

Quantum Effect in D. C. and Hall Conductivities*—An Application of Wigner Representation—*

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The Wigner representation formalism is applied to investigating the effect of the momentum-coordinate commutation relation on the d.c. and Hall conductivities of a system of non-interacting electrons moving in a potential field of randomly distributed impurities. The conductivities are expanded in powers of \hbar and the second- and fourth-order terms are shown to vanish within the Born approximation, as far as the expansion is reasonable. This situation is discussed in comparison with the result of the kinetic theory.

§ 1. Introduction

The quantum operators of momentum and coordinate do not commute. As is well known, this fact leads to the momentum-coordinate uncertainty. The effect of this uncertainty can be discussed by examining the dependence of physical quantities on \hbar which is the Planck constant divided by 2π . \hbar -expansion is systematically done by use of the Wigner representation^{1),2)} in which one can directly calculate contributions from each order term in \hbar .

In this paper we discuss the quantum effect on the d.c. and Hall conductivities, i.e., whether the conductivities increase, decrease or otherwise are affected when the momentum-coordinate uncertainty is introduced to a classical system.

Several years ago, Kubo¹⁾ presented a description of quantal systems in terms of the Wigner representation, and pointed out that the magnetic field comes into the expression of the Hall conductivity in two ways, firstly in the propagation of current and secondly in the equilibrium distribution. The latter contribution is proportional to \hbar^2 , i.e., essentially quantal, and shown to give the Landau diamagnetism of conduction electrons. However, the usual naive theory of the Hall conductivity seems to neglect this contribution. We will show that such a neglect is allowed when the scattering potential is very weak compared with the kinetic energy.**)

The general formulae for the conductivities in the Wigner representation have been given by Kubo.¹⁾ To simplify the explicit calculations, we assume

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***) In the case of the Coulomb potential, the potential energy near the origin overcomes the kinetic energy, so this discussion is not valid for the Coulomb potential. (See §9.)

that the relaxation of the electron system is dominated by the scattering by randomly distributed static impurities. We consider no other interaction, therefore, the quantum effect comes only from the coordinate dependence of the impurity potential.*)

In this work we seek the conductivities to the lowest order of the impurity potential. This approximation corresponds to the quantum Born approximation and will be simply called the Born approximation. The validity of this approximation is related to the weakness and the space dependence of the impurity potential and to the density of impurities. On the other hand, \hbar -expansion is related only to the coordinate dependence of the impurity potential, as is easily seen from the form of the Liouville operator (see § 2). Thus, if the impurity potential is sufficiently weak (compared with the kinetic energy) and the density of the impurities is low enough, we can consider \hbar -expansion within the framework of the Born approximation. With respect to this point we will give some comments in the last section. Anyway, we show formally that the quantum correction up to the fourth order of \hbar does not appear within the Born approximation, as far as \hbar -expansion is possible. This is consistent with the result of the kinetic theory. Furthermore the quantum correction related to the change of the equilibrium distribution is shown to be of higher order in the strength of the impurity potential than the Born approximation. If one wants to discuss the contribution from the equilibrium distribution to the quantum correction, one must calculate a number of terms which give contributions of the same order in the impurity potential strength.

The Coulomb potential is the typical one for which the Born approximation in the sense stated above is not valid. In this case the result of the kinetic theory, which is also obtainable by the Wigner representation, shows that the momentum-coordinate uncertainty saves the difficulty which is due to the divergence of the potential at the origin.

In § 2, we formulate the problem in terms of the Wigner representation, and in § 3, a graphical method is introduced for the expansion of the conductivities with respect to the impurity potential. In §§ 4 and 5, we calculate the d.c. conductivity in the classical limit ($\hbar \rightarrow 0$) and its quantum correction, respectively, both within the Born approximation. The same procedure is applied to the Hall conductivity in § 6. Section 7 is dedicated to the comparison with the kinetic theory, which provides us with a good insight into the properties of the higher-order terms in \hbar . The validity of the expansion is discussed in § 8. In § 9 we will state some concluding remarks including comments on the validity condition for the Born approximation.

*) As we take the Boltzmann statistics electrons, the effect of the Fermi statistics is not considered in this paper.

§ 2. Formulation

In what follows, we consider a system of non-interacting electrons moving in the potential field of randomly distributed impurities. The total Hamiltonian for each electron in the presence of electric and magnetic fields may be written as

$$\mathcal{H}_T = \mathcal{H} + \mathcal{H}_F \tag{2.1}$$

and

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_I + \mathcal{H}_H, \tag{2.2}$$

where \mathcal{H}_0 describes the free motion of the electron, \mathcal{H}_I the interaction between the electron and impurities, \mathcal{H}_F and \mathcal{H}_H the interactions of the electron with the applied uniform electric and magnetic field, respectively. These Hamiltonians are explicitly expressed as

$$\mathcal{H}_0 + \mathcal{H}_H = \frac{1}{2m} \left(\mathbf{p} + \frac{e}{c} \mathbf{A} \right)^2, \tag{2.3}$$

