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Kinetic equation having the integral scattering term with a linear form of external electrical and magnetic fields

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Abstract. In many cases, nobody consider any kinetic equation where the collision integral does not use clearly the values of external electric and magnetic fields. But there is some reason to use in the collision integral the above fields and to consider the ratio of the averaged deBroglie wavelength to the free-path length.

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1. Introduction

Along the way to construct the kinetic equation from some "first principles", the rightful place belongs to the influence of external macroscopic and microscopic fields on movement of charged band carriers. The scattering fields give the main, principal contribution to the existence and form of the collision integral. The evident influence of macroscopic fields on the scattering system is not usually taken into account, and one supposes that for the scheme of the second order perturbation theory, and the external field can be omitted (see [1]). Special consideration shows that direct influence of macroscopic fields on the form of collision integral and of corresponding non-equilibrium distribution function can change the value of kinetic coefficients.

2. One-particle density matrix Hamiltonian and scattering system

Let us design by using the symbols *A*, *B etc*. some set of quantum numbers (for instance, components of space wave vector), which characterize the state of each separate band particle; farther, for simplicity, we say here about electrons. In what follows, we do not use the direct designations for spin variables, because processes of spin overturn are not considered here. The act of averaging we designate by angle brackets; formally that procedure is performed using the non-equilibrium statistical operator of total system of electrons and external system, representing the selected scattering field that interact with electron system (see, for example, [9–12]).

Define the one-particle density matrix $\rho_{AB}(t)$ by the following manner:

$$\rho_{AB}(t) = a_B^+(t)\, a_A(t)\,. \tag{1}$$

Here, t is time, a_A^+ and a_A are operators of generation and annihilation of electron at the state *A*. The averaged value of given matrix (we call it below as the one-particle density matrix) is

$$f_{AB}(t) = \langle \rho_{AB}(t) \rangle = \left\langle a_B^+(t)\, a_A(t) \right\rangle. \tag{2}$$

The dynamic value $C = \sum_{n=1}^{N} C(\vec{r}_n)$ that belongs to an additive type, in the representation of secondary quantization has the form $\hat{C} = \sum_{A,B} C_{BA}\, a_B^+ a_A$, where $C_{BA} = \int \Psi_B^*(\vec{r})\hat{C}(\vec{r})\Psi_A(\vec{r}) d^3\vec{r}$. In this formula, the value $\Psi_A(\vec{r})$ is the wave function of separate band particle, which belongs to the state *A*.

Deduce an equation, solution of which is the one-particle density matrix f_{AB} of the considered non-equilibrium system of particles. As a start point, we use the standard motion equation for the operator $\rho_{AB}(t)$ in the Heisenberg representation:

$$i\hbar \frac{\partial \rho_{AB}}{\partial t} = \left[\rho_{AB}(t)\,, H^{tot} \right] \equiv \rho_{AB}(t)\, H^{tot} - H^{tot} \rho_{AB}(t). \tag{3}$$

One can represent the Hamiltonian of considered total system H^{tot} as the sum of four parts: Hamiltonian H_e for electrons non-interacting with microscopic scattering fields, Hamiltonian H_{ee} related to inter-electron interaction, individual Hamiltonian H_S of external scattering system and Hamiltonian H_{eS} that is related to interaction of band electrons with the scattering system:

$$H^{tot} = H_{ee} + H_e + H_S + H_{eS}. \tag{4}$$

In this paper, we assume only the point charged impurities as external scattering system $(S \to I)$.

Here, we use the constant uniform electrical $\vec{E}$ and magnetic $\vec{H}$ fields. Then the Hamiltonian of free band carriers is

$$H_e = \varepsilon\left(\hat{\vec{p}} + \frac{e}{c}\vec{A}(\vec{r})\right) - e\vec{E}\vec{r}\,. \tag{5}$$

Here, $\hat{\vec{p}} = \hbar\hat{\vec{k}} = -i\hbar\dfrac{\partial}{\partial\vec{r}}$ is the momentum operator, $\varepsilon(\vec{p})$ – dispersion law, $\varepsilon(\hat{\vec{p}})$ – operator of the kinetic energy, and $\vec{A}$ – vector-potential of magnetic field. In this work, we suppose that the dispersion law has the simple form:

$$\varepsilon(\vec{p}) = p^2/2m = \hbar^2k^2/2m, \tag{6}$$

where *m* is the effective mass.

The quantum limit of strong magnetic field in this paper is not considered. Therefore, in the Hamiltonian (5) we omit the terms of the order A^2; the latter is acceptable at the condition $|eH|\hbar/2mc << \langle\varepsilon\rangle$. Let $(A_1A_2)_+ = (1/2)(A_1A_2 + A_2A_1)$. Then it follows from Eq. (5):

$$H_e = H^{(0)} + H^{(E)} + H^{(H)} = \varepsilon(\hat{\vec{p}}) - e\vec{E}\vec{r} + \frac{e}{mc}\left(\vec{A}(\vec{r})\cdot\hat{\vec{p}}\right)_+ \tag{7}$$

Assume the following orientations of electrical $\vec{E}$ and magnetic $\vec{H}$ fields:

$$\vec{E} = (E_x, 0, 0),\ \vec{H} = (0, 0, H_z),\ \vec{A} = (-H_z y, 0, 0). \tag{8}$$

For the considered case (see Eq. (6)), the separate items of Hamiltonian H_e are

$$H^{(0)} = \varepsilon(\hat{\vec{p}}) = (\hat{\vec{p}})^2/2m = \hbar^2\hat{\vec{k}}^2/2m,$$
$$H^{(E)} = -exE_x, \tag{9}$$
$$H^{(H)} = -\frac{e\hbar H_z\hat{k}_x}{mc}y.$$

In the representation of secondary quantization, the Hamiltonian of electrons that do not interact with microscopic scattering fields is (see Eqs (7) and (9))

$$H_e = \sum_{AB}(H_e)_{AB}a_A^+a_B = \sum_{AB}(H_e)_{AB}\rho_{BA} = \\ = \sum_{AB}\left\{\left(H^0\right)_{AB} + \left(H^{(E)}\right)_{AB} + \left(H^{(H)}\right)_{AB}\right\}\rho_{BA}. \tag{10}$$

