A DIAGRAM TECHNIQUE FOR EVALUATING TRANSPORT QUANTITIES

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We have developed a diagram technique to evaluate the single-electron density matrix. Quantum mechanics is used to obtain a transport equation which takes into account the inhomogeneity of an external electrical field and the self-consistent electron field.

It is well known that the evaluation of transport quantities requires the summation of an infinite number of terms of a perturbation-theory series, however small the coupling constant. It must therefore always lead to the formulation and solution of some kind of integral equation. Boltzmann's classical transport equation is an example of such an equation.

Many papers[1-5] have been devoted to the derivation of a transport equation. In some of them[1] the problem is studied using classical mechanics. In the papers by Kohn and Luttinger[3] and van Hove,[4] which are based upon quantum theory, there is no diagram technique. The technique proposed by Montroll and Ward[5] and by Prigogine and Ono[6] does not use the convenient second quantization formalism and is thus complicated (in reference 6 three-dimensional diagrams are even used). Also, if there is no simple and convenient diagram technique, it is extremely difficult to apply it in those cases where the classical Boltzmann equation is inapplicable (for instance, the problem of plasma kinetics or the polaron). In a paper by Abrikosov, Gor'kov, and Dzyaloshinskiĭ[7] a simple diagram technique was proposed which enabled one in principle to evaluate transport coefficients directly. However, the straightforward evaluation of transport coefficients, even in the case where the transport equation is valid, is a difficult problem. Also, the authors of the cited paper did not derive a transport equation, and its derivation by means of their technique is difficult. We must note that the idea of analytical continuation, proposed in reference 7 and used with success by Larkin,[8] turns out to be extremely helpful for evaluating the internal block diagrams obtained in the present paper. We restrict ourselves here to a derivation of a generalized transport equation and we show that it turns into the usual transport equation when the latter is valid. In a subsequent paper we shall obtain a transport equation for a plasma on the basis of the technique developed here.

1. THE SINGLE ELECTRON DENSITY MATRIX IN AN EXTERNAL ELECTROMAGNETIC FIELD

We consider a system of electrons and some other particles interacting with them (phonons or impurity centers). We assume that in the initial state, $t \to -\infty$, the system was in contact with a thermostat and could be described by a density matrix

$$F_0 = Z^{-1}\exp(-\beta H'), \quad Z = \mathrm{Sp}\exp(-\beta H'),$$
$$\beta = (kT)^{-1}, \quad H' = H - \mu\hat{N},$$

where μ is the chemical potential and $\hat{N}$ the operator of the total number of electrons. At $t \to -\infty$ an adiabatically increasing weak electromagnetic field is applied to the system and at the same time the contact with the thermostat is broken. The time variation of the density matrix F of the system is determined by the equation

$$i\hbar\partial F/\partial t = [(H + H_t), F],$$

$$H_t = \int \rho(\mathbf{x})\, U(\mathbf{x}, t)\, d\mathbf{x} - \frac{1}{c}\int J_\mu(\mathbf{x})\, A_\mu(\mathbf{x}, t)\, d\mathbf{x},$$

where $\rho(\mathbf{x})$ is the charge density operator, $J_\mu(\mathbf{x})$ the current density operator of the system, and $U(\mathbf{x}, t)$ and $A_\mu(\mathbf{x}, t)$ are respectively the scalar and vector potentials of the weak electromagnetic field.

In the approximation which is linear in the field, the solution of the equation for the density matrix can be written in the form $F = F_0 + F_t$, where

$$F_t = \int_{-\infty}^{0} d\tau \int d\mathbf{x} E_\mu(\mathbf{x}, t+\tau) \int_0^\beta d\lambda\, J_\mu(\mathbf{x}, \tau + i\hbar\lambda)\, F_0$$
$$+ \frac{1}{c}\int d\mathbf{x}\, A_\mu(\mathbf{x}, t) \int_0^\beta d\lambda J_\mu(\mathbf{x}, i\hbar\lambda)\, F_0. \qquad (1)$$

To derive this formula we used the relation $\operatorname{div} \mathbf{J}(\mathbf{x}) = \dot{\rho}(\mathbf{x})$ and the identity[9]

$$[F_0, L] = i\hbar \int_0^\beta d\lambda \dot{L}\,(i\hbar\lambda) F_0,$$

where

$$L(t) = \exp(-H't/i\hbar)\, L \exp(H't/i\hbar),$$

$$\dot{L} = (i\hbar)^{-1}[L, H'].$$

The average value $\overline{B}$ of a quantity B can be evaluated using the formula

$$\overline{B} = \operatorname{Sp} F_0 B_0 + \operatorname{Sp} F_t B_0 + \operatorname{Sp} F_0 B_t, \quad B = B_0 + B_t,$$

where B_t is the correction to the operator B, necessitated by the perturbing vector potential in the approximation which is linear in the field. If, for instance, B is the current density operator, we have

$$\mathbf{B}_t = -(e^2/mc)\,\mathbf{A}(\mathbf{x}, t)\,\Psi^+(\mathbf{x})\,\Psi(\mathbf{x}),$$