$$\mathcal{H}_I = \sum_{i=1}^{N_i} V(\mathbf{r} - \mathbf{R}_i) = V_I(\mathbf{r}), \tag{2.4}$$

$$\mathcal{H}_F = e\mathbf{E}x, \tag{2.5}$$

where N_i is the number of impurities, $-e$ the charge of an electron, and $V(\mathbf{r} - \mathbf{R}_i)$ the interaction potential between an electron located at \mathbf{r} and an impurity at \mathbf{R}_i . The electric field is applied along the x -axis. As is usual in the calculation of the Hall conductivity, we take the direction of the magnetic field, which is related to the vector potential \mathbf{A} as $\text{rot } \mathbf{A} = \mathbf{H}$, to be parallel to the z -axis, i.e., perpendicular to the electric field.

We apply the Wigner representation to the above-mentioned system. The details of the procedure have been given by Kubo,¹⁾ therefore only the results are presented here.

In the Wigner representation, one can define the distribution function $f(\mathbf{p}, \mathbf{r}, t)$ of an electron in the phase space, even for a quantal system. The Liouville equation for $f(\mathbf{p}, \mathbf{r}, t)$ is written as

$$\frac{\partial}{\partial t} f(\mathbf{p}, \mathbf{r}, t) = i\mathcal{L}_T f(\mathbf{p}, \mathbf{r}, t). \tag{2.6}$$

In the present case, the Liouville operator $i\mathcal{L}_T$ is divided into two parts:

$$i\mathcal{L}_T = i\mathcal{L} + eE \frac{\partial}{\partial p_x}. \tag{2.7}$$

According to Kubo, the operator $i\mathcal{L}$ can be formally expanded in the power of \hbar as

$$i\mathcal{L} = i\mathcal{L}_0 + i\mathcal{L}_H + i\mathcal{L}_2 + i\mathcal{L}_4 + O(\hbar^6), \tag{2.8}$$

where

$$i\mathcal{L}_0 = -\frac{\mathbf{p}}{m} \frac{\partial}{\partial \mathbf{r}} + \frac{\partial V_I}{\partial \mathbf{r}} \frac{\partial}{\partial \mathbf{p}}, \quad (2.9)$$

$$i\mathcal{L}_H = -\omega_c \left(p_x \frac{\partial}{\partial p_y} - p_y \frac{\partial}{\partial p_x} \right), \quad (2.10)$$

$$i\mathcal{L}_3 = -\frac{\hbar^2}{3! 2^3} \frac{\partial^3 V_I(\mathbf{r})}{\partial x_\alpha \partial x_\beta \partial x_\gamma} \frac{\partial^3}{\partial p_\alpha \partial p_\beta \partial p_\gamma}, \quad (2.11)$$

$$i\mathcal{L}_4 = \frac{\hbar^4}{5! 2^4} \frac{\partial^5 V_I(\mathbf{r})}{\partial x_\alpha \partial x_\beta \partial x_\gamma \partial x_\delta \partial x_\eta} \frac{\partial^5}{\partial p_\alpha \partial p_\beta \partial p_\gamma \partial p_\delta \partial p_\eta}. \quad (2.12)$$

In the above expressions and in what follows, the usual dummy suffixes (Greek letters) are used and the summation should be taken over x, y and z components, and

$$\omega_c = \frac{cH}{mc}. \quad (2.13)$$

The operator $i\mathcal{L}_0$ represents the classical motion of the electron, for which the Maxwell-Boltzmann distribution is a stationary solution, and $i\mathcal{L}_H$ corresponds to the Lorentz force in a magnetic field. The other operators, $i\mathcal{L}_3$ and $i\mathcal{L}_4$, etc., have no such classical meaning and are due to the uncertainty between the momentum and the coordinate, i.e., to the fact that the quantum operators of the momentum and the coordinate do not commute with each other.

In the following discussions, we shall confine ourselves to the first order with respect to the magnetic field, i.e., the weak field limit.

The equilibrium distribution function in the absence of electric field is obtained by solving

$$i\mathcal{L}f_{\text{eq}} = 0. \quad (2.14)$$

Expanding f_{eq} in the power of \hbar , we have the following result to the second power of \hbar ,

$$f_{\text{eq}}(\mathbf{p}, \mathbf{r}) = f_0(\mathbf{p}, \mathbf{r}) + f_2(\mathbf{p}, \mathbf{r}) + f_{2H}(\mathbf{p}, \mathbf{r}) + O(\hbar^4), \quad (2.15)$$

where

$$f_0(\mathbf{p}, \mathbf{r}) = e^{-\beta(p^2/2m + V_I(\mathbf{r}))}, \quad (2.16)$$

$$f_2(\mathbf{p}, \mathbf{r}) = -\frac{\hbar^2 \beta^2}{8m} \left[\frac{\partial^2 V_I}{\partial \mathbf{r}^2} - \frac{\beta}{3} \left(\frac{\partial V_I}{\partial \mathbf{r}} \right)^2 - \frac{\beta}{3m} \frac{\partial^2 V_I}{\partial x_\alpha \partial x_\beta} p_\alpha p_\beta \right] f_0(\mathbf{p}, \mathbf{r}), \quad (2.17)$$