As a result, the total Hamiltonian presented in Eq. (3) has the form

$$H^{tot} = \sum_{AB}\left\{(H_e)_{AB} + (H_{eI})_{AB}\right\}\rho_{BA}. \tag{11}$$

The plane waves are the natural basis for spatially uniform system of electrons:

$$\Psi_A(\vec{r}) \to L^{-3/2}\exp\left(i\vec{k}_A\vec{r}\right). \tag{12}$$

Substituting the expression (11) into (3) and performing necessary commutations of Fermi operators, one obtains the following equation for the density matrix:

$$i\hbar\frac{\partial\rho_{AB}(t)}{\partial t} = \sum_{\Gamma}\left\{(H_e)_{A\Gamma}\rho_{\Gamma B}(t) - (H_e)_{\Gamma B}\rho_{A\Gamma}(t)\right\} + \\ + \sum_{\Gamma}\left\{(H_{eI}(t))_{A\Gamma}, \rho_{\Gamma B}(t)_+ - (\rho_{A\Gamma}(t), (H_{eI}(t))_{\Gamma B})_+\right\}. \tag{13}$$

3. Averaged values and fluctuations

Separate the density matrix $\rho_{AB}(t)$ and Hamiltonian $H^{tot}(t)$ into averaged values and fluctuations. Let us assume that the averaged scattering potential is zero. Then

$$\rho_{AB}(t) = \langle\rho_{AB}(t)\rangle + \delta\rho_{AB}(t) = f_{AB}(t) + \delta\rho_{AB}(t), \tag{14}$$

$$(H_{eI}(t))_{AB} = \langle(H_{eI}(t))_{AB}\rangle + \delta(H_{eI}(t))_{AB} = \delta(H_{eI}(t))_{AB}. \tag{15}$$

Non-dependence (or very weak dependence) of the electron density on spatial coordinates is provided by the following condition:

$$f_{AB}(t) = \delta_{AB}f_{AA}(t) \equiv \delta_{AB}f_A(t). \tag{16}$$

Accept also the condition below (see [6]):

$$\langle\partial\rho_{AB}/\partial t\rangle = \partial\langle\rho_{AB}\rangle/\partial t = \partial f_{AB}/\partial t. \tag{17}$$

Averaging the latter expression, we find:

$$i\hbar\frac{\partial f_{AB}(t)}{\partial t} = \sum_{\Gamma}\left\{(H_e)_{A\Gamma}f_{\Gamma B}(t) - (H_e)_{\Gamma B}f_{A\Gamma}(t)\right\} + i\hbar\,\mathrm{St}\,f_{AB}(t), \tag{18}$$

where

$$\mathrm{St}\ f_{AB}(t) = -\frac{i}{\hbar}\sum_{\Gamma}\left\{\left(\delta H(t)\right)_{A\Gamma},\delta\rho_{\Gamma B}(t))_{+} - \left(\delta H(t)\right)_{\Gamma B},\delta\rho_{A\Gamma}(t))_{+}\right\}. \quad (19)$$

Thereof (see (16)):

$$i\hbar\frac{\partial f_A}{\partial t} = \sum_B\left[\left(H_e\right)_{AB} f_{BA}(t) - \left(H_e\right)_{BA} f_{AB}(t)\right] + i\hbar\,\mathrm{St}\ f_A(t), \quad (20)$$

$$\mathrm{St}\ f_A = -\frac{i}{\hbar}\sum_B\left\{\left\langle\left(\delta H(t)\right)_{AB},\delta\rho_{BA}(t))_{+}\right\rangle - \left\langle\left(\delta H(t)\right)_{BA},\delta\rho_{AB}(t))_{+}\right\rangle\right\}. \quad (21)$$

One calls Eq. (20) as the kinetic equation and the expression (21) as the collision integral.

Subtracting Eq. (18) from Eq. (20), we find (terms of second order of trifle are here omitted):

$$i\hbar\frac{\partial}{\partial t}\{\delta\rho_{AB}(t)\} = \sum_{\Gamma}\left[\left(H_e\right)_{A\Gamma}\delta\rho_{\Gamma B}(t)) - \left(H_e\right)_{\Gamma B}\delta\rho_{A\Gamma}(t)\right] + \left[f_B(t) - f_A(t)\right]\left(\delta H(t)\right)_{AB}. \quad (22)$$

Farther in Eq. (31), we consider the averaged distribution function to be smooth in comparison with fluctuating values. Using the Laplas transformation [15]:

$$\xi(\omega) = \int_0^{\infty}\xi(t)\exp(i\omega t)\,dt\ ,$$
$$\xi(t) = \frac{1}{2\pi}\int_{-\infty+i0}^{\infty+i0}\xi(\omega)\exp\left(-i\omega t\right)d\omega\,, \quad (23)$$

one obtains:

$$-i\hbar\delta\rho_{AB}\left(t=0\right) + \hbar\omega\delta\rho_{AB}(\omega) = \sum_{\Gamma}\left\{\left(H_e\right)_{A\Gamma}\delta\rho_{\Gamma B}(\omega)) - \left(H_e\right)_{\Gamma B}\delta\rho_{A\Gamma}(\omega)\right\} + \left(f_B - f_A\right)\left(\delta H(\omega)\right)_{AB}, \quad (24)$$

$$\mathrm{St}\ f_A = -\frac{1}{2\pi^2\hbar}\times \left\{\int d\omega\int d\omega'\exp\left[-i\left(\omega+\omega'\right)\right]\sum_B\left\langle\delta\rho_{AB}(\omega),\delta H_{BA}\left(\omega'\right)_{+}\right\rangle\right\}. \quad (25)$$

4. Correlation for scattering potential of charged impurities

Designate the non-screened electrical potential created by charge disposed in the point $\vec{r}=0$ by the symbol $\varphi^{(I)}\left(\vec{r},t\right) = H_{eI}\left(\vec{r}\right)/e$. The total potential created by all centers has the form

$$\varphi^{(I)}\left(\vec{r}\right) = \sum_{j=1}^{N}\varphi_I\left(\vec{r}-\vec{r}_j\right), \quad (26)$$

$$\varphi^{(I)}\left(\omega,\vec{q}\right) = C\left(\omega,0\right)\varphi^{(I)}(\vec{q})\sum_{j=1}^{N}\exp\left(-i\vec{q}\vec{r}_j\right)\to \to 2\pi\delta(\omega)\,\varphi^{(I)}\left(\vec{q}\right)\sum_{j=1}^{N}\exp\left(-i\vec{q}\vec{r}_j\right). \quad (27)$$

Here, $\vec{r}_j$ is the radius-vector of *j*-th impurity, $\varphi^{(I)}(\vec{q}) = 4\pi e/q^2\varepsilon_L$ and N – total number of impurities in crystal.

