have

$$\sigma_{xy}^{(1)} = (ec/H) \left(\sum N_+ - \sum N_- \right), \tag{48}$$

which is the same as the previously obtained classical result. As in the classical case, when the topology of the Fermi surfaces is more complicated, Eq. (48) is not valid.

When the number of "holes" and "electrons" is equal,

$$\sigma_{xy}^{(1)} = 0. \tag{49}$$

We have thus shown that there are no quantum corrections to those terms the expansion of σ_{ik} in powers of γ which vanish in the classical case.

This means that, at least in the quasi-classical approximation, significant effects can be expected only in the temperature dependence of the conductivity and in the occurrence of quantum fluctuations. We shall now go on to a consideration of these questions.

3. THE RELATION BETWEEN THE QUANTUM MECHANICAL AND CLASSICAL EXPRESSIONS FOR THE CONDUCTIVITY IN A MAGNETIC FIELD

The expression for the conductivity tensor $\sigma^{xx'}$ is, according to (42) and (13),

$$\sigma^{xx'} = -e^2 t_0 \operatorname{Sp} \hat{v}^x \hat{\psi}^{x'}. \tag{50}$$

Noting that $\hat{v}$ and $\hat{\psi}$ are Hermitian and diagonal with respect to p_z, we have

$$\begin{aligned}\sigma^{xx'} &= A \int \sum_{n, n'} v^x_{n'n} \psi^{x'}_{n'n} dp_z \\ &= A \int \Big\{ \sum_n v^x_{nn} \psi^{x'}_{nn} + 2\operatorname{Re} \sum_{n'>n} v^x_{nn'} \psi^{x'}_{n'n} \Big\} dp_z \\ &= A \sum_n \int \{ v^x_0 \psi^{x'}_0 + 2\operatorname{Re} \sum_{k=1}^{\infty} v^x_{-k} \psi^{x'}_k \} \, dp_z.\end{aligned} \tag{51}$$

The normalizing constant A is most simply determined by comparison with the classical limit $\hbar\omega \to 0$ (see Eq. (42) of Ref. 1). Noting that $m^*\Delta\varepsilon_n = eH\hbar/c$, we have

$$A = -2 (e^2 t_0 / h^3) (eHh / c). \tag{52}$$

The ψ^x_k to be substituted into Eq. (51) must be a solution of the kinetic equation (25). In view of the linearity of (25) and (51) with respect to ψ^x_k and g_k, the results of this substitution can be written in the form of a certain "scalar product"

$$\sigma^{xx'} = -2 \frac{e\hbar H}{c} (\chi^{xx'}, g);$$

$$(\chi^{xx'}, g) = \sum_n \int \Big\{ \sum_{k=0}^{\infty} \chi^{xx'}_k g_k \Big\} dp_z; \quad \chi = \chi_k (\varepsilon_n, p_z). \tag{53}$$

Since v^x_0 and v^y_0 vanish, and the term g_0 enters only into the equation for ψ^z, none of the components of $\sigma^{xx'}$ containg $g_0 = \partial f^0/\partial\varepsilon$, except σ^{zz}:

$$\sigma^{xx'} = -2 \int \sum_{p_{zn}} \Big\{ \sum_{k=1}^{\infty} \chi^{xx'}_k g_k \Big\} m^* \Delta p_{zn} \, d\varepsilon, \quad (x, x' \neq z, z), \tag{54}$$

$$\sigma^{zz} = -2 \int \sum_{p_{zn}} \Big\{ \chi^{zz}_0 \frac{\partial f^0}{\partial \varepsilon} + \sum_{k=1}^{\infty} \chi^{zz}_k g_k \Big\} m^* \Delta p_{zn} \, d\varepsilon. \tag{55}$$

Thus, for instance, in the case $\tilde{W} = 1$ we have, according to (22),

$$\chi^{xx'}_k = \frac{2\pi e^2 t_0}{h^3} \operatorname{Re} \frac{2\gamma}{ik + \gamma} v^x_{-k} v^x_k. \tag{56}$$