where $\Psi(\mathbf{x})$ is the operator of the quantized wave function. Using Eq. (1) we can write $\overline{B}$ in the form

$$\overline{B} = \operatorname{Sp} F_0 B_0 + \overline{B}^{(1)} + \overline{B}^{(2)},$$

$$\overline{B}^{(1)} = \int_{-\infty}^0 d\tau \int d\mathbf{x} E_\mu(\mathbf{x}, t+\tau) \int_0^\beta d\lambda \operatorname{Sp}\{F_0 B_0 J_\mu(\mathbf{x}, \tau + i\hbar\lambda)\},$$

$$\overline{B}^{(2)} = \frac{1}{c}\int d\mathbf{x} A_\mu(\mathbf{x}, t) \int_0^\beta d\lambda \operatorname{Sp}\{F_0 B_0 J_\mu(\mathbf{x}, i\hbar\lambda)\} + \operatorname{Sp} F_0 B_t. \tag{2}$$

Although the quantity $\overline{B}^{(2)}$ contains the vector potential, we can show that it is gauge invariant. We can verify that this quantity owes its existence purely to the magnetization current. Indeed, if $E_\mu = 0$ the total change in the average value of B is due to $\overline{B}^{(2)}$. Also, $\overline{B}^{(2)}$ does not contain a time retardation relative to the vector potential. $\overline{B}^{(2)}$ is thus that value of $\overline{B}$ which would have been obtained if the magnetic field were constant and if there were no electrical field. Then, of course, only the magnetization current would exist in the system. We have studied earlier[10] the properties and the physical meaning of $\overline{B}^{(2)}$ for the case where B is the current density operator. In the present paper we shall not be interested any further in the quantity $\overline{B}^{(2)}$.

Let us consider the quantity $\overline{B}^{(1)}$ in more detail.

Bearing in mind that in the second quantization representation

$$B_0 = \int \Psi^+(\mathbf{x})\, b_0 \Psi(\mathbf{x})\, d\mathbf{x} = \sum_{nn'} (b_0)_{nn'} a_n^+ a_{n'}.$$

(where b_0 is a single-electron operator and the n are the quantum numbers of the set of single-electron states) we get

$$\overline{B}^{(1)} = \sum_{nn'} (b_0)_{nn'} f^{(1)}_{nn'}(t). \tag{3a}$$

Here

$$f^{(1)}_{nn'}(t) = \int_{-\infty}^0 d\tau \int d\mathbf{x} E_\mu(\mathbf{x}, t+\tau) \int_0^\beta d\lambda \operatorname{Sp}\{F_0 a_n^+ a_{n'} J_\mu(\mathbf{x}, \tau + i\hbar\lambda)\}. \tag{3b}$$

We can call the quantity $f^{(1)}_{nn'}(t)$ the correction to the single-electron density matrix.

Let

$$E_\mu(\mathbf{x}, t) = E_\mu(\mathbf{x}, s) \exp(i\varkappa\mathbf{x} + st), \quad s = -i\omega + \nu,$$

where ω is the frequency of the field and ν the adiabatic parameter, which we shall let tend to zero in the final formulae. If we write the operator $J_\mu(\mathbf{x}, \tau + i\hbar\lambda)$ in the second-quantization representation, Eq. (3b) becomes

$$f^{(1)}_{nn'}(t) = E_\mu(\mathbf{x}, s)\, e^{st} \sum_{mm'} G^{m'n'}_{mn}(s, \beta) \int e^{i\varkappa\mathbf{x}} j_\mu(\mathbf{x})_{mm'} d\mathbf{x}, \tag{4b}$$

$$G^{m'n'}_{mn}(s, \beta) = \int_{-\infty}^0 e^{s\tau} d\tau \int_0^\beta d\lambda \operatorname{Sp}\left\{F_0 \exp\left[\frac{H'}{i\hbar}(\tau + i\hbar\lambda)\right] a_n^+ a_{n'} \times \exp\left[-\frac{H'}{i\hbar}(\tau + i\hbar\lambda)\right] a_m^+ a_{m'}\right\}. \tag{4a}$$

Let $H = H_0 + V$, then

$$\exp\left[\frac{H_0'}{i\hbar}(z_1 - z_2)\right] = \exp\left(\frac{H_0' z_1}{i\hbar}\right)\left[T_c \exp\left(\frac{1}{i\hbar}\int_{z_2}^{z_1} V_z dz\right)\right] \exp\left(-\frac{H_0' z_2}{i\hbar}\right),$$

$$V_z = \exp\left(-\frac{H_0' z}{i\hbar}\right) V \exp\left(\frac{H_0' z}{i\hbar}\right).$$

z_1 and z_2 are here complex numbers and the integration is along an arbitrary contour C in the complex plane from z_2 to z_1. The T_C sign indicates an ordering of the operators along this contour in such a way that points on the contour which lie nearer to z_2 along the contour are assumed to be earlier. Using this formula we can write the exponents in Eq. (4b) in the following form