Calculating correlations over positions of impurities, we have (see [3] and [9])

$$\left\langle\delta\varphi^{(I)}\left(\omega,\vec{q}\right)\delta\varphi^{(I)}\left(\omega',\vec{q}'\right)\right\rangle = 4\pi^4\delta\left(\omega+\omega'\right)\delta\left(\vec{q}+\vec{q}'\right)\left\langle\delta\varphi_I^2\right\rangle_{\vec{q},\,\omega} \quad (28)$$

Here,

$$\left\langle\delta\varphi_I^2\right\rangle_{\vec{q},\,\omega} = \left\langle\delta\varphi_I^2\right\rangle_{\vec{q}}\cdot\delta(\omega)\,,$$
$$\left\langle\delta\varphi_I^2\right\rangle_{\vec{q}} = 2\pi n_I\left[\varphi^I\left(\left(\vec{q}\right)\right]^2 = 32\pi^3e^2\ n_I/\varepsilon_L^2q^4\right.. \quad (29)$$

Turn out to the equation for fluctuation of the density matrix in the form (31) and use the following approximation:

$$\left(H_e\right)_{A\Gamma} = \delta_{A\Gamma}\hbar\omega_A = \delta_{A\Gamma}\varepsilon_A\,. \quad (30)$$

Usually, for the standard approach (see [1–3]), they use neglecting the field terms in the collision integral; in particular the form (7) can be used, where

$$H_e \to H^{(0)} \quad (31)$$

and the equation for fluctuation of the density matrix (24) accepts the simplified form

$$-i\hbar\delta\rho_{AB}\left(t=0\right) + \left(\hbar\omega\ -\varepsilon_A+\varepsilon_B\right)\delta\rho_{AB}(\omega) + \left(f_A - f_B\right)\left(\delta H(\omega)\right)_{AB} = 0. \quad (32)$$

If the field terms, maintained in the Hamiltonian H_e (here, we consider some non-standard or "field" approach), are used in the form (31), it leads to the following equation:

$$\left(H_e\right)_{A\Gamma}\to\left(\overline{H}^0\right)_{A\Gamma} = \delta_{A\Gamma}\hbar\overline{\omega}_A = \delta_{A\Gamma}\overline{\varepsilon}_A\ , \quad (33)$$

$$-i\hbar\delta\rho_{AB}\left(t=0\right) + \left(\hbar\omega\ -\overline{\varepsilon}_A+\overline{\varepsilon}_B\right)\delta\rho_{AB}(\omega) + \left(f_A - f_B\right)\left(\delta H(\omega)\right)_{AB} = 0. \quad (34)$$

Then, after formal transition $i/\left(x+i0\right)\to 2\pi\delta(x)$ and designation $\overline{\varepsilon}_{AB} = \overline{\varepsilon}_A - \overline{\varepsilon}_B = \hbar\overline{\omega}_{AB}$, we obtain

$$\delta\rho_{AB}(\omega) = 2\pi\,\hbar\delta\left(\hbar\omega - \overline{\varepsilon}_{AB}\right)\times \times\left[\delta\rho_{AB}\left(t=0\right) - \left(i/\hbar\right)\left(f_B - f_A\right)\delta H_{AB}(\omega)\right]. \quad (35)$$

The standard approach can be considered as a limited case of non-standard approach. For this approach, we apply the simple approximation:

$$\bar{\varepsilon}_A \to \varepsilon_A . \tag{36}$$

As the initial form of density matrix $\rho_{AB}(t)$, we use

$$\rho_{AB}(t=0) = a_B^+ a_A . \tag{37}$$

Here and farther, we don't show the argument $t = 0$ for Fermi operators a_A and a_A^+.

Let us construct the correlator for $\delta\rho_{AB}(t=0) = a_B^+ a_A - \left\langle a_B^+ a_A \right\rangle$ and

$$\left\langle \delta\rho_{AB}(t=0)\,\delta\rho_{A'B'}(t=0)\right\rangle = \left\langle a_B^+ a_A a_{B'}^+ a_{A'}\right\rangle - \left\langle a_B^+ a_A\right\rangle\left\langle a_{B'}^+ a_{A'}\right\rangle. \tag{38}$$

Using Bogolubov's principle of weakening of correlations and performing weak-coupling for two-particle correlator $\left\langle a_B^+ a_A a_{B'}^+ a_{A'}\right\rangle$, one obtains the following expression:

$$\left\langle \left(\delta\rho_{AB}^{(0)}(\omega)\,,\,\delta\rho_{A'B'}^{(0)}(\omega')\right)_+ \right\rangle = \\ = 2\pi^2\delta(\omega+\omega')\delta(\omega-\bar{\omega}_{AB})\delta_{A'B}\delta_{AB'}\left[f_A(1-f_B)+f_B(1-f_A)\right]. \tag{39}$$

Completing calculation of the corresponding correlators, represent the selected collision integral in the form

$$\mathrm{St}\ f_A = \mathrm{St}_{eI} f_A . \tag{40}$$

Introducing the designations $A \to \vec{k}$ and $B \to \vec{k}'$ to Eq. (35), we obtain (here, $f_{\vec{k}} \equiv f(\vec{k})$)

$$\mathrm{St}_{eI} f(\vec{k}) = \frac{1}{(2\pi)^3\hbar}\int d^3\vec{q}\ \delta\left(\bar{\varepsilon}_{\vec{k}} - \bar{\varepsilon}_{\vec{k}-\vec{q}}\right)\left(f_{\vec{k}-\vec{q}} - f_{\vec{k}}\right)\left\langle \delta H_I^2\right\rangle_{\vec{q}}. \tag{41}$$

For practical calculations, further we use the following approximation for dielectric function (here $1/q_0$ is the screening length, $\vartheta(q)$ – standard step-function):

$$1/\varepsilon(\omega,\vec{q}) \to (1/\varepsilon_L)\vartheta(q-q_0). \tag{42}$$

