ON THE QUANTUM ANALOG OF THE COLLISION INTEGRAL FOR ELECTRONS IN MAGNETIC AND ELECTRIC FIELDS

A. M. KOSEVICH and V. V. ANDREEV

Physico-technical Institute, Academy of Sciences, Ukrainian S. S. R.

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The influence of an electric field on the quantum analog of the collision integral for electrons in a magnetic field is investigated. For this purpose the quantum mechanical transport equation for electrons in a metal in crossed magnetic and electric fields is derived for low temperatures when the electron scattering occurs mainly on impurities. It is found that the purely quantum mechanical term in the "collision integral" which is proportional to the electric field and was not taken into account in the transport equation in reference 1 plays an important role in the discussion of quantum effects in strong magnetic fields. The oscillations of the elements of the "transverse" electrical conductivity tensor due to variations of the magnetic field are considered.

INTRODUCTION

I. M. LIFSHITZ[1] has constructed a quantum theory of the conduction of metals in a magnetic field at low temperatures. In this work essential use is made of the correspondence principle, according to which the kernel of the integral transformation that describes the collisions of the electrons with the impurities can be replaced by its classical value in the quasi-classical approximation. By making this replacement one neglects, of course, the effect of the electric field on the collision integral, as in the classical case.

In the present paper it is our aim to investigate the influence of the electric field on the quantum analog of the collision integral in a magnetic field and to point out possible consequences arising from taking this circumstance into account. Our interest in this problem was prompted to a large extent by remarks contained in the paper by Adams and Holstein.[2]

To obtain a qualitative idea of the possible role of those corrections in the quantum mechanical transport equation which are caused by the influence of the electric field $\mathbf{E}$ on the "collision integral" we consider the fundamental equation of the paper by I. M. Lifshitz,[1] which is in its simplest form

$$\{i(n-n')\omega^* + 1/\tau\}\rho^1_{nn'} = -e\mathbf{E}\mathbf{v}_{nn'}(f^0_n - f^0_{n'})/(\varepsilon_n - \varepsilon_{n'}). \quad (1)$$

Here ρ^1 is a correction to the equilibrium density matrix for the electrons, n is the quantum number of the orbital motion of the electron in the magnetic field $\mathbf{H}$, $f^0_n \equiv f_0(\epsilon_n)$ is the Fermi function, $\omega^* = eH/m^*c$, m^* is the effective mass of the electron, τ is the relaxation time, and $\mathbf{v}$ is the velocity of the electron.

The most interesting region for the application of equation (1) is the region of strong magnetic fields, when $\omega^*\tau \gg 1$. In the following we will be interested only in this region of fields, so that we shall regard $1/\omega^*\tau$ as a small parameter the powers of which define the order of smallness of the corresponding expressions.

When the electric field is taken account of in the "collision integral" in (1), a small quantum term of the order of

$$(eEa/\hbar\omega^*)(f_0/\tau), \quad (2)$$

will appear, where a is some characteristic length related to the collision process. Observing that the estimate (2) depends on f_0 but not on ρ^1, we consider the largest possible alteration of Eq. (1). The estimate (2) depends critically on the determination of the order of magnitude of the parameter a. In the case of a longitudinal electric field ($\mathbf{E} \parallel \mathbf{H}$), the parameter a is of the same order of magnitude as the de Broglie wavelength of the electron. With such an a, the quantity (2) is so small that the longitudinal electric field may be neglected in the "collision integral." In the case of a transverse electric field ($\mathbf{E} \perp \mathbf{H}$) the parameter a should be of the order of magnitude of the classical radius of the Larmor orbit of the electron, r. This is easily understood by noting that the motion of the

electron is quantized in a direction perpendicular to the magnetic field, so that even in the scattering from a point center the result depends on the radius of the orbit as on one of the parameters describing the state of the electron

Since the right hand side of (1) has for $n \neq n'$ the order of magnitude

$$eEv\,(f_0/\hbar\omega^*), \tag{3}$$

it may turn out that even in the case of a transverse field the correction (2) is smaller than the leading term of the right hand side of (1) by the factor $r/v\tau \sim 1/\omega^*\tau \ll 1$. However, for uniform fields the basic term on the right hand side of (1) does not give any contribution to the electric current in the zeroth approximation with respect to $1/\omega^*\tau$; to investigate the role of the additional term in the transport equation we must therefore estimate the ratio of the quantities (2) and (3) multiplied by $\omega^*\tau$. This last circumstance permits us to believe that in quantum phenomena the role of the term due to the influence of the electric field on the "collision integral" is comparable to that of the basic term included in Eq. (1).