$$f_{2H}(\mathbf{p}, \mathbf{r}) = \frac{\beta^2 \hbar \hbar'}{12m^2} \left[p_y \frac{\partial V_I}{\partial x} - p_x \frac{\partial V_I}{\partial y} \right] f_0(\mathbf{p}, \mathbf{r}) \quad (2.18)$$

and the following abbreviation is employed:

$$\hbar' = \frac{e\hbar}{c} H. \quad (2.19)$$

In the above, f_0 is the well-known Maxwell-Boltzmann distribution, f_1 the lowest-order quantum correction to it in the absence of magnetic field, f_{1H} the additional correction due to the applied magnetic field and related to the Landau diamagnetism.¹⁾

According to the linear response theory, the conductivity tensor of the electron system is expressed as

$$\sigma_{\mu\nu}(z) = \int_0^\infty dt e^{-zt} \phi_{\mu\nu}(t), \quad (2.20)$$

where

$$\phi_{\mu\nu}(t) = -\frac{ne^2}{m} \int d\Gamma \left(\frac{\partial}{\partial p_\nu} f_{eq} \right) e^{-tL_t} p_\mu \Big/ \int d\Gamma f_{eq}. \quad (2.21)$$

Here, the denominator comes from the normalization of the distribution function. The conductivity tensor can be expanded in powers of \hbar as follows:

$$\sigma_{\mu\nu}(z) = \sigma_{\mu\nu}^{(0)}(z) + \sigma_{\mu\nu}^{(2)}(z) + \dots, \quad (2.22)$$

where

$$\sigma_{xx}^{(0)}(z) = -\frac{ne^2}{m} \int d\Gamma \frac{\partial f_0}{\partial p_x} \frac{1}{z+iL_0} p_x \Big/ \int d\Gamma f_0, \quad (2.23)$$

$$\begin{aligned} \sigma_{xx}^{(2)}(z) = & -\frac{ne^2}{m} \int d\Gamma \frac{\partial f_0}{\partial p_x} \frac{1}{z+iL_0} (-iL_2) \frac{1}{z+iL_0} p_x \Big/ \int d\Gamma f_0 \\ & -\frac{ne^2}{m} \int d\Gamma \frac{\partial f_2}{\partial p_x} \frac{1}{z+iL_0} p_x \Big/ \int d\Gamma f_0 \\ & +\frac{ne^2}{m} \int d\Gamma \frac{\partial f_0}{\partial p_x} \frac{1}{z+iL_0} p_x \int d\Gamma f_2 \Big/ \left(\int d\Gamma f_0 \right)^2, \end{aligned} \quad (2.24)$$

$$\sigma_{yx}^{(0)}(z) = -\frac{ne^2}{m} \int d\Gamma \frac{\partial f_0}{\partial p_x} \frac{1}{z+iL_0} (-iL_H) \frac{1}{z+iL_0} p_y \Big/ \int d\Gamma f_0, \quad (2.25)$$

$$\begin{aligned} \sigma_{yx}^{(2)}(z) = & -\frac{ne^2}{m} \int d\Gamma \left(\frac{\partial f_{1H}}{\partial p_x} \right) \frac{1}{z+iL_0} p_y \Big/ \int d\Gamma f_0 \\ & -\frac{ne^2}{m} \int d\Gamma \frac{\partial f_0}{\partial p_x} \frac{1}{z+iL_0} \left\{ (-iL_2) \frac{1}{z+iL_0} (-iL_H) \right. \\ & \left. + (-iL_H) \frac{1}{z+iL_0} (-iL_2) \right\} \frac{1}{z+iL_0} p_y \Big/ \int d\Gamma f_0 \\ & -\frac{ne^2}{m} \int d\Gamma \left(\frac{\partial f_2}{\partial p_x} \right) \frac{1}{z+iL_0} (-iL_H) \frac{1}{z+iL_0} p_y \Big/ \int d\Gamma f_0 \\ & +\frac{ne^2}{m} \int d\Gamma \left(\frac{\partial f_0}{\partial p_x} \right) \frac{1}{z+iL_0} (-iL_H) \frac{1}{z+iL_0} p_y \int d\Gamma f_2 \Big/ \left(\int d\Gamma f_0 \right)^2 \end{aligned} \quad (2.26)$$

and higher-order terms such as $\sigma_{xx}^{(4)}$, $\sigma_{yx}^{(4)}$ and so forth can be written similarly,

but they are too lengthy to be presented here and have been omitted. Up to this point the expansion with respect to \hbar is exact if it is possible.

For the explicit evaluation of the tensor given above, one has to expand each element in the power of the impurity potential and to take an ensemble average over the configurations of the impurities. In the following section, we introduce a graphical method for clearer understanding of the problem.