5. Calculation of the energies $\bar{\varepsilon}_A$

Accept the components of wave vectors $\vec{k}$ as quantum numbers:

$$A \to \vec{k} = (k_x\,,\,k_y\,,\,k_z), \\ B \to \vec{k}-\vec{q} = (k_x - q_x\,,\,k_y - q_y\,,\,k_z - q_z). \tag{43}$$

The set of matrix elements of Hamiltonian H_e is as follows (see Eq. (7))

$$\left(\hat{H}_e\right)_{AB} = \left(\hat{H}^{(0)}\right)_{AB} + \left(\hat{H}^{(E)}\right)_{AB} + \left(\hat{H}^{(H)}\right)_{AB}. \tag{44}$$

Here (see Exs (9)),

$$\left(\hat{H}^{(0)}\right)_{AB} = \left(\hbar^2/2m\right)\left(\hat{\vec{k}}^2\right)_{AB},\ \left(\hat{H}^{(E)}\right)_{AB} = -e(x)_{AB}E_x, \\ \left(\hat{H}^{(H)}\right)_{AB} = -\frac{e\hbar H_z}{mc}\left(y\,\hat{k}_x\right)_{AB}. \tag{45}$$

Note that Hamiltonian $\hat{H}_e$ containing field-dependent terms is not arbitrary invariant in space. The following wave functions are most convenient for calculations:

$$\Psi(A_w; w) \equiv \Psi(k_w; w) = L^{-1/2}\exp(i\,k_w w), \tag{46}$$

$$\Psi(B_w; w) \equiv \Psi\left[(k_w + q_w)w\right] = L^{-1/2}\exp\left[i(k_w+q_w)w\right]. \tag{47}$$

Here and farther, $w = x$ or $w = y$ or $w = z$, and

$$-L/2 < w < L/2 . \tag{48}$$

The linear dimension L of the system exceeds utmost an every characteristic length ($L \to \infty$). The noted functions are proper for the operator of momentum $\hbar\hat{\vec{k}}$ (and for the operator of kinetic energy):

$$-i\nabla_w\Psi(k_w; w) = k_w\Psi(k_w; w), \\ \nabla_x^2\Psi(k_w; w) = -k_w^2\Psi(k_w; w). \tag{49}$$

For the parabolic dispersion law

$$\hat{\varepsilon}\,\Psi(\vec{k};\vec{r}) = \varepsilon(\hbar k)\Psi(\vec{k};\vec{r}) = \left(\hbar^2k^2/2m\right)\Psi(\vec{k};\vec{r}). \tag{50}$$

When one uses the field variant, the Hamiltonian H_e evidently depends on spatial coordinates. But at the same time, all the points of $\vec{r}$ -space are equivalent. Note that wave functions are invariant relatively to the shift of argument w on the length that is proportional to the deBroglie wavelength.

Now calculate the matrix components of radius-vector (here $L \to \infty$):

$$(w)_{AB} = \int_{-L/2}^{L/2} w\Psi^*(k_A; w)\,\Psi(k_B; w)\,dw = \\ = (1/L)\int_{-L/2}^{L/2} w\exp(-iq_w w)\,dw = \left(1/Lq_w^2\right)\int_{-Lq_w/2}^{Lq_w/2}\xi\exp(-i\xi)\,d\xi \tag{51}$$

or

$$(w)_{AB} \to F(L\,,q_w) = \\ = \left(1/Lq^2\right)\int_{-Lq_w/2}^{Lq_w/2}\xi\cos(\xi)d\xi - i\left(1/Lq^2\right)\int_{-Lq_w/2}^{Lq_w/2}\xi\sin(\xi)d\xi. \tag{52}$$

Shift the edges of area (49) to some little distance l_w, which is sufficiently small as compared to the length L. Then,

$$F(L,q_w)\to F(L,q_w,l_w)=\left(1/Lq_w^2\right)\int\limits_{q_w(l_w-L/2)}^{q_w(l_w+L/2)}\xi\cos(\xi)d\xi- \\ -i\left(1/Lq^2\right)\int\limits_{q_w(l_w-L/2)}^{q_w(l_w+L/2)}\xi\sin(\xi)d\xi. \tag{53}$$

Let us introduce the following designations:

$$D_w=q_w(l_w+L/2),\quad B_w=q_w(-l_w+L/2). \tag{54}$$

Then,

$$\int\limits_{-B_w}^{D_w}\xi\cos\xi\,d\xi=D_w\sin D_w-B_w\sin B_w+\cos D_w-\cos B_w\to \\ \to D_w\sin D_w-B_w\sin B_w\to(q_wL/2)(\sin D_w-\sin B_w), \tag{55}$$

$$\int\limits_{-B_w}^{D_w}\xi\sin\xi\,d\xi=-D_w\cos D_w+B_w\cos B_w+\sin D_w+\sin B_w\to \\ \to -D_w\cos D_w+B_w\cos B_w\to(q_wL/2)(\cos B_w-\cos D_w). \tag{56}$$

It follows:

$$\int\limits_{-B_w}^{D_w}\xi\cos\xi\,d\xi\to q_wL\cos(q_wL/2)\sin(q_wl_w), \\ \int\limits_{-B_w}^{D_w}\xi\sin\xi\,d\xi\to q_wL\sin(q_wL/2)\sin(q_wl_w). \tag{57}$$

Now one finds the possibility to refuse from imaginary part in the equation of matrix $(w)_{AB}$. We rely to the factor $\sin(q_wL/2)\to 0$; then we take $|\cos(q_wL/2)|\to 1$. The length q_wl_w is selected with the relation $\sin(q_wl_w)\to 1$ and $l_w\to 1/|q_w|$.

As a result (here $AB\to A,\ B\to k_w-q_w$), approximately $\int\limits_{-B_w}^{D_w}\xi\sin\xi\,d\xi\to 0$ and

$$(\omega)_{AB}\to\left(1/Lq_w^2\right)\int\limits_{-B_w}^{D_w}\xi\exp(-i\xi)d\xi= \\ =q_w\,L\left(1/Lq_w^2\right)\cos(q_wL/2)\sin(q_wl_w)\to 1/q_w. \tag{58}$$

The transformation (63) is not obviously single. We accept the shown form, because just this one gives the expected physical result (see below (124) and (125)).