$$F_0 \exp\left[\frac{H'}{i\hbar}(\tau + i\hbar\lambda)\right] = Z^{-1} \exp\left\{\frac{H'}{i\hbar}[(\tau - i\hbar\beta) - (-i\hbar\lambda)]\right\}$$

$$= Z^{-1} \exp\left[\frac{H_0'}{i\hbar}(\tau - i\hbar\beta)\right] \exp\left[\frac{1}{i\hbar}\int_{-i\hbar\lambda}^{\tau - i\hbar\beta} V_z dz\right] \exp(\lambda H'_0),$$

$$\exp\left[-\frac{H'}{i\hbar}(\tau + i\hbar\lambda)\right] = \exp(-H_0'\lambda) \exp\left[\frac{1}{i\hbar}\int_{\tau}^{-i\hbar\lambda} V_z dz\right] \exp\left(-\frac{H_0'\tau}{i\hbar}\right).$$

Substituting these expressions into Eq. (4b) we write $G^{m'n'}_{mn}$ in a form which is convenient for a series expansion in the coupling constant:

$$G_{mn}^{m'n'}(s,\beta) = \int_{-\infty}^{0} e^{s\tau} d\tau G_{mn}^{m'n'}(\tau,\beta), \qquad (5a)$$

$$G_{mn}^{m'n'}(\tau,\beta) = \int_0^\beta d\lambda \,\mathrm{Sp}\left\{e^{-\beta H_0} T_c \exp\left[\frac{1}{i\hbar}\int_C V_z dz\right](a_n^+ a_{n'})_{-i\hbar\lambda}\,(a_m^+ a_{m'})_\tau\right\} Z^{-1}. \qquad (5b)$$

The integration in the exponent is over the contour C shown in Fig. 1. The sign T_c orders the operators along the same contour.

$G_{mn}^{m'n'}$ is thus some kind of temperature-dependent Green function with the peculiar feature that the S-matrix contains an integral over a contour in the complex "time" plane.

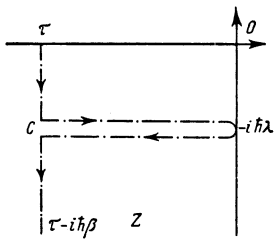

FIG. 1

2. A DIAGRAM TECHNIQUE TO EVALUATE THE FUNCTION $G_{mn}^{m'n}$

1. Let V_{ph} be the electron-phonon interaction operator

$$V_{ph} = \sum_{f,\, q\neq 0} (c_q b_q a_f^+ a_{f-q} + c_q^* b_q^+ a_f^+ a_{f+q}),$$

where b_q^+ and b_q are the creation and annihilation operators of the phonons. We have taken for the set of single-electron states plane waves, and **f** is the electron and **q** the phonon wave vector. After expanding the exponent in Eq. (5b) in a series, we get the usual Feynman expansion for the function $G_{kp}^{k'p'}(\tau,\beta)$. It occurs as a sum of terms, in which every term corresponds to a diagram. All points of the diagram lie on the contour C. Each point is the start of one and the end of another electron line and either the start (phonon emission) or the end (absorption) of a phonon line. The points τ and $-i\hbar\lambda$ are excepted, and we call them the terminal points.

No phonon lines go to them. The line **k'** ends and the line **k** starts at the terminal point τ. The line **p'** ends and the line **p** starts at the terminal point $-i\hbar\lambda$.

To each electron line going from the point z_2 to the point z_1 there corresponds a factor

$$g_\alpha(z_1,z_2) = \mathrm{Sp}\{e^{-\beta H_0'} T_c (a_\alpha)_{z_1} (a_\alpha^+)_{z_2}\} Z_0^{-1} = \exp\frac{\varepsilon_\alpha'(z_1-z_2)}{i\hbar}\begin{cases}(1-n_\alpha) & \text{if } z_2 \text{ is earlier than } z_1\\ -n_\alpha & \text{if } z_2 \text{ is later than } z_1\end{cases}$$

(here $\epsilon_\alpha' = \epsilon_\alpha - \mu$), and to a phonon line a factor

$$d_q(z_1,z_2) = |c_q|^2 \mathrm{Sp}\{e^{-\beta H_0'} T_c (b_q)_{z_1} (b_q^+)_{z_2}\} Z_0^{-1} = |c_q|^2 \exp[-i\omega_q(z_1-z_2)] \times \begin{cases}(1+m_q) & \text{if } z_2 \text{ is earlier than}\\ m_q & \text{if } z_2 \text{ is later than } z_1\end{cases}$$

where ϵ_α is the electron energy, ω_q the phonon frequency, and

$$Z_0 = \mathrm{Sp}\exp[-\beta(H_0-\mu N)],$$

$$n_\alpha = [\exp\beta(\varepsilon_\alpha-\mu)+1]^{-1}, \qquad m_q = [\exp\beta\hbar\omega_q - 1]^{-1}.$$

To each point (except the terminal points) there corresponds a factor $dz/i\hbar$. For each z one must integrate along the contour C. Moreover, λ is integrated from 0 to β.