§ 3. Graphical method

In this section we describe a graphical method to treat the impurity potential, which is included in the equilibrium distribution function, i.e., f_0, f_1, f_{2H} and so on, and in the Liouville operators, $i\mathcal{L}_0, i\mathcal{L}_2$ and so on. In order to take an average over the random configurations, we have to perform a systematic expansion with respect to the impurity potential. We develop here a graphical method which is useful for this purpose.

The definition of the ensemble average over the configurations is described as follows: The impurity potential $V_I(\mathbf{r})$ is transformed into the form of a Fourier integral:*)

$$V_I(\mathbf{r}) = \sum_{i=1}^{N_s} \frac{1}{(2\pi)^3} \int d^3k V_k e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{R}_i)}, \quad (3.1)$$

then the average over the configuration in the thermodynamic limit is expressed as^{5), 6)}

$$\begin{aligned} \left\langle \sum_{i=1}^{N_s} e^{-i\mathbf{k}\cdot\mathbf{R}_i} \right\rangle &= (2\pi)^3 n_s \delta(\mathbf{k}), \\ \left\langle \sum_{i=1}^{N_s} \sum_{j=1}^{N_s} e^{-i\mathbf{k}\cdot\mathbf{R}_i - i\mathbf{k}'\cdot\mathbf{R}_j} \right\rangle &= (2\pi)^3 n_s \delta(\mathbf{k} + \mathbf{k}') + (2\pi)^6 n_s^2 \delta(\mathbf{k}) \delta(\mathbf{k}') \end{aligned} \quad (3.2)$$

and so forth, where n_s is the concentration of the impurities.

For a while, we take $\sigma_{zz}^{(0)}$ as an example. In the expression of $\sigma_{zz}^{(0)}$, Eq. (2.23), the impurity potential is included in $i\mathcal{L}_0$ and f_0 , the latter appearing in both of the numerator and the denominator. Expanding $(z - i\mathcal{L}_0)^{-1}$ in powers of the impurity potential and averaging over the configurations, we have, for example, such diagrams as shown in Figs. 1 (a) to (c) for the fourth power of the potential. We assign n_s and V_k to each cross and to each dotted line, respectively, the latter of which will be called the interaction line. The horizontal line and each point on it (the foot of the interaction line) represent the operators $(z + \mathbf{p}/m \cdot \partial/\partial \mathbf{r})^{-1}$ and $i\mathbf{k} \cdot \partial/\partial \mathbf{p}$ respectively, where the latter corresponds to $\partial V_I/\partial \mathbf{r} \cdot \partial/\partial \mathbf{p}$ in $i\mathcal{L}_0$ and \mathbf{k} is the wave vector of the interaction line. The algebraic sum of the wave vectors of the interaction lines flocking to one cross should be zero, because of the δ -functions appearing on averaging over the impurity con-

*) We may put $V_{\mathbf{k}=0} = 0$ because $V_{\mathbf{k}=0}$ gives only a constant energy shift.

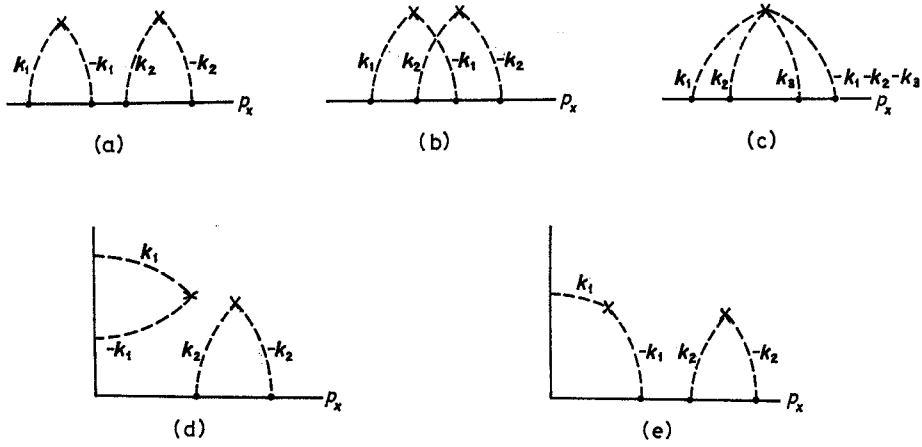


Fig. 1. Typical diagrams for $\sigma_{xx}^{(0)}$. The meanings of the notation are shown in the paragraph.

figures.

The contributions from f_0 in the numerator will be expressed for example as in Figs. 1(d) and (e), where a vertical line is used to distinguish the source of V_k 's. Some numerical factors are needed for the contributions from f_0 , because V_I is included in f_0 as $e^{-\beta V_I}$. However the terms related to f_0 are found to be unnecessary for further manipulations in this paper (see the next section). Therefore we shall not be bothered any more by the contributions from f_0 's in the numerator and denominator.