Using the designations $\vec{k}_A\to\vec{k}$ and $\vec{k}_B\to\vec{k}-\vec{q}$, one obtains the forms (see (9))

$$\varepsilon_{AA}\to\varepsilon_A\to\varepsilon\left(\vec{k}\right)=\frac{\hbar^2\vec{k}^2}{2m}-\frac{2\pi eE_x}{k_x}-\hbar\,\Omega\frac{k_x}{k_y}\,, \tag{59}$$

$$\varepsilon_{AB}=\varepsilon_A-\varepsilon_B\to\ \varepsilon_{\vec{k}}-\varepsilon_{\vec{k}-\vec{q}}=\frac{\hbar^2}{2m}\left(2\vec{k}\vec{q}-q^2\right)+ \\ +\frac{2\pi eE_xq_x}{k_x\left(k_x-q_x\right)}+\hbar\,\Omega\frac{k_xq_y-k_yq_x}{k_y\left(k_y-q_y\right)} \tag{60}$$

(here, $\Omega=\pi eH_z/mc$). $\varepsilon_{AA}\to\varepsilon_A\to\varepsilon\left(\vec{k}\right)=\dfrac{\hbar^2\vec{k}^2}{2m}$.

Let us simplify the calculations by using the approximation $|q_w|<<|k_w|$ and these changes:

$$k_x^2\to\left\langle k_x^2\right\rangle=(1/3)\left\langle k^2\right\rangle=2m\langle\varepsilon\rangle/3\hbar^2, \\ k_y^2\to\left\langle k_y^2\right\rangle=(1/3)\left\langle k^2\right\rangle=2m\langle\varepsilon\rangle/3\hbar^2. \tag{61}$$

Here, $\langle\varepsilon\rangle=3k_BTF_{3/2}(\eta)/2F_{1/2}(\eta)$ is the averaged energy,

$$F_r(\eta)=\frac{1}{\Gamma(r+1)}\int\limits_0^\infty\frac{w^r\,dw}{1+\exp(w-\eta)},\quad \eta=\varepsilon_F/k_BT\ . \tag{62}$$

As a result,

$$\varepsilon_{\vec{k}}-\varepsilon_{\vec{k}-\vec{q}}=\frac{\hbar^2}{2m}\left(2\vec{k}\vec{q}-q^2\right)+\frac{3\pi e\hbar^2}{m\langle\varepsilon\rangle}E_xq_x+\frac{3\hbar^3\Omega\left(k_xq_y-k_yq_x\right)}{m\langle\varepsilon\rangle}. \tag{63}$$

We don't consider here quantazing the magnetic field (that is only $b << 1$); therefore, values of the order b^2 will be omitted in every case. With the designations

$$3\pi e\vec{E}/\langle\varepsilon\rangle=\vec{k}^{(E)},\quad 3\hbar\Omega/\langle\varepsilon\rangle=b \tag{64}$$

the expression (66) can be written as

$$\varepsilon_{\vec{k}}-\varepsilon_{\vec{k}-\vec{q}}=\frac{\hbar^2}{m}\left\{\left(k_x^{(E)}+k_x-bk_y\right)q_x+\left(k_y+bk_x\right)q_y+k_zq_z-\frac{q^2}{2}\right\}. \tag{65}$$

The latter expression prompts to introduce a new vector $\vec{\kappa}\left(\vec{k}\right)$:

$$\vec{\kappa}\left(\vec{k}\right)=\left(\kappa_x\left(\vec{k}\right),\kappa_y\left(\vec{k}\right),\kappa_z\left(\vec{k}\right)\right), \tag{66}$$

where

$$\kappa_x\left(\vec{k}\right)=k_x+k_x^{(E)}-bk_y, \\ \kappa_y\left(\vec{k}\right)=k_y+bk_x,\ \kappa_z\left(\vec{k}\right)=k_z\,. \tag{67}$$

The reverse transformation (by using the inequality $b^2 << 1$) is

$$k_x = \kappa_x + b\kappa_y - k_x^{(E)} - bk_y^{(E)}, \quad k_y = \kappa_y - b\kappa_x + bk_x^{(E)}. \quad (68)$$

Then (with account of the approximations shown before), one obtains from (65)

$$\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}-\vec{q}} = \hbar\left(\omega_{\vec{k}} - \omega_{\vec{k}-\vec{q}}\right) = \frac{\hbar^2}{m}\left\{\vec{\kappa}\vec{q} - \frac{q^2}{2}\right\}. \quad (69)$$

6. Balance of forces for electrons and impurities

For a stationary spatially uniform system, the kinetic equation (20) acquires the form

$$\frac{e}{\hbar}\left\{\vec{E} + \frac{1}{c}\left[\vec{v}\left(\vec{k}\right)\times\vec{H}\right]\right\}\frac{\partial f_{\vec{k}}}{\partial \vec{k}} = \mathrm{St}\, f_{\vec{k}}. \quad (70)$$

Construct the first moment of the equation (70), applying there the following operator

$$2(2\pi)^{-3}\int \vec{k}\, d^3\vec{k} \quad (71)$$

to both sides.

Then, we obtain a vector equation having the sense of balance of dynamical and statistical fields forced by all the system of band carriers:

$$e\left[\vec{E} + (1/c)\left(\vec{H}\times\vec{u}\right)\right] + \frac{2\hbar}{(2\pi)^3 n}\int \vec{k}\,\mathrm{St}_{e-I} f_{\vec{k}}\, d^3\vec{k} = \\ = e\left[\vec{E} + (1/c)\left(\vec{H}\times\vec{u}\right)\right] + \vec{F}_{eI} = 0. \quad (72)$$

Here, the value $\vec{F}_{eI}$ is the resistant force acting from the side of charged impurities (something like to the "friction force"). The values

$$n = \frac{2}{(2\pi)^3}\int f_{\vec{k}}\, d^3\vec{k}\ ,$$

$$\vec{u} = \frac{\int \vec{v}\left(\vec{k}\right) f\left(\vec{k}\right) d^3\vec{k}}{\int f\left(\vec{k}\right) d^3\vec{k}} = \frac{2}{(2\pi)^3 n}\int \vec{v}\left(\vec{k}\right) f_{\vec{k}}\, d^3\vec{k} \quad (73)$$

are the density of electrons and drift velocity of whole band electrons.