In particular, for the diagonal components of σ^{xx}

$$\chi^{xx}_k = \frac{4\pi e^2 t_0}{h^3} \frac{\gamma^2}{k^2 + \gamma^2} |v^x_k|^2. \tag{57}$$

Expressions (56) and (57) agree exactly with the classical ones, since as has already been indicated the $\mathbf{v}_k$ are the Fourier amplitudes of the classical velocity vector; in order to obtain the classical expression for $\sigma^{xx'}$ it is sufficient to replace g_k by $\partial f^0/\partial\varepsilon$ in (54) and (55), and to go from summation over n to integration over $d\varepsilon$.

In the general case, the $\chi^{xx'}$ can be expressed in terms of the Green function of the kinetic equation (25)

$$\begin{aligned} &ik\mathfrak{G}_k + \gamma \hat{W}_{kk'} \mathfrak{G}_{k'} = \gamma \delta(\varepsilon - \varepsilon^0) \delta_{pzn,\, pzn^0} \delta_{kk^0} / \Delta p_{zn}; \\ &\mathfrak{G}_k = \mathfrak{G}(\varepsilon^0 p_z^0 k^0 \,|\, \varepsilon p_z k); \quad p_z = p_{zn} = p_z(n, \varepsilon); \\ &p_z^0 = p_{zn^0} \end{aligned} \tag{58}$$

by means of the equation

$$\begin{aligned} m^*(\varepsilon^0, p_z^0) \chi^{xx'}_{k^0}(\varepsilon^0, p_z^0) = \frac{2\pi e^2 t_0}{h^3} 2\operatorname{Re} \int \sum_{p_z} \Big\{ \sum_k v^x_{k_0}(\varepsilon^0, p_z^0) \\ \times \mathfrak{G}(\varepsilon^0 p_z^0 k^0 \,|\, \varepsilon p_z k) \, v^{x'}_{-k}(\varepsilon, p_z) \Big\} m^*(\varepsilon, p_z) \, d\varepsilon \, \Delta p_z. \end{aligned} \tag{59}$$

The classical "Green function" is a solution of the equation

$$ik\mathfrak{G}_k + \gamma \hat{W}_{kk'} \mathfrak{G}_{k'} = \gamma \delta(\varepsilon - \varepsilon^0) \delta(p_z - p_z^0) \delta_{kk^0}, \tag{60}$$

where $\hat{W}_{kk'}$ is the classical limit of the collision integral; in order to obtain $\chi^{xx'}$, one must go from summation to integration over p_z in Eq. (59).

When only elastic scattering by impurities is of importance, the collision integral does not contain the temperature. Therefore $\chi^{xx'}$ does not contain the parameter $\mu^*H/\Theta = \hbar\omega^*/\Theta$ and the transition to the classical limit for $\chi^{xx'}$ means just neglecting quantities of the order of $\hbar\omega^*/\zeta$ in comparison with $\hbar\omega^*/\Theta$ entering into the quantum effects through the expressions

$$g_k = [f^0(\varepsilon + k\hbar\omega^*) - f^0(\varepsilon)] / k\hbar\omega^*.$$

Thus in the case indicated, we may consider the $\chi^{xx'}_k$ in (54) and (55) to be equal to their classical analogs.

The classical expression for the conductivity is obtained by the substitution $g_k \to \partial f^0/\partial\varepsilon$ and transition to the integral

$$\begin{aligned} &\sigma^{xx'} = -2 \iint \frac{\partial f^0}{\partial \varepsilon} \chi^{xx'} m^* \, dp_z \, d\varepsilon; \quad x, x' \neq z, z; \\ &\sigma^{zz} = -2 \iint \frac{\partial f^0}{\partial \varepsilon} \{ \chi^{zz}_0 + \chi^{zz} \} m^* \, dp_z \, d\varepsilon; \end{aligned} \tag{61}$$