In order to clarify the correspondence between the diagrams and the explicit expressions, we write the following expressions equivalent to Figs. 1(a) to (e):

$$\begin{aligned}
 \text{(a)} = & \hat{A} \left\{ p_x \frac{1}{z} n_s^2 \int d^3 k_1 \int d^3 k_2 |V_{k_1}|^2 |V_{k_2}|^2 \left(i\mathbf{k}_1 \cdot \frac{\partial}{\partial \mathbf{p}} \right) \right. \\
 & \times \frac{1}{z - i(\mathbf{p} \cdot \mathbf{k}_1/m)} \left(-i\mathbf{k}_1 \cdot \frac{\partial}{\partial \mathbf{p}} \right) \frac{1}{z} \left(i\mathbf{k}_2 \cdot \frac{\partial}{\partial \mathbf{p}} \right) \frac{1}{z - i(\mathbf{p} \cdot \mathbf{k}_2/m)} \\
 & \left. \times \left(-i\mathbf{k}_2 \cdot \frac{\partial}{\partial \mathbf{p}} \right) \frac{1}{z} p_x \right\}, \tag{3.3a}
 \end{aligned}$$

$$\begin{aligned}
 \text{(b)} = & \hat{A} \left\{ p_x \frac{1}{z} n_s^2 \int d^3 k_1 \int d^3 k_2 |V_{k_1}|^2 |V_{k_2}|^2 \left(i\mathbf{k}_1 \cdot \frac{\partial}{\partial \mathbf{p}} \right) \frac{1}{z - i(\mathbf{p} \cdot \mathbf{k}_1/m)} \right. \\
 & \times \left(i\mathbf{k}_2 \cdot \frac{\partial}{\partial \mathbf{p}} \right) \frac{1}{z - i\mathbf{p} \cdot \mathbf{m} \cdot (\mathbf{k}_1 + \mathbf{k}_2)} \left(-i\mathbf{k}_1 \cdot \frac{\partial}{\partial \mathbf{p}} \right) \frac{1}{z - i(\mathbf{p} \cdot \mathbf{k}_2/m)} \\
 & \left. \times \left(-i\mathbf{k}_2 \cdot \frac{\partial}{\partial \mathbf{p}} \right) \frac{1}{z} p_x \right\}, \tag{3.3b}
 \end{aligned}$$

$$\text{(c)} = \hat{A} \left\{ p_x \frac{1}{z} n_s \int d^3 k_1 \int d^3 k_2 \int d^3 k_3 V_{k_1} V_{k_2} V_{k_3} V_{-\mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3} \left(i\mathbf{k}_1 \cdot \frac{\partial}{\partial \mathbf{p}} \right) \right.$$

$$\begin{aligned} & \times \frac{1}{z-i \cdot (\mathbf{p} \cdot \mathbf{k}_1/m)} \left(i\mathbf{k}_2 \cdot \frac{\partial}{\partial \mathbf{p}} \right) \frac{1}{z-i \cdot \mathbf{p}/m \cdot (\mathbf{k}_1 + \mathbf{k}_2)} \left(i\mathbf{k}_3 \cdot \frac{\partial}{\partial \mathbf{p}} \right) \\ & \times \frac{1}{z-i \cdot \mathbf{p}/m \cdot (\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3)} \left(-i(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3) \cdot \frac{\partial}{\partial \mathbf{p}} \right) \frac{1}{z} p_x \Big\}, \end{aligned} \quad (3.3c)$$

$$\begin{aligned} (d) = \hat{A} \Big\{ p_x \frac{(-\beta)^2}{2!} n_s \int d^3 k_1 |V_{\mathbf{k}_1}|^2 \frac{1}{z} n_s \int d^3 k_2 |V_{\mathbf{k}_2}|^2 \left(i\mathbf{k}_3 \cdot \frac{\partial}{\partial \mathbf{p}} \right) \\ \times \frac{1}{z-i \cdot (\mathbf{p} \cdot \mathbf{k}_2/m)} \left(-i\mathbf{k}_2 \cdot \frac{\partial}{\partial \mathbf{p}} \right) \frac{1}{z} p_x \Big\}, \end{aligned} \quad (3.3d)$$

$$\begin{aligned} (e) = \hat{A} \Big\{ p_x \frac{(-\beta)}{1!} n_s \int d^3 k_1 |V_{\mathbf{k}_1}|^2 \frac{1}{z-i \cdot (\mathbf{p} \cdot \mathbf{k}_1/m)} \left(-i\mathbf{k}_1 \cdot \frac{\partial}{\partial \mathbf{p}} \right) \frac{1}{z} \\ \times \left(i\mathbf{k}_2 \cdot \frac{\partial}{\partial \mathbf{p}} \right) \frac{1}{z-i \cdot (\mathbf{p} \cdot \mathbf{k}_2/m)} \left(-i\mathbf{k}_2 \cdot \frac{\partial}{\partial \mathbf{p}} \right) \frac{1}{z} p_x \Big\}, \end{aligned} \quad (3.3e)$$