In order to substantiate the qualitative remarks made above, we must analyze the equation for the density matrix of the electrons in the magnetic field and establish rigorously the corresponding quantum mechanical transport equation. Without pretense to completeness we consider, in Sec. 1, the quantum mechanical transport equation obtained from the general equation for the density matrix of perturbation theory, i.e., in the same approximation as in the work of Adams and Holstein.[2] The "collision integral" of this equation is derived by the method developed by Bogolyubov[3] and used by Gurzhi[4] for the calculation of the electron-phonon interaction in the field of an electromagnetic wave. This method is similar to that proposed by Kohn and Luttinger.[5]

In Sec. 2 we illustrate the role of the additional term in the transport equation on the example of the calculation of the oscillations of the tensor of the "transverse" electric conductivity (Shubnikov-de Haas effect). It will be shown in this section that the quantum oscillations of the tensor of electrical conductivity can, as has also been done earlier,[6] be expressed in terms of the classical "mobility" tensor and the oscillatory part of the magnetic moment of the electron gas. This connection between the classical and quantum characteristics was obtained for the first terms of the expansion of the tensor of electrical conductivity in powers of $1/\omega^*\tau$, but it is not essentially linked to perturbation theory by which τ was computed.

1. THE QUANTUM MECHANICAL TRANSPORT EQUATION IN MAGNETIC AND ELECTRIC FIELDS

Let us consider a gas of electrons which interact with particles of a different kind. As we are interested in the elastic scattering by the impurities, we consider only the interactions of the electrons with the heavy neutral particles (the interaction with the phonons can be treated in an analogous fashion). If the mass of the heavy particle is M, we can assume that $M \gg m$ (m is the mass of the electron), and consider the interaction of the electrons with fixed impurities. We assume that the heavy particles are distributed uniformly in space (the state of free motion of the particle is described by the momentum $\mathbf{s}$). The energy of the interaction between the electron and the heavy particle will be denoted by $V(\mathbf{r})$, where $\mathbf{r}$ is the distance between the two particles.

Following Bogolyubov,[3] we can write down a chain of equations for the partial statistical operators of the system of electrons and heavy particles and cut it off at the equation for the binary density matrix. We can then use perturbation theory to obtain a system of two equations for the one-particle density matrices of the electrons, ρ, and the heavy particles. The equation for ρ has the form

$$\partial\rho/\partial t + (i/\hbar)[\mathcal{H}, \rho] + D\{\rho\} = 0, \tag{4}$$

where $D\{\rho\}$ is the quantum analog of the collision integral. The expression for $D\{\rho\}$ is quadratic in the matrix elements of V and depends on the density matrix of the heavy particles.

In writing down the expression for $D\{\rho\}$ for the elastic scattering by the impurities, we regard the gas of heavy particles to be in equilibrium (the corresponding density matrix is diagonal in $\mathbf{s}$), and assume that the mass of the heavy particle is infinite as compared to the mass of the electron ($M \gg m$). These assumptions replace the usual averaging over the positions of the impurities and lead to the following expression for $D\{\rho\}$ in the representation in which the Hamiltonian of the electron in the given fields, $\mathcal{H}$, is diagonal ($\mathcal{H}_{\mu\nu} = \epsilon_\mu\delta_{\mu\nu}$):*

$$(D\rho)^{\mu\nu} = N(2\pi/\hbar)\sum\delta_+(\varepsilon_l - \varepsilon_\mu)[\rho^{\mu l'}V_s^{l'l}V_{-s}^{l\nu} - V_s^{\mu l'}\rho^{l'l}V_{-s}^{l\nu}]$$
$$- \delta_+(\varepsilon_\nu - \varepsilon_l)[V_s^{\mu l}\rho^{ll'}V_{-s}^{l'\nu} - V_s^{\mu l}V_{-s}^{ll'}\rho^{l'\nu}]. \tag{5}$$

The summation in (5) goes over all Latin indices, N is the number of scattering centers per unit

*All calculations leading to (5) are completely analogous to the calculations of references 3 and 4 and can therefore be omitted.

volume, and

$$\delta_+(x) = \tfrac{1}{2}\delta(x) + i/2\pi x. \quad (6)$$

If we assume that $\rho^{\mu\nu}$ is diagonal, i.e., that there exists a distribution function, then formula (5) goes over into the classical collision integral for impurities.