$$\chi^{xx'} = \sum_{k=1}^{\infty} \chi_k^{xx'}. \qquad (62)$$

Noting that the fundamental part of the quantum corrections is due to neighborhoods in which the function f^0 is highly nonstationary (that is, where $\varepsilon_n \cong \zeta$), and the functions $m^*(\varepsilon, p_z)$ and $\chi(\varepsilon, p_z)$ are smoothly varying, with the same accuracy, according to (54) and (17), we obtain the difference between the quantum and classical expressions for $\sigma^{xx'}$ (for $x, x' \neq z, z'$):

$$-\frac{1}{2}(\sigma^{xx'} - \sigma^{xx'}_{\text{class}}) = \sum_{k=1}^{\infty} \int \sum_n \left\{ \chi_k^{xx'} \frac{f^0(\varepsilon_n + k\hbar\omega^*)}{k\hbar\omega^*} - \chi_k^{xx'} \frac{f^0(\varepsilon_n)}{k\hbar\omega^*} \right\} \Delta\varepsilon_n \, dp_z$$

$$- \sum_{k=1}^{\infty} \iint \chi_k^{xx'} \frac{\partial f^0}{\partial \varepsilon} m^* \, d\varepsilon \, dp_z = \sum_{k=1}^{\infty} \int dp_z \left\{ \sum_{n \geqslant k} m^* \chi_k^{xx'}(\varepsilon - k\hbar\omega^*) \frac{f_n^0}{k} - \right.$$

$$\left. - \sum_{n \geqslant 0} m^* \chi_k^{xx'}(\varepsilon_n) \frac{f_n^0}{k} - f^0(\varepsilon_0) m^*(\varepsilon_0, p_z) \chi_k^{xx'}(\varepsilon_0, p_z) + \int f^0 (\partial(\chi_k^{xx'} m^*)/\partial\varepsilon) \, d\varepsilon \right\}$$

$$= - \sum_{k=1}^{\infty} \int dp_z \left\{ \sum_{\varepsilon_n} (\partial(\chi_k^{xx'} m^*)/\partial\varepsilon_n) f^0(\varepsilon_n) \Delta\varepsilon_n - \int (\partial(\chi_k^{xx'} m^*)/\partial\varepsilon) f^0 \, d\varepsilon \right\}.$$

Summing over k, we obtain

$$\sigma^{xx'} - \sigma^{xx'}_{\text{class}} = -2 \iint f^0 (\partial(\chi^{xx'} m^*)/\partial\varepsilon) \, d\varepsilon \, dp_z + \int \sum_n f^0 (\partial(\chi^{xx'} m^*)/\partial\varepsilon) \Delta\varepsilon \, dp_z.$$

Let us now go over to integration over n, making use of the fact that $\partial\varepsilon/\partial n = \hbar\omega^* = \Delta\varepsilon$ and Poisson's formula

$$\sigma^{xx'} - \sigma^{xx'}_{\text{class}} = \int \varphi^{xx'}(n) \, dn - \sum \varphi^{xx'}(n) = -\frac{1}{2} \varphi^{xx'}(0) + \sum_k I_k^{xx'};$$

$$\varphi^{xx'}(n) = -2 \int f^0 \frac{\partial(\chi^{xx'} m^*)}{\partial\varepsilon} \Big|_{\varepsilon = \varepsilon(n, p_z)} \hbar\omega^* \, dp_z;$$

$$I_k^{xx'} = 2 \int \varphi^{xx'}(n) e^{2\pi i k n} \, dn.$$

The expression obtained for the quantum corrections contains both an oscillating part and terms varying smoothly with the field. In the latter, however, a large contribution comes from levels with small n (in particular, from $\varphi(0)$). For these levels the quasi-classical approximation is exact only for the quadratic dispersion law. In general we need maintain only the oscillating part of the conductivity, since the smoothly varying part merely contributes a small correction to the basic classical value. Thus

$$\sigma^{xx'} - \sigma^{xx'}_{\text{class}} = m \sum_{k=1}^{\infty} I_k;$$

$$I_k = 2 \iint f^0 \frac{\partial(\chi^{xx'} m^*)}{\partial\varepsilon} \hbar\omega^* e^{2\pi i k n} \, dn \, dp_z \qquad (63)$$