where the operator \hat{A} is defined by

$$\hat{A} \{ \varphi(\mathbf{p}) \} = \frac{n e^2}{m} \left(\frac{\beta}{2\pi m} \right)^{3/2} \frac{\beta}{m} \int d^3 p e^{-\beta(\mathbf{p}^2/2m)} \varphi(\mathbf{p}) \quad (3.4)$$

and the following relations have been used:

$$\frac{1}{z + \mathbf{p}/m \cdot \partial/\partial \mathbf{r}} B = B \frac{1}{z + \mathbf{p}/m \cdot \partial/\partial \mathbf{r}}, \quad (B; \text{independent of } \mathbf{r}) \quad (3.5)$$

$$e^{i\mathbf{k} \cdot \mathbf{r}} \frac{1}{z + \mathbf{p}/m \cdot \partial/\partial \mathbf{r}} e^{-i\mathbf{k} \cdot \mathbf{r}} = \frac{1}{z - i \cdot (\mathbf{p} \cdot \mathbf{k}/m) + \mathbf{p}/m \cdot \partial/\partial \mathbf{r}} \quad (3.6)$$

and

$$V_{-\mathbf{k}} = V_{\mathbf{k}}^*. \quad (3.7)$$

The last one is due to the fact that the impurity potential $V(\mathbf{r})$ is real.

In calculating other terms, i.e., $\sigma_{yx}^{(0)}$, $\sigma_{xx}^{(2)}$ and so on, we will introduce other diagrammatic notations corresponding to the operators $i\mathcal{L}_B$, $i\mathcal{L}_3$, $i\mathcal{L}_4$ and so on, about which explanations will be given where they are necessary.

If one sums up the contributions from all the possible diagrams, one has exact expressions for the conductivities. However, it seems impossible, therefore in the following sections we employ an approximation and sum selectively certain kind of diagrams.

§ 4. D. C. conductivity in the classical limit

In this section we evaluate $\langle \sigma_{xx}^{(0)}(0) \rangle$, using an approximation which will be valid in the case of a weak impurity potential.

At first, among those diagrams having the same number of crosses which represent n_s , we take a group of diagrams with the least number of impurity

lines. Next we pick up from the group such a diagram as gives the most divergent contribution (in the group) in the limit $z \rightarrow 0$ (the static limit). It will be called "the n -th Born term" where n is the number of the crosses. One easily finds the n -th-order Born term for the d.c. conductivity to be of the form

$$\frac{1}{z} \left(\frac{n_s |V_k|^2}{z} \right)^n \tag{4.1}$$

and that the corresponding diagrams are expressed as in Fig. 2. Those terms including contributions from the equilibrium distribution function f_0 are clearly less divergent than the Born terms in the above-mentioned sense; for example the contributions from Figs. 1(d) and (e) are of the form

$$\left(\frac{n_s |V_k|^2}{z} \right)^2. \tag{4.2}$$

Those diagrams such as Fig. 1(b) are also less divergent; for example Fig. 1(b) contributes as is expressed in (4.2).

The summation of the diagrams depicted in Fig. 2 is formally a Neumann expansion of an reciprocal operator shown in Fig. 3. Therefore, using a differential operator $\hat{O}_0(\mathbf{p}, z)$ defined by Fig. 4 and expressed as

$$\hat{O}_0(\mathbf{p}, z) = n_s \int d^3k |V_k|^2 \left(i\mathbf{k} \cdot \frac{\partial}{\partial \mathbf{p}} \right) \frac{1}{z - i \cdot (\mathbf{p} \cdot \mathbf{k} / m)} \left(-i\mathbf{k} \cdot \frac{\partial}{\partial \mathbf{p}} \right), \tag{4.3}$$

we can write the classical d.c. conductivity in the Born approximation,^{*)} which means to sum up only Born terms, as follows:

$$\langle \sigma_{xx}^{(0)}(0) \rangle = \lim_{\omega \rightarrow 0} \hat{A} \left\{ p_x \frac{1}{z - \hat{O}_0(\mathbf{p}, z)} p_x \right\}, \tag{4.4}$$

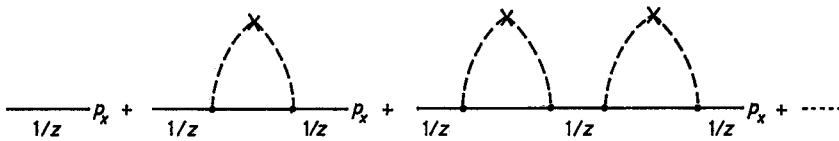


Fig. 2. Summation of "Born terms" for $\sigma_{xx}^{(0)}$.

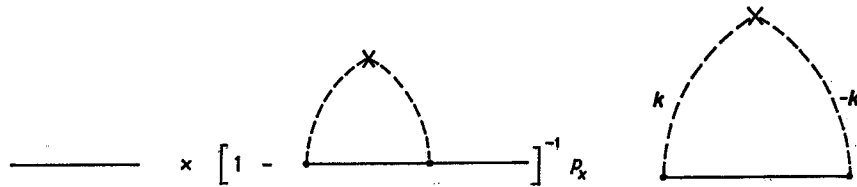


Fig. 3.