Equation (4), with a Hamiltonian $\mathcal{H}$ which allows stationary states of the electron, determines the equilibrium density matrix of the electron gas. It is easy to verify that, up to terms which are quadratic in V [with accuracy corresponding to expression (5)], the equilibrium density matrix ρ_0 has the form

$$\rho_0^{\mu\nu} = f_0(\varepsilon_\mu)\,\delta_{\mu\nu} + F_0^{\mu\nu}, \quad (7)$$

$$F_0^{\mu\nu} = N\sum_{l,s} V_s^{\mu l} V_{-s}^{l\nu}\,(g^{\mu l} - g^{\nu l})/(\varepsilon_\mu - \varepsilon_\nu),$$

$$g^{\mu\nu} = (f_\mu^0 - f_\nu^0)/(\varepsilon_\mu - \varepsilon_\nu). \quad (8)$$

The physical meaning of the nondiagonal part of ρ_0 (i.e., of the matrix F_0) is very simple: expression (7) gives the first terms of the expansion of the operator $f_0(\mathcal{H} + W)$ in powers of $W = \Sigma V$ (sum over all impurities) averaged over the positions of the fixed impurities.

In order to establish the explicit form of Eq. (4) for the electron gas in constant magnetic (**H**) and electric (**E**) fields with $\omega^*\tau \gg 1$, we must take account of the existence of stationary states of the electron for mutually perpendicular **H** and **E**. This last circumstance leads, as we shall see below, to the dependence of $D\{\rho\}$ on the component of **E** perpendicular to **H**. A simple analysis shows at the same time that in our approximation $D\{\rho\}$ does not depend on the component of **E** along **H**. This means that the longitudinal electric field is fully included in the equations of type (1) in reference 1. In order to keep the appearance of the equations simple, we shall in the following not consider the component of **E** along the magnetic field at all, i.e., we shall investigate the simplest case of mutually perpendicular **H** and **E** ($H = H_z$, $E = E_y$).

Let $\hat{\epsilon}$ be the Hamiltonian for the motion of the electron in the magnetic field (its eigenvalues are $\epsilon_\mu \equiv \epsilon_n(p_z)$, $\mu = n, p_x, p_z$). We use the representation corresponding to this Hamiltonian in order to facilitate the comparison of our equation with the equations of reference 1 (the result given below can be obtained in a more direct way by using the representation in which the total Hamiltonian $\mathcal{H} = \hat{\epsilon} - eE\hat{y}$ is diagonal).

In the representation $\hat{\epsilon}$ the total Hamiltonian takes the form

$$\mathcal{H}_{\mu\nu} = (\varepsilon_\mu - eEy_0)\,\delta_{\mu\nu} - eE\xi_{\mu\nu}, \quad (9)$$

where $y_0 = -cp_x/eH$ plays the role of y, the coordinate of the center of the classical Larmor orbit of the electron,[7,8] and ξ is the displacement of the electron with respect to this center.

It is an essential characteristic of Eq. (9) that the electric field enters in the diagonal part of $\mathcal{H}$. It then follows by straight mathematical manipulation that the δ-functions of the "collision integral" $D\{\rho\}$, which describe the law of energy conservation, will also contain E explicitly. From a physical point of view this is extremely reasonable, since the term $-eEy_0$ in (9) has the meaning of the potential energy of the electron in the electric field. However, by virtue of the quantum nature of the motion of the electron in the Larmor orbit in the magnetic field (the electron is "smeared out" over the orbit), its "potential" energy depends on the location of the center of this orbit. Since the location of the center of the classical orbit changes in collisions, it is natural that E enters explicitly in the law of energy conservation.*

The nondiagonal part of $\mathcal{H}$ is very simply accounted for in writing down $D\{\rho\}$. If we express the density matrix ρ in the form $\rho = \rho_0 + \rho_1$ (ρ_0 is determined by (7), where ϵ_μ are the energy levels of the electron in the magnetic field) and linearize Eq. (4) with respect to E, we obtain as a result the following form of the quantum mechanical transport equation:

$$\partial\rho_1/\partial t + (i/\hbar)[\varepsilon, \rho_1] + eEgv_y + D\{\rho_1\} = eED\{(cp_x/eH)\,df_0/d\varepsilon - \xi g\} + (i/\hbar)[eEy, F_0]. \quad (10)$$

The matrix product ga in (10) is to be understood as a direct product: $(ga)^{\mu\nu} = g^{\mu\nu}a^{\mu\nu}$. The matrix F_0 is given by formula (8).