Noting that according to (55) the expression for σ^{zz} contains an additional term with $\chi_0^{zz} \partial f^0/\partial\varepsilon$, we obtain in a similar way

$$\sigma^{zz} - \sigma^{zz}_{\text{class}} = \sum I_k^{zz} - \sum L_k^{zz};$$

$$L_k^{zz} = 2 \iint \frac{\partial f^0}{\partial\varepsilon} \chi_0^{zz} m^* \hbar\omega^* e^{2\pi i k n} \, dn \, dp_z. \qquad (64)$$

The structure of Eqs. (63) and (64) is such that it is easy to separate out the oscillating terms in I_k and L_k. Their detailed analysis, and a discussion of the various aspects of the Shubnikov–de Haas effect, is taken up in a separate article.

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Vacuum Polarization in Mesonic Atoms

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Level shifts in mesonic atoms due to vacuum polarization produced by the nuclear electric field are computed. The recursion relations between the meson wave functions are used to derive equations in closed form for the first six level shifts. The shifts for the first three levels of heavy mesonic atoms are computed with allowance for the finite volume of the nucleus.

1. INTRODUCTION

TO STUDY THE PROPERTIES of mesonic atoms it is important to know the position of the energy levels of the meson. In light mesonic atoms (up to $Z \sim 20$), the energy level is determined principally by nonrelativistic formulas of the Keppler problem of hydrogen-like atoms, in which the electron mass is replaced by a reduced meson mass.[1] The most significant corrections for these formulas are the relativistic corrections, the level shifts due to the vacuum polarization by the electric field of the nucleus,[2] the shift due to the distribution of the positive charge over the volume of the nucleus, and in π-mesoatoms also the shift due to nuclear interaction between the meson and the nucleons of the nucleus.[3] In heavy mesonic atoms the effect of the finite volume of the nucleus on the position of the levels is so considerable that it can no longer be considered a small perturbation. For example, when the volume of the nucleus is taken into account, the energy of the 1S muon in μ-meso-lead turns out to have half the value given by the equation for point-like nuclei.[1] In the case of heavy mesonic atoms it therefore becomes necessary to solve from the very beginning for the motion of the meson in the electric field of a nucleus occupying a finite volume. As to the remaining significant corrections to the energy levels of heavy mesonic atoms, to which one must add also the influence of the quadrupole electric moment of the nucleus[4,5] and the polarization (deformation) of the nucleus by the meson,[6,7] these do not exceed 1 – 2% of the level energy.

While in the hydrogen atom the Lamb shift of the electron energy levels is due fundamentally to the correction for the field electromagnetic mass, and approximately 1/25 th of the shift is caused by vacuum polarization, the situation in mesonic atoms is different. The vacuum polarization of electrons and positrons changes the electrostatic potential of the nucleus at a distance on the order of the Compton wavelength of the electron ($\sim 10^{-11}$ cm), regardless of what particle, electron or meson, moves around the nucleus. Since the Bohr radius of the orbit is inversely proportional to the mass of the particle, the radii of the meson orbits are 200 – 300 times smaller than the radii of the electron orbits and their dimensions are on the order of $10^{-11} - 10^{-12}$ cm. As a result, the meson spends a greater part of its time in a region where the electrostatic potential of the nucleus is changed by the influence of the vacuum polarization, which leads to a considerable level shift. At the same time, the correction for the electromagnetic intrinsic mass, which is inversely proportional to the square of the mass of the moving particle, will be considerably smaller in mesonic atoms than the Lamb shift for electrons, as a consequence of the greater mass of the meson.

The energy level shift due to vacuum polarization is a substantial correction for all mesonic atoms ($\sim$ 0.1 – 2% of the energy of the level). The influence of vacuum polarization is noticeable at