Fig. 4.

Fig. 3. Result of the summation shown in Fig. 2.

Fig. 4. The operator $\hat{O}_0(\mathbf{p}, z)$.

^{*)} The result shows that this is equivalent to the usual Born approximation in the quantum theory.

where \hat{A} is defined by Eq. (3.4) and

$$z = i\omega + 0. \quad (4.5)$$

For brevity we restrict ourselves to the case of a spherically symmetric potential in what follows, then in the limit of $\omega \rightarrow 0$, the differential operator $\hat{\mathcal{O}}_0$ takes a very simple form (the details of the calculation are shown in Appendix A) as

$$\hat{\mathcal{O}}_0(\mathbf{p}, \omega \rightarrow 0) = \pi^2 m n_s C_3 \frac{\partial}{\partial p_\alpha} \frac{1}{p} [\alpha, \beta] \frac{\partial}{\partial p_\beta}, \quad (4.6)$$

where we have used the following abbreviations:

$$[\alpha, \beta] = \delta_{\alpha\beta} - \frac{p_\alpha p_\beta}{p^2}, \quad (4.7)$$

$$C_n = \int_0^\infty dk k^n |V_k|^2. \quad (4.8)$$

The integration (4.8) will be finite if there exists k_m such that

$$V_k \begin{cases} = 0 & \text{for } k > k_m \\ \text{or} \\ \sim e^{-(k/k_m)^a} & \text{for } k \rightarrow \infty. \quad (a > 0) \end{cases} \quad (4.9)$$

However if one assumes a screened-Coulomb-type potential for V_k , the integration will be divergent for $n \geq 3$.

Making use of the relation

$$[\hat{\mathcal{O}}_0(\mathbf{p}, \omega \rightarrow 0)]^n p^l p_x = \left(\frac{-2\pi^2 m n_s C_3}{p^3} \right)^n p^l p_x, \quad (l; \text{arbitrary}) \quad (4.10)$$

we have

$$\begin{aligned} \langle \sigma_{xx}^{(0)}(0) \rangle &= \hat{A} \left\{ \frac{p^3 p_x^2}{2\pi^2 m n_s C_3} \right\} \\ &= \frac{ne^2}{m} \frac{32}{\sqrt{2\pi}} \left(\frac{m}{\beta} \right)^{3/2} \frac{1}{2\pi^2 m n_s C_3}, \end{aligned} \quad (4.11)$$

which is of the order of inverse square of the impurity potential. If one adds non-Born terms, one will have higher-order terms with respect to the impurity potential as corrections to the above expressions. When the potential is sufficiently weak, these corrections will be small.

§ 5. On the quantum corrections to the d.c. conductivity

The quantum corrections to the d.c. conductivity are estimated within the Born approximation. It is easily seen that the contributions from f_s belong to

non-Born terms as well as those from f_0 .*) Hence we have only to replace one of the operators, $(i\mathbf{k} \cdot \partial/\partial \mathbf{p})$, on the horizontal line by a quantum-correction operator, e.g., for the second order in \hbar ,

$$-\frac{\hbar^2}{3!2^2} \left(i\mathbf{k} \cdot \frac{\partial}{\partial \mathbf{p}} \right)^3 \tag{5.1}$$

which is derived from $i\mathcal{L}_2$ in Eq. (2.11) and expressed diagrammatically by a circle shown in Fig. 5.

First, we evaluate the second-order term in \hbar , $\langle \sigma_{xx}^{(2)}(0) \rangle$. The diagrams to be summed up within the Born approximation are shown in Fig. 6. Thus we obtain the following expression for $\langle \sigma_{xx}^{(2)}(z) \rangle$:

$$\begin{aligned} \langle \sigma_{xx}^{(2)}(z) \rangle = & \hat{A} \left\{ p_x \frac{1}{z - \hat{\mathcal{O}}_0(\mathbf{p}, z)} \left(-\frac{\hbar^2}{3!2^2} \right) [\hat{\mathcal{O}}_2^{(1)}(\mathbf{p}, z) + \hat{\mathcal{O}}_2^{(2)}(\mathbf{p}, z)] \right. \\ & \left. \times \frac{1}{z - \hat{\mathcal{O}}_0(\mathbf{p}, z)} p_x \right\}, \tag{5.2} \end{aligned}$$

where the differential operators $\hat{\mathcal{O}}_2^{(1)}$ and $\hat{\mathcal{O}}_2^{(2)}$, corresponding to the diagrams in Fig. 7, are expressed as

$$\hat{\mathcal{O}}_2^{(1)}(\mathbf{p}, z) = -n_s \int d^3k |V_k|^2 \left(i\mathbf{k} \cdot \frac{\partial}{\partial \mathbf{p}} \right)^2 \frac{1}{z - i \cdot (\mathbf{p} \cdot \mathbf{k}/m)} \left(-i\mathbf{k} \cdot \frac{\partial}{\partial \mathbf{p}} \right), \tag{5.3}$$

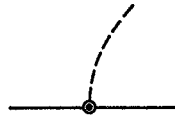


Fig. 5. The second-order quantum correction operator $(\hbar^2/3!2^2) (i\mathbf{k} \cdot \partial/\partial \mathbf{p})^3$.