The right hand side of (10), which vanishes in the classical case of scattering by point centers, takes account of the influence of E on $D\{\rho\}$ and distinguishes (10) from the quantum mechanical transport equation used by I. M. Lifshitz.[1]

In the stationary case ($\partial\rho_1/\partial t = 0$) a solution of (10) can be found in the form of an expansion of ρ_1 in powers of $1/\omega^*\tau$: $\rho_1 = \rho_1^{(0)} + \rho_1^{(1)}$. The first term, which is independent of the relaxation time, has the form

$$\rho_1^{(0)} = -eE\xi g. \quad (11)$$

*Noting that in the quasi-classical approximation the inclusion of E is essential only in the conservation law, the influence of the electric field on the "collision integral" can be described within the framework of the basic transport equation of reference 1 by using the representation in which the Hamiltonian $\mathcal{H}$ is diagonal and by replacing $\delta(\epsilon - \epsilon')$ by $\delta(\epsilon - eEy_0 - \epsilon' + eEy_0')$ in formula (27) of reference 1.

For $\rho_1^{(1)}$ we obtain the relation

$$(i/\hbar)[\varepsilon, \rho_1^{(1)}] = eED\{(cp_x/eH)\,df_0/d\varepsilon\} + (i/\hbar)[eEy, F_0], \quad (12)$$

which is in agreement with the result of Adams and Holstein.[2] The last term on the right hand side of (12) does not contribute to the current along the y axis and was therefore neglected.

In the classical approximation, expressions (11) and (12) go over into

$$\rho_1^{(0)} = -eE\xi df_0/d\varepsilon, \quad (13)$$

$$\partial\rho_1^{(1)}/\partial\varphi = eED_0\{(cp_x/eH)\,df_0/d\varepsilon\}, \quad (14)$$

respectively, where φ is an angular variable that describes the position of the electron on the classical orbit in momentum space, which we introduce following Lifshitz et al.[1,9] The determination of $D_0\{\rho\}$ is formally the same as before, with the only difference that the matrix elements of V which enter in the expression are replaced by the corresponding Fourier components,[1] and the functions $\delta_+(x)$ are changed to $\frac{1}{2}\delta(x)$.

It is easily seen that expressions (13) and (14) give the first terms of the expansion of the solution of the classical transport equation in a magnetic field in powers of $1/\omega^*\tau$.

2. THE TRANSVERSE ELECTRICAL CONDUCTIVITY OF A METAL IN A MAGNETIC FIELD

The electric current transverse to the magnetic field is given by the usual expression

$$j^\alpha = e\,\mathrm{Sp}\{\rho_1 v^\alpha\} \quad (\alpha = x, y). \quad (15)$$

It immediately follows from (15) and (11) that the terms proportional to $1/H$ in the expansion of the elements of the electrical conductivity tensor $\sigma^{\alpha y}$ are determined in the obvious way:[1]

$$\sigma_{yy}^{(0)} = 0, \quad \sigma_{xy}^{(0)} = (ec/H)(n_e - n_h), \quad (16)$$

where n_e is the number of electrons and n_h is the number of "holes" in the case of a closed Fermi surface. The expression (16) for $\sigma_{xy}^{(0)}$ includes the current along the x axis due to the last term in (12); it gives the following contribution to σ_{xy}:

$$\Delta\sigma_{xy}^{(0)} = (ec/H)\,\mathrm{Sp}\{F_0\}. \quad (17)$$

It is clear from the meaning of the diagonal elements of the matrix $F_0^{\mu\nu}$ that the additional term (17) can be included in the renormalized chemical potential of the electron gas, so that it is indeed taken account of in expression (16).