After non-complicated transformations of the formula (45), we obtain the following expression:

$$\vec{F}_{eI} = -\frac{e^4 n_I m}{\pi^3\hbar^2 n\varepsilon_L^2}\int f\left(\vec{k}\right) d^3\vec{\kappa}\int \vec{q}\, d^3\vec{q}\ \delta\left(\vec{\kappa}\vec{q} - q^2/2\right) q^{-4}. \quad (74)$$

Performing here integration over the components of vector $\vec{q}$ (see (74)), we find

$$\vec{F}_{eI} = -\frac{2me^4 n_I}{\pi^3\hbar^2 n\varepsilon_L^2}\ln\left(\frac{q_M}{q_0}\right)\int f\left(\vec{k}(\vec{\kappa})\right)\kappa^{-3}\left(\vec{k}\right)\vec{\kappa}\, d^3\vec{\kappa}. \quad (75)$$

7. The model of non-equilibrium distribution function

As one can see, the friction force (75) is the linear integral of non-equilibrium distribution function $f(\vec{k})$. As the sufficiently simple model of $f(\vec{k})$, we accept here the Fermi function with the shifted argument (see also [9]):

$$f\left(\vec{k}\right) = f_0\left(\vec{k} - \vec{k}_u\right) = \left[1 + \exp\left(\frac{\hbar^2\left(\vec{k} - m\vec{u}/\hbar\right)^2/2m - \varepsilon_{\mathrm{F}}}{k_{\mathrm{B}}T}\right)\right]^{-1}. \quad (76)$$

Introduce three-dimensional vectors $\vec{K}$, $\vec{K}^{(u)}$ and several dimensionless values:

$$\vec{K}^{(u)} = \left(K_x^{(u)}, K_y^{(u)}, 0\right), \quad K_x^{(u)} = k_x^{(E)} + mu_x/\hbar, \\ K_y^{(u)} = -bk_x^{(E)} + mu_y/\hbar, \quad (77)$$

$$\vec{K} = \left(K_x, K_y, K_z\right) = \left(\kappa_x + b\kappa_y, \kappa_y - b\kappa_x, \kappa_z\right), \quad (78)$$

$$\hbar\vec{K}/\sqrt{2mk_{\mathrm{B}}T} = \vec{t}\ , \quad \hbar\vec{K}^{(u)}/\sqrt{2mk_{\mathrm{B}}T} = \vec{Y}\ , \quad \varepsilon_{\mathrm{F}}/k_{\mathrm{B}}T = \eta. \quad (79)$$

Then, the "friction" force (75) takes the form

$$\vec{F}_{eI} = -\frac{2^{13/2} m^{3/2}\left(k_{\mathrm{B}}T\right)^{1/2} e^4 n_I}{\pi^3\hbar^3 n\varepsilon_L^2}\ln\left(\frac{q_M}{q_0}\right)\times \\ \times\int \frac{t^{1-p}\left[\vec{t} + \chi b\left(\vec{e}_z\times\vec{t}\right)\right]}{\left[1 + \exp\left(\left(\vec{t} - \vec{Y}\right)^2 - \eta\right)\right]} d^3\vec{t}. \quad (80)$$

Introduce the dimensionless electric field and current density:

$$\vec{W} = \vec{E}/E_T\ , \quad \vec{J} = \vec{j}/j_0 = \sqrt{m/k_{\mathrm{B}}T}\ \vec{u}. \quad (81)$$

Here,

$$E_T = \langle\varepsilon\rangle\sqrt{2mk_{\mathrm{B}}T}/3\pi e\hbar\ , \quad j_0 = en\sqrt{k_{\mathrm{B}}T}/\sqrt{m}. \quad (82)$$

It follows from (79) and (81) that

$$\vec{Y} = \vec{J} + \vec{W} + b\left(\vec{W}\times\vec{e}_z\right). \quad (83)$$

Then, the balance equation acquires the form

$$\vec{W} + b\left(\vec{e}_z\times\vec{J}\right) = \frac{\Theta_{(I)}}{F_{3/2}(\eta)}\times \\ \times\int \frac{t^{1-p}\left[\vec{t} - \chi b\left(\vec{t}\times\vec{e}_z\right)\right] d^3\vec{t}}{1 + \exp\left\{\left[\vec{t} - \chi\vec{W} - \chi b\left(\vec{W}\times\vec{e}_z\right) - \vec{J}\right]^2 - \eta\right\}}\ , \quad (84)$$

where

$$\Theta_{(I)} = \frac{2^{5/2}\pi^3 e^4 \hbar n_I}{\varepsilon_L^2 m^{1/2} (k_B T)^{5/2}} \ln\left(\frac{q_M}{q_0}\right). \quad (85)$$

For $q_M >> q_0$,

$$\ln(q_M/q_0) \approx \frac{1}{2}\ln\left\{\frac{4\varepsilon_L\sqrt{8k_BT}\hbar F_1^2(\eta)}{e^2\sqrt{m\pi}F_{1/2}^2(\eta)F_{-1/2}(\eta)}\right\}. \quad (86)$$

If the external magnetic field b is absent, the equation (84) passes to the following equation:

$$\vec{W}(H_y = 0) = \frac{\Theta_{(I)}}{F_{3/2}(\eta)}\int \frac{\vec{t}\, t^{1-p} d^3\vec{t}}{1+\exp\left\{\left[\vec{t}-\vec{J}\right]^2 - \eta\right\}}. \quad (87)$$

Designate the mobility tensor with the symbol $\hat{\mu}$ and write here:

$$\vec{j} = en\hat{\mu}\vec{E}, \quad \vec{J} = (\hat{\mu}/\mu_{\min})\vec{W}, \quad (88)$$

$$\mu_{\min} = \frac{j_0}{enE_T} = \frac{3\pi e\hbar}{\sqrt{2}m\langle\varepsilon\rangle} = \frac{\sqrt{2}\pi e\hbar}{mk_BT}\frac{F_{1/2}(\eta)}{F_{3/2}(\eta)} = M\frac{F_{1/2}(\eta)}{F_{3/2}(\eta)}. \quad (89)$$

The dimensionless magnetic field $b = \mu_{\min} H_z/c$. In absence of magnetic field, $\mu_{ij} = \mu\delta_{i,j}$. For the system CGSE and $m = 2\cdot10^{-28}$, $T = 100$ K, we find $M = 8.1\cdot10^5$ CGSE.