Unconnected diagrams, similar to vacuum loops, need not be taken into account as they are cancelled by diagrams from the expansion of Z.

We need $G_{kp}^{k'p'}(s,\beta)$ to evaluate the single-particle density matrix [see Eq. (5a)]. It is in fact more convenient to evaluate the function*

$$G_{kp}^{k'p'}(s,\sigma) = \int_0^\beta e^{-\beta\sigma} G_{kp}^{k'p'}(s,\beta)\, d\beta.$$

We do not consider β, which enters into n_α and m_q, as an integration variable.

We proceed now to justify the rules for evaluating $G_{kp}^{k'p'}(s,\beta)$. These rules will be formulated later on. The integration over τ and β is easily performed if each Feynman diagram is broken up into a sum of diagrams with different relative arrangements of points. As an example we give in Fig. 2 some modified diagrams of second order,† which must be considered to be different and which originate from the same Feynman diagram. The horizontal sections of the "time" contour are pulled apart for the sake of convenience. Owing to this modification, the order of the integrals in each diagram containing n points on the horizontal and r points on the vertical sections of the contour C is of the form

$$\int_{-\infty}^{0} e^{s\tau} d\tau \int_0^\tau dt_1 \ldots \int_0^{t_{n-1}} dt_n \int_0^\infty e^{-\beta\sigma} d\beta \int_0^\beta d\gamma_1 \ldots \times \int_0^{\gamma_m} d\lambda \int_0^\lambda d\gamma_{m+1} \ldots \int_0^{\gamma_{r-1}} d\gamma_r.$$

*V. V. Tolmachev has drawn our attention to the fact that C. Bloch[11] has used essentially a similar method to evaluate the partition function.

†We do not for the present turn our attention to the thin intersecting straight lines.

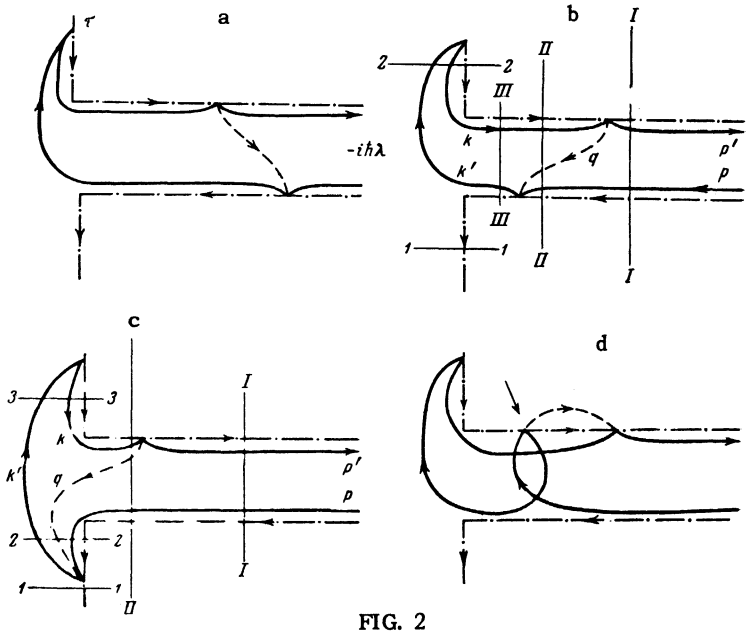

FIG. 2

Here $t_1, \ldots, t_n$ are the real parts of the complex "time" points on the horizontal sections of the contour C (the imaginary part of the "time" is for all these points equal to $-\hbar\lambda$). The quantities $-\hbar\gamma_1, \ldots, -\hbar\gamma_m$ are the imaginary parts of the "time" points on the upper vertical section of the contour C; and $-\hbar\gamma_{m+1}, \ldots, -\hbar\gamma_r$ the imaginary parts of the "time" points on the lower vertical section of the contour C (the real part of the times is for all these points equal to τ).

The time dependent exponents contained in g_α and d_q are best referred to the points. Each point z (including the terminal points) will then correspond to a factor $\exp(i\Omega_{AB}z)$, where $\hbar\Omega_{AB} = E_A - E_B$, with E_A the energy of the line starting at the point z and E_B the energy of the line ending at the point z. For a point on the horizontal section we have $z = t - i\hbar\lambda$. We set the factor $\exp(i\Omega_{AB}t)$ along a suitable differential dt, and the factor $\exp(\hbar\lambda\Omega_{AB})$ along $d\lambda$. For points on the vertical sections we have $z = \tau - i\hbar\gamma$. We set the exponent $\exp(\hbar\Omega_{AB}\gamma)$ along the differential $d\gamma$ and the factor $\exp(i\Omega_{AB}\tau)$ along $d\tau$. After this, all integrals can easily be evaluated by consecutive integrations by part. As a result we get the following rules for writing down the expression corresponding to the modified diagram for the function $G^{k'p'}_{kp}(s, \sigma)$.

1) A line going from an earlier point on the contour to a later point will be called a regular line. To each regular line there corresponds a factor $1 - n_\alpha$ for the electrons and $|c_q|^2(1 + m_q)$ for the phonons. For an irregular line we have respectively n_α and $m_q|c_q|^2$.