The part of $\sigma^{\alpha y}$ which is determined by the "collision integral" can be written in the form

$$\sigma_{\alpha y}^{(1)} = -2\sum_{\varepsilon_n}\int\frac{df_0}{d\varepsilon_n}\chi_{qu}^{\alpha y}m^*\Delta\varepsilon_n dp_z. \quad (18)$$

The quantities $\chi_{qu}^{\alpha y}$ entering in (18) are given in an obvious way by (15) and (12). They correspond to the linear terms of the expansion in powers of $1/\omega^*\tau$ of the analogous quantities χ introduced in reference 1.

The classical part of $\sigma_{\alpha y}^{(1)}$ is obtained from (18) by going directly from the summation over ϵ_n to the integration over ϵ and replacing $\chi_{qu}^{\alpha y}$ by its classical value $\chi^{\alpha y}$:

$$\sigma_{\alpha y}^{(1)} = -2\int\int\frac{df_0}{d\varepsilon}\chi^{\alpha y}m^*d\varepsilon dp_z. \quad (19)$$

Following reference 1, we replace the quantities $\chi_{qu}^{\alpha y}$ in (18) by their classical values $\chi^{\alpha y}$. This operation was discussed in reference 1, and its validity was proven for the scattering by impurities. Its meaning is merely that we consider only the basic term in the expansion of the quantum corrections to $\sigma^{\alpha y}$ in powers of λ/r, where λ is the de Broglie wavelength, and r is the radius of the Larmor orbit of the electron. Since $\lambda/r \ll 1$ in metals, the magnitude of any quantum effect is determined by the basic term of the expansion.

Starting from (18) and (19) and using the method of calculation developed earlier,[6,7] we easily obtain the oscillatory parts of the elements of $\sigma^{\alpha y}$:

$$\Delta\sigma_{osc}^{\alpha y} = h^3(\gamma m^*)_m^\zeta\frac{dS_m^{-1}(\zeta)}{d\zeta}H^2\frac{\partial\Delta M_z}{\partial H}, \quad (20)$$

where $S_m(\zeta)$ is the maximal area of the intersection of the Fermi surface with the plane perpendicular to **H**; the index m indicates that the corresponding quantity is evaluated at the maximal section of this surface. ΔM_z denotes the oscillatory part of the component of the magnetic moment of the electron gas along the magnetic field and is determined in reference 7.

We note that the classical formula for $\sigma_{\alpha y}^{(1)}$ with $kT \ll \zeta_0$ (ζ_0 is the chemical potential of the electron gas at $T = 0°K$) can be written in terms of the same quantities which determine the amplitude of the oscillations in (20):

$$\sigma_{\alpha y}^{(1)} = n_0\bar{u}_{\alpha y}(\zeta), \quad (21)$$

where n_0 is the number of current carriers in a given group and $u_{\alpha y}$ has the meaning of an element of the "mobility tensor":

$$u^{\alpha y}(\varepsilon, p_z) = \chi^{\alpha y}m^*/S(\varepsilon, p_z) \quad (22)$$

the averaging is performed over the Fermi surface:

$$\bar{u}(\zeta) = \int u(\zeta, p_z)S(\varepsilon, p_z)\,dp_z \Big/ \int S(\varepsilon, p_z)\,dp_z. \quad (23)$$

The quantity $S(\zeta, p_z)$ in (23) denotes the area of

the intersection of the Fermi surface with the plane p_z = const, so that the integral $\int S(\zeta, p_z)\, dp_z$ gives the volume bounded by the Fermi surface.

Using (22), we rewrite (20) in the form

$$\Delta\sigma_{osc}^{\alpha y} = -H^2 u_m^{\alpha y}(\zeta)\left(\frac{d \ln S_m(\zeta)}{d\zeta}\right)\frac{\partial \Delta M_z}{\partial H}. \qquad (24)$$

In this way we see that, as in the work of I. M. Lifshitz,[1] the oscillations of $\sigma^{\alpha y}$ are expressed in terms of the oscillations of ΔM_z, where the amplitude of the oscillations is determined by the classical "mobility tensor."

The oscillation amplitudes given by formula (24) are in agreement with the results of Adams and Holstein[2] and are larger than the amplitudes determined in reference 6 by the factor $\zeta_0/\hbar\omega^*$. This last circumstance allows us to neglect the oscillations of the chemical potential of the electron gas in the investigation of the oscillations.

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