Determine the conditional free-path length $\overline{L}$ and averaged length of deBroglie wave $\overline{\lambda}$ by using the relations:

$$\overline{L} = \left|\hat{\mu}\right|\sqrt{2m\langle\varepsilon\rangle}/e, \quad \overline{\lambda} = \hbar/\sqrt{2m\langle\varepsilon\rangle}. \quad (90)$$

Then, the equality

$$\overline{L}^{(\chi)} >> \overline{\lambda} \quad (91)$$

can be written as $J >> W$ or $\left|\hat{\mu}\right| >> \mu_{\min}$. At the condition $\overline{L} \le \overline{\lambda}$, or $\left|\vec{J}\right| \le \left|\vec{W}\right|$, the concept "mobility", how we shall see below, loses its usual meaning, and description of macroscopic movement of band carriers requires other ways.

If electrical field and current density are weak, that is

$$\left|\vec{W}\right| + \left|\vec{J}\right| << 1, \quad (92)$$

one can linearize the model non-equilibrium distribution $f(\vec{k})$. In this case, the relation of dimensionless electrical field $\vec{W}$ with the dimensionless density of current $\vec{J}$ becomes the linear equation

$$\vec{W} + b\left(\vec{e}_z \times \vec{J}\right) = \frac{2\Theta_{(I)}}{F_{3/2}(\eta)}\int \frac{\left[\vec{t} + b\left(\vec{t}\times\vec{e}_z\right)\right]}{t^3\left[1+\exp\left(t^2-\eta\right)\right]^2} \times \times\left\{\vec{t}\cdot\left[\vec{J} + \vec{W} + b\left(\vec{W}\times\vec{e}_z\right)\right]\right\}\exp\left(t^2-\eta\right)d^3\vec{t}. \quad (93)$$

8. Current-voltage characteristics in absence of magnetic fields

At $b = 0$ (that is for $H = 0$), the linear equation (93) has the form (external macroscopic electrical field is directed along the x-axis):

$$W_x = J_x Q_{(I)}(\eta) = \Theta_{(I)}\cdot\alpha(\eta)J_x, \quad (94)$$

$$\alpha(\eta) = \frac{8\pi}{3F_{3/2}(\eta)}\int_0^\infty \frac{t\exp\left(t^2-\eta\right)}{\left[1+\exp\left(t^2-\eta\right)\right]^2}dt = = \frac{4\pi}{3}\frac{F_{-1}(\eta)}{F_{3/2}(\eta)} = \frac{4\pi}{3\left[1+\exp(-\eta)\right]F_{3/2}(\eta)}. \quad (95)$$

Accordingly to (94) and (95), the current-voltage characteristic has the form

$$J_x = \frac{1}{\mu_{\min}}\mu^{(1)}W_x = W_x\left(1/Q_{(I)}(\eta) - 1\right). \quad (96)$$

It follows thereof:

$$\mu^{(0)} = \mu(W=0) = \mu_{\min}/Q_{(I)},$$
$$\mu^{(1)} = \mu(W\neq 0) = \mu_{\min}\left(1-Q_{(I)}\right)/Q_{(I)}, \quad (97)$$
$$\mu^{(1)}/\mu^{(0)} = 1 - Q_{(I)}. \quad (98)$$

One can see from the formula (85) that for field variant the concept "mobility" has a meaning only at this condition:

$$Q_{(I)} < 1. \quad (99)$$

In this case, $0 < \mu^{(1)} < \mu^{(0)}$. As it also follows from (85), the distinction between results of calculations for standard field variants disappears at the conditions $Q_{(I)} << 1$ or $\mu^{(0)} >> \mu_{\min}$.

9. Galvanomagnetic kinetic effects

9.1. Kinetic characteristics calculated for typical linear equation of forces balance

For the typical case, we write the vector equation (97) as the system

$$W_x - bJ_y = Q_{(I)}(\eta)J_x, \quad (100)$$
$$W_y + bJ_x = Q_{(I)}(\eta)J_y. \quad (101)$$

Here, we accept $b^2 << 1$. The components of mobility tensor $\hat{\mu}^{(0)}$ are

$$\mu_{xy}^{(0)}(H) = -\mu_{yx}^{(0)}(H) = -b(H)\frac{\mu_{\min}}{Q_{(I)}^2 + b^2(H)}. \quad (102)$$

At presence of magnetic field $\vec{H} = H_z\vec{e}_z$ and current $\vec{j} = (j_x, 0)$, the longitudinal component j_x, transverse component of electrical field E_y and Hall constant $R_H^{(0)}$ are

$$j_x(H) = en\left[\mu_{xx}^{(0)}(H) + \frac{\left(\mu_{xy}^{(0)}(H)\right)^2}{\mu_{xx}^{(0)}(H)}\right]E_x = en\mu_{\|}^{(0)}(H)E_x, \quad (103)$$

$$\mu_{\|}^{(0)}(H) = \frac{\mu_{\min}}{Q_{(I)}},$$

$$E_y(H) = \vartheta^{(0)}(H)E_x = \frac{\mu_{yx}^{(0)}(H)}{\mu_{xx}^{(0)}(H)}E_x = \frac{b(H)}{Q_{(I)}}E_x, \quad (104)$$

$$R_H^{(0)}(H) = \left|\frac{E_y(H)}{H_z j_x(H)}\right| = \left|\frac{1}{enc}\right|. \quad (105)$$

As one can see, in the typical variant the longitudinal conductivity $\sigma_{\|}^{(0)} = en\mu_{\|}^{(0)}$ and Hall constant $R_H^{(0)}$ do not depend on the intensity of magnetic field.