2) To each point on the upper horizontal section of the contour there corresponds a factor $(i\hbar)^{-1}$, on the lower section a factor $(-i\hbar)^{-1}$, and on the vertical sections (-1); momentum is conserved at each point.

3) We imagine a vertical line taking up consecutively the positions I, II, . . . in the intervals between the points on the horizontal section as is shown, for example, in Figs. 2b and 2c.

To each interval there corresponds a factor $(s + i\omega_{MN})^{-1}$ where $\hbar\omega_{MN} = E_M - E_N$, with E_M the total energy of the lines entering the interval on the right of the intersecting line and E_N the total energy of the lines leaving this region. For instance, in Fig. 2c the intersection I corresponds to a factor $(s + i\omega_{p'p})^{-1}$ and the intersection II to a factor $[s + i(\omega_{kp} - \omega_q)]^{-1}$ where $\omega_{kp} = (\epsilon_k - \epsilon_p)/\hbar$.

Similarly we imagine a horizontal line taking up consecutively the positions 1, 2, . . . between the points on the vertical axis (see Figs. 2b and 2c). To each vertical interval there corresponds a factor $(\sigma + \hbar\omega_{MN})^{-1}$, where E_M is the total energy of the lines entering the region below the intersecting line and E_N the energy of the lines coming from that region. For instance, in Fig. 2c the intersection 1 corresponds to a factor σ^{-1} and the intersection 2 to a factor $[\sigma + \hbar(\omega_{pk'} + \omega_q)]^{-1}$.

4) Each diagram is multiplied by $(-1)^M$, where M is the number of mutual intersections of electron lines. One must draw here the electron line to the point "in the same sense" as the time axis (see in Fig. 2d the point indicated by an arrow).

We give as an example the expression corre-

sponding to the diagram 2b:

$$[(1-n_{p'})(1-n_p)(1+m_q)]\frac{(-1)}{(i\hbar)^2}\frac{(c_q)^2}{s+i\omega_{p'p}}\frac{n_{k'}(1-n_k)}{s+i(\omega_{kp}-\omega_q)}$$
$$\times\frac{1}{\sigma}\frac{1}{\sigma+\hbar\omega_{kk'}}\frac{1}{s+i\omega_{kk'}}\delta_{k,\,p'+q}\delta_{k',\,p+q}. \qquad (6)$$

Summation over $\mathbf{q}$ is implied.

Let us consider some properties of the modified diagrams.

If we transfer one point from the lower horizontal axis to the upper one (or the other way round) without changing its coordinates in the complex plane, only the regularity of the lines joining it from the right is changed. Also, the sign of the expression may change. Examples of diagrams obtained from one another by the transfer of a point are the diagrams of Figs. 2b and 2d (the transferred point is indicated by an arrow). It is convenient to consider such diagrams together, transferring the points mentally. For instance, the sum of all diagrams obtained from 2b by a transfer of points differs from (6) only in that now the square brackets contain

$$\{(1-n_p)(1+m_q)+n_pm_q\}(1-n_p+n_p)=1+m_q-n_p.$$

When all lines from a point on the horizontal axis go to the left (right-hand return) the transfer of a point changes only the sign of the diagram (the sign changes because when such a point is transferred the parity of the number of intersections is not changed, but the upper point becomes the lower one and vice versa). We can therefore in general neglect diagrams with a right-hand return. An example is shown in Fig. 3. The arrow indicates the right-hand return.

2. The presence of an interelectronic interaction

$$V_e=\frac{1}{2}\sum_{q\neq q',\,ff'}u_{q-q'}a_q^+a_{q'}a_f^+a_{f'}\delta_{q+f,\,q'+f'}$$

only leads to the occurrence in the diagrams of points where four electron lines meet. Such a point can conveniently be indicated in the way shown in Fig. 4.

It will correspond to a factor $u_{q-q'}$ (apart from those mentioned in the preceding subsection).

3. Let the perturbation V contain the operator for the interaction of the electrons with heavy impurities

$$V_n=\sum_{q\neq q'}v_{q-q'}a_q^+a_{q'}\sum_\nu\exp[-i(\mathbf{q}-\mathbf{q}')\mathbf{r}_\nu],$$

where $\mathbf{r}_\nu$ is the coordinate of the ν-th impurity center. In that case averaging over all $\mathbf{r}_\nu$ is implied in the operation $\mathrm{Sp}\{\exp(-\beta H')\ldots\}$. The changes introduced in this case into the diagram technique are confined to the following ones:

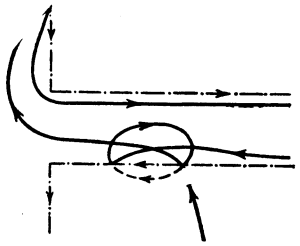

FIG. 3

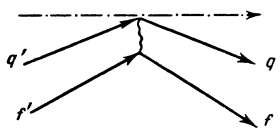

FIG. 4

a) Impurity points appear along the contour C.

b) Such a point gives rise to a factor $v_{q-q'}$ (apart from these mentioned in subsection 1).

c) The loose ends of the impurity lines are tied up in bundles in such a way that there are at least two lines going to each knot* (examples can be seen in Figs. 5a and 5b). To each bundle there corresponds a factor N: the total number of impurity centers. There are no factors corresponding to an impurity line as it does not carry any energy (in contradistinction to the phonon line). They need therefore not be taken into account when ω_{MN} is calculated for each intersection and when the right-hand return is determined. For instance, in Fig. 5b there is a right-hand return. In each bundle the sum of the momenta of the electron lines entering into all the points corresponding to the bundle is equal to the sum of the momenta of the lines leaving these points.

We note in conclusion that we can directly draw the diagrams for the single-particle density matrix $f_{pp'}$. They will differ from the diagrams described in the foregoing only by the fact that the terminal point τ will now correspond to a factor

$$E_\mu(\mathbf{x},\,s)\,e^{st}\frac{e\hbar}{2m}(\mathbf{k}+\mathbf{k}')\,\delta_{k',\,k-\varkappa}$$

[see Eq. (4a)] and that one sums over $\mathbf{k}$ and $\mathbf{k}'$.

To emphasize the difference between the diagrams for $f_{pp'}$ and for $G_{kp}^{k'p'}$, we shall draw the diagrams for $f_{pp'}$ in a way which is similar to the diagrams for the vertex part in electro-dynamics,

*The bundling of the impurity lines can be elucidated as follows. We consider, for instance, the term of fourth order in the interaction. It contains the quantity

$$\Big\langle\sum_{\nu_1\nu_2\nu_3\nu_4}\exp[-i(q_1-q_1')r_{\nu_3}]\ldots\exp[-i(q_4-q_4')r_{\nu_4}]\Big\rangle$$

(the angular brackets indicate the averaging over the positions of the impurity centers). In this sum there will be a term for which $\nu_1=\nu_2=\nu_3=\nu_4$. To this term there corresponds a diagram with one bundle, where all four impurity lines are tied together. Furthermore, there will be one for which $\nu_1=\nu_2$, $\nu_3=\nu_4$. To this term there corresponds a diagram with two bundles with two lines going to each of them. There will clearly be altogether three such diagrams. There are no diagrams where the bundle contains only one line (for instance, $\nu_1=\nu_2=\nu_3\neq\nu_4$) as there is no term with $\mathbf{q}=\mathbf{q}'$ in the expression for V_n.

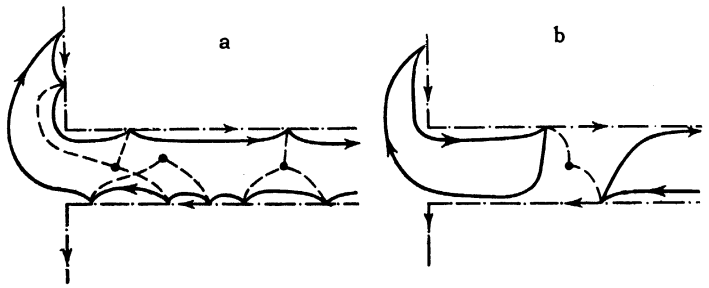

FIG. 5

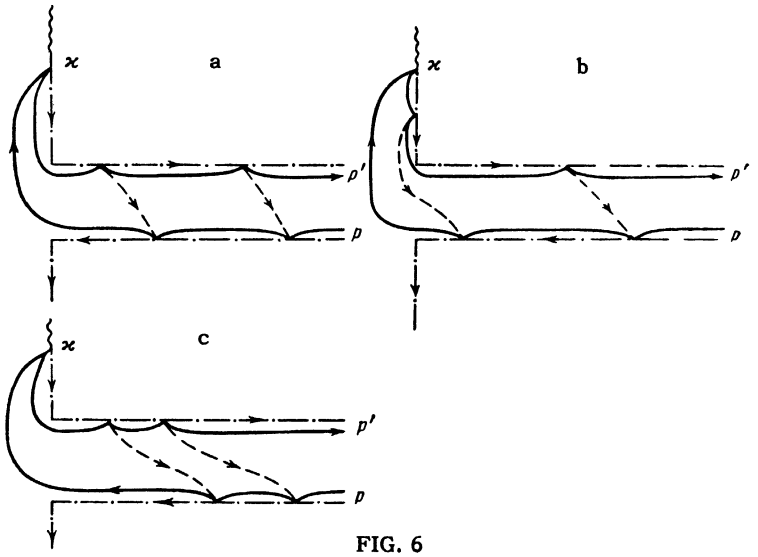

FIG. 6

with a "photon" wavy line included at the terminal point τ (see Fig. 6).

3. THE TRANSPORT EQUATION

Let us classify the modified diagrams. We call an intersection (vertical or horizontal) which cuts only two electron lines and nothing else a free intersection. That part of a diagram which is bounded by two vertical free intersections and which does not contain free intersections in the intervals between its points we call a horizontal irreducible part. A vertical irreducible part is defined in a similar way. A part of a diagram which contains points both on the vertical and on the horizontal segments which can not be cut by a free intersection is called an angular part. For instance, in Fig. 5a there is one horizontal irreducible part and an angular part.