9.2. Kinetic characteristics calculated for specific linear equation of forces balance

Write the components of linear vector equation (see formula (96)):

$$W_x - bJ_y = Q_{(I)}(\eta)\left(J_x + W_x - bJ_y\right), \quad (106)$$

$$W_y + bJ_x = Q_{(I)}(\eta)\left(J_y + W_y + bJ_x\right). \quad (107)$$

Solving this system of equations, one applies the magnetic field to be not quantized, that is $|b| = \mu^{(0)}H/c << 1$. But the value $|b|$ can be comparable with $Q_{(I)}$ and even exceed it. As a result

$$\mu_{xx}^{(1)} = \mu_{yy}^{(1)} = \mu_{\min}\frac{\left(1-Q_{(I)}\right)Q_{(I)}}{Q_{(I)}^2 + b^2\left(1-Q_{(I)}\right)^2},$$

$$\mu_{xy}^{(1)} = -\mu_{yx}^{(1)} = -\mu_{\min}b\frac{\left(1-Q_{(I)}\right)^2}{Q_{(I)}^2 + b^2\left(1-Q_{(I)}\right)^2}. \quad (108)$$

Consider the case $\vec{j} = (j_x, 0)$. Then

$$j_x = en\left[\mu_{xx}^{(1)} + \frac{\left(\mu_{xy}^{(1)}\right)^2}{\mu_{xx}^{(1)}}\right]E_x = en\mu_{\|}^{(1)}E_x,$$

$$\mu_{\|}^{(1)}(b) = \mu_{\min}\frac{\left(1-Q_{(I)}\right)}{Q_{(I)}}, \quad (109)$$

$$\vartheta^{(1)}(b) = \frac{E_y(b)}{E_x} = \frac{\mu_{yx}^{(1)}(b)}{\mu_{xx}^{(1)}(b)} = b\frac{1-Q_{(I)}}{Q_{(I)}} = \vartheta^{(0)}(b)\left(1-Q_{(I)}\right),$$

$$R_H^{(1)}(b) = \left|\frac{E_x\vartheta^{(1)}(b)}{H_z j_x(b)}\right| = \left|\frac{1}{enc}\right|. \quad (110)$$

Comparing the results obtained in the sections (9.1) and (9.2), we find:

$$\mu_{\|}^{(1)} = \mu_{\|}^{(0)}\left(1-Q_{(I)}\right), \quad \vartheta^{(1)} = \vartheta^{(0)}\left(1-Q_{(I)}\right),$$

$$R_H^{(1)}(b) = R_H^{(0)}(b) = R_H. \quad (111)$$

It follows that formulae (119), (120) and the meanings of mobility and Hall angle have a sense at the following condition only:

$$Q_{(I)} < 1. \quad (112)$$

The distance of free-path (see (90)) is

$$\bar{L}^{(1)} = \bar{L}^{(0)}\left(1-Q_{(I)}\right). \quad (113)$$

If at the inequality (112) the value $Q_{(I)}$ is sufficiently close to unity, one can say about a low mobility or about definite "demobilization" of band electrons due to the extremely high intensity of scattering. The limit of mobility $\mu_{\|}^{(1)} = 0$ is achieved at $Q_{(I)} = 1$.

One obtains from (90) and (91):

$$\frac{\bar{L}}{\bar{\lambda}} = \frac{3\pi}{\sqrt{2}\,Q_{(S)}}\left(1-Q_{(I)}\right), \quad Q_{(I)} = 3\pi\bar{\lambda}/\sqrt{2}\,\bar{L}^{(0)}. \quad (114)$$

It follows thereof that retention of field terms in the collision integral is the reason of appearance of quantum amendment to kinetic coefficients, for instance:

$$\mu_{\|}^{(1)} = \mu_{\|}^{(0)}\left(1 - \frac{3\pi}{\sqrt{2}}\frac{\bar{\lambda}}{\bar{L}^{(0)}}\right). \quad (115)$$

As a result, we obtain the important conclusion: the quantum kinetic equation distinguishes from the classical kinetic one by retention of field terms in the collision integral.

10. Conclusion

One can make the conclusion that account of the field terms in the collision integral results there in appearance of deBroglie wavelength λ and comparability of it with the free-path distance *L*. Taking into account the finite ratio of λ and *L*, we can say about a quantum kinetic equation in total. If a consideration does not use directly the field terms in the collision integral, the kinetic equation leaves to be the classic one.

References

1. Anselm A.I. *Introduction to Semiconductor Theory*. Prentice Hall, 1982.
2. Lifshitz E.M. and Pitaevskii L.P. *Physical Kinetics.* Moscow, Nauka, 1984 (in Russian).
3. Klimontovich Yu.L. *Statistical Physics*. Moscow, Nauka, 1978 (in Russian).
4. Gantmaher V.F. and Levinson I.B. *Scattering of Current Carriers in Metals and Semiconductors.* Nauka, Moscow, 1984 (in Russian).
5. Bogolubov N.N. *Lectures on Quantum Statistics*. Kiev, Radianska Shkola, 1949 (in Ukrainian).
6. Bogolubov N.N. *Non-equilibrium Statistical Mechanics*. Collected works in 12 volumes, vol. 5. Moscow, Nauka, 2006 (in Russian).
7. Zubarev D.N. *Non-equilibrium Statistical Thermodynamics*. Moscow, Nauka, 1971 (in Russian).
8. Boiko I.I. *Transport of Band Carriers in Semiconductor*. Palmarium Academic Publishing, Saarbruken, 2013.
9. Boiko I.I. *Kinetics of Electron Gas Interacting with Fluctuating Potential*. Naukova dumka, Kyiv, 1993 (in Russian).
10. Boiko I.I. Impurity scattering of band carriers. *Semiconductor Physics, Quantum Electronics & Optoelectronics.* 2010. **13**, No 2. P. 214–220.
11. Boiko I.I. Dependence of the collision integral on electric field. *Semiconductor Physics, Quantum Electronics & Optoelectronics.* 2015. **18**, No 2. P. 138–143.

Кінетичне рівняння, яке містить інтегральний член розсіювання з лінійною формою зовнішніх електричного та магнітного полів

І.І. Бойко

Анотація. У багатьох випадках при розгляді кінетичного рівняння в інтегралі зіткнення даремно не враховується наявність зовнішніх електричного та магнітного полів у явному вигляді. Насправді існує певна причина уважно використовувати в інтегралі зіткнення вищезазначені поля і правильно оцінювати кінцеві результати, приймаючи відношення усередненої довжини хвилі деБройля до середньої довжини вільного пробігу.

Ключові слова: кінетичне рівняння, інтеграл зіткнень, рухливість.