In the case where the frequency ω and the wave vector κ of the electrical field tend to zero, there occurs an important singularity in the perturbation-theory series. The factors corresponding to the vertical free intersections increase without bound. Therefore the number of terms cannot be kept finite in an expansion in any interaction parameter, however small. In that case we must compare with one another only those diagrams which contain the same number of vertical free intersections (and hence the same number of horizontal irreducible parts). For instance, we can neglect the diagram 2c compared with a free line, but we can not neglect diagrams 2a, 2b, and 2d. In exactly the same way, we can neglect diagrams 6b and 6c compared to 2a, but not diagram 6a. If the frequency and the wave vector of the electrical field are thus sufficiently small it is necessary to sum an infinite number of terms. This summation leads to an exact integral equation for $f_{pp'}$ which is depicted in Fig. 7 (the first diagram is equal to the sum of the next two):

$$f_{pp'}(s,\ \sigma) = r_{pp'}(s,\ \sigma)(s + i\omega_{p'p})^{-1} + f_{qq'}W^{qp'}_{q'p}(s)(s + i\omega_{p'p})^{-1} \qquad (7)$$

(summation over q is implied). $r_{pp'}(s, \sigma)$ is here the sum of all diagrams which do not contain horizontal irreducible parts without the last free intersection on the right; $W^{qp'}_{q'p}$ is the sum of all possible horizontal irreducible parts. The term corresponding to each irreducible part includes the factors from all points occurring in it, from all intersections (except the last, free ones), and from all lines except the two last ones on the left.

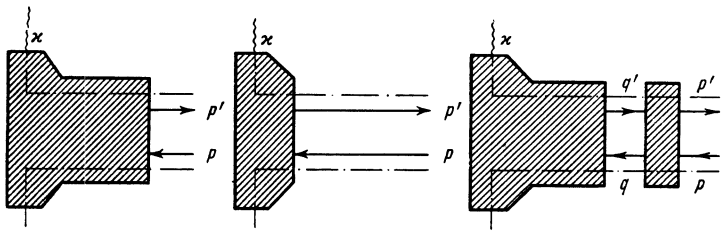

FIG. 7

Because of the conservation of momentum we have $\mathbf{p}' = \mathbf{p} + \kappa$, $\mathbf{q}' = \mathbf{q} + \kappa$. For simplicity denoting $W^{\mathbf{q},\mathbf{p}+\kappa}_{\mathbf{q}+\kappa,\mathbf{p}}$ by $W_{\mathbf{qp}}$ we can write Eq. (7) in the form

$$(s + i\omega_{\mathbf{p}+\varkappa,\,\mathbf{p}}) f_{\mathbf{p},\,\mathbf{p}+\varkappa} = r_{\mathbf{p},\,\mathbf{p}+\varkappa}(s,\ \beta) + \sum_{\mathbf{q}} f_{\mathbf{q},\,\mathbf{q}+\varkappa} W_{\mathbf{qp}}(s),$$

$$r_{\mathbf{pp}'}(s,\beta) = (2\pi i)^{-1} \int_{-i\infty+a}^{i\infty+a} r_{\mathbf{pp}'}(s,\ \sigma)\, e^{\beta\sigma} d\sigma. \qquad (8)$$

This equation is a generalized transport equation. It is important to note that the quantities W and r occurring in it do not contain free intersections.

If we take into account that the distribution function is

$$f_{\mathbf{p}}(x) = \int e^{i\varkappa\mathbf{x}} f_{\mathbf{p}-\varkappa/2,\ \mathbf{p}+\varkappa/2}\, d\varkappa,$$

the meaning of the different terms in Eq. (8) becomes clear: the term on the left hand side corresponds to the expression $\partial f_{\mathbf{p}}/\partial t + v_{\mathbf{p}}\nabla_{\mathbf{x}} f_{\mathbf{p}}$ when $\kappa \ll p$, the first term on the right hand side describes the change in $f_{\mathbf{p}}(x, t)$ under the action of the electrical field, and the second one the influence of collisions (it will become clear in the following that the second term also includes the self-consistent field).

As examples we shall consider the interaction of electrons with phonons and with impurities.

1. Interaction with phonons. We shall assume that the interaction is weak. We can then restrict ourselves to second order diagrams when evaluating W. Typical diagrams are given in Fig. 8. We shall for simplicity assume that the wave length of the electrical field is much larger than the electron de Broglie wave length and that $\hbar\omega \ll kT$ ($s = -i\omega - \nu$). Diagrams of the type 8b give them a contribution to W equal to

$$W^{(b)}_{\mathbf{qp}} = 2\pi\hbar^{-2} |c_{\mathbf{p}-\mathbf{q}}|^2 [(1 + m_{\mathbf{q}-\mathbf{p}} - n_{\mathbf{p}})\, \delta(\omega_{\mathbf{pq}} + \omega_{\mathbf{p}-\mathbf{q}}) + (m_{\mathbf{p}-\mathbf{q}} + n_{\mathbf{p}})\, \delta(\omega_{\mathbf{pq}} - \omega_{\mathbf{p}-\mathbf{q}})].$$

The contribution of diagrams of type 8a is equal to

$$W^{(a)}_{\mathbf{qp}} = -\delta_{\mathbf{pq}} \sum_{\mathbf{r}} W^{(6)}_{\mathbf{pr}}.$$

If we restrict ourselves to diagrams such as 8a and 8b, the second term on the right hand side of (8) takes on the usual form of the collision term in the transport equation, where diagrams of type 8b correspond to an electron entering a state $\mathbf{p}$, and diagrams of type 8a to an electron leaving this state. Diagrams of type 8a give a contribution

$$W^{(c)}_{\mathbf{qp}} = -\frac{|c_{\varkappa}|^2}{\hbar^2} \frac{2\omega_{\varkappa}}{\omega_{\varkappa}^2 - \omega^2} i(\mathbf{x}\mathbf{v}_p) \frac{\partial n_{\mathbf{r}}}{\partial \varepsilon_{\mathbf{p}}}, \qquad v_{\mathbf{p}} = \frac{1}{\hbar}\frac{\partial \varepsilon_{\mathbf{p}}}{\partial \mathbf{p}}.$$

The corresponding term in the transport equation (8) describes the influence of the self-consistent field created by the electrons through the phonons. The potential energy for the interaction between two electrons has the Fourier components

$$G_{\varkappa\omega} = -\hbar^2 |c_{\varkappa}|^2 2\omega_{\varkappa}/(\omega_{\varkappa}^2 - \omega^2).$$

We must note that a study of the actual value of this potential requires that the direct Coulomb interaction between the electrons is taken into account at the same time.

The diagram of lowest order in the interaction is for the quantity r a free line. If $\kappa \ll p$, we have then

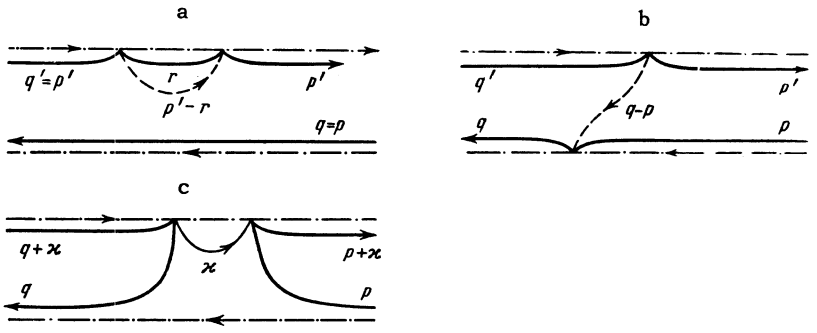

FIG. 8

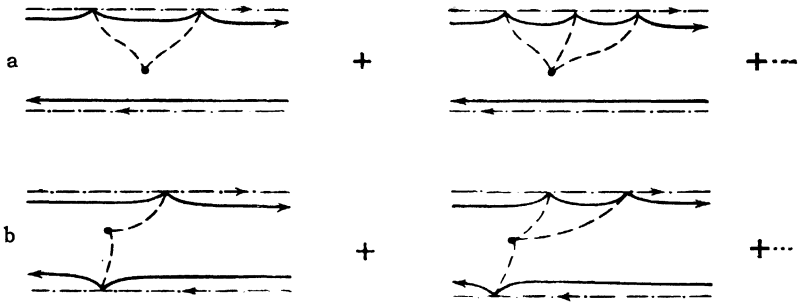

FIG. 9

$$r_{\mathbf{p},\,\mathbf{p}+\varkappa} = -e\mathbf{E}(\varkappa, s)\, e^{st}\, \mathbf{v}_{\mathbf{p}}\, dn_{\mathbf{p}}/d\varepsilon_{\mathbf{p}},$$

which corresponds to the field term in the transport equation.

2. Interaction with neutral impurities. We shall assume the impurity concentration to be small. We can therefore restrict ourselves to diagrams with one bundle when evaluating W. Typical diagrams are given in Fig. 9. As before we shall assume $\kappa \to 0$ and $s \to 0$. After transferring each point we find that each line occurring in W will correspond to a factor 1. One can verify that the sum of diagrams 9b, $W^{(b)}$, is the exact probability that an electron through scattering at an impurity center makes a transition from a state $\mathbf{q}$ into a state $\mathbf{p}$ per unit time (the first term of this sum is the first Born approximation). The sum of diagrams of type 9a gives

$$W_{\mathbf{qp}}^{(a)} = -\delta_{\mathbf{qp}} \sum_{r} W_{\mathbf{pr}}^{(b)}.$$

The second term on the right hand side of (8) takes thus the usual form of the collision term, linearized in the field. The diagram of the self-consistent field type is in this case equal to zero (right hand return).

If we restrict ourselves for the quantity r to the zeroth approximation in the impurity concentration we obtain the usual transport equation.

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