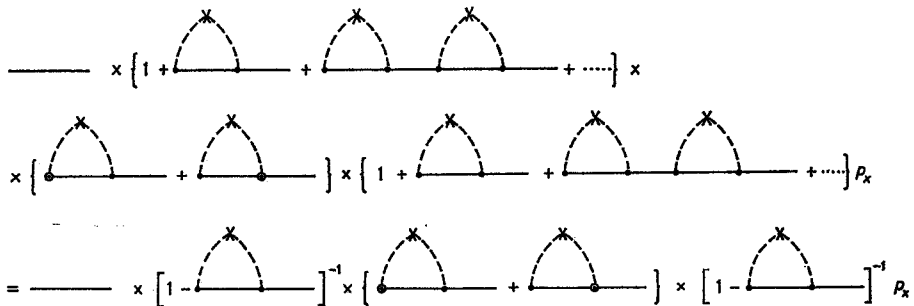


Fig. 6. The second-order quantum correction for the d.c. conductivity in the "Born approximation".

*) When one discusses the effect of f_2 , one must take into account non-Born terms in a consistent manner. By the way, naturally f_{2H} does not contribute to the d.c. conductivity.

$$\hat{\mathcal{O}}_2^{(2)}(\mathbf{p}, z) = -n_s \int d^3k |V_{\mathbf{k}}|^2 \left(i\mathbf{k} \cdot \frac{\partial}{\partial \mathbf{p}} \right) \frac{1}{z - i \cdot (\mathbf{p} \cdot \mathbf{k} / m)} \left(-i\mathbf{k} \cdot \frac{\partial}{\partial \mathbf{p}} \right)^3. \quad (5.4)$$

For the spherically symmetric potential, these operators take simpler forms in the static limit $\omega \rightarrow 0$ as

$$\begin{aligned} \hat{\mathcal{O}}_2^{(1)}(\mathbf{p}, \omega \rightarrow 0) &= \frac{\pi^2 m n_s C_s}{4} \frac{\partial^3}{\partial p_\alpha \partial p_\beta \partial p_\gamma} \frac{1}{p} \left\{ [\alpha, \beta] [\gamma, \xi] + [\alpha, \gamma] [\beta, \xi] \right. \\ &\quad \left. + [\alpha, \xi] [\beta, \gamma] \right\} \frac{\partial}{\partial p_\xi}, \end{aligned} \quad (5.5)$$

$$\begin{aligned} \hat{\mathcal{O}}_2^{(2)}(\mathbf{p}, \omega \rightarrow 0) &= \frac{\pi^2 m n_s C_s}{4} \frac{\partial}{\partial p_\xi} \frac{1}{p} \left\{ [\alpha, \beta] [\gamma, \xi] + [\alpha, \gamma] [\beta, \xi] \right. \\ &\quad \left. + [\alpha, \xi] [\beta, \gamma] \right\} \frac{\partial^3}{\partial p_\alpha \partial p_\beta \partial p_\gamma}, \end{aligned} \quad (5.6)$$

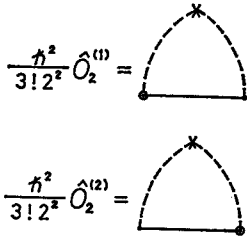


Fig. 7. The operators $\hat{\mathcal{O}}_2^{(1)}$ and $\hat{\mathcal{O}}_2^{(2)}$.

where C_s and $[\alpha, \beta]$ are defined by Eqs. (4.7) and (4.8), respectively. The derivation of these expressions are given in Appendix B.

Using Eq. (4.10) and the following relations:

$$\hat{\mathcal{O}}_2^{(1)}(\mathbf{p}, \omega \rightarrow 0) p^l p_x = 2\pi^2 m n_s C_s l p^{l-5} p_x, \quad (5.7)$$

$$\hat{\mathcal{O}}_2^{(2)}(\mathbf{p}, \omega \rightarrow 0) p^l p_x = -2\pi^2 m n_s C_s l p^{l-5} p_x, \quad (5.8)$$

we find that

$$\langle \sigma_{xx}^{(2)}(0) \rangle = 0, \quad (5.9)$$

if C_s is well-defined.

We continue the calculation to the fourth order in \hbar . The fourth-order operator is

$$\frac{\hbar^4}{5! 2^4} \left(i\mathbf{k} \cdot \frac{\partial}{\partial \mathbf{p}} \right)^5, \quad (5.10)$$

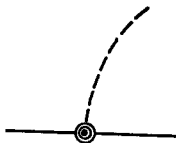


Fig. 8. The fourth-order quantum correction operator $(\hbar^4/5!2^4) (i\mathbf{k} \cdot \partial/\partial \mathbf{p})^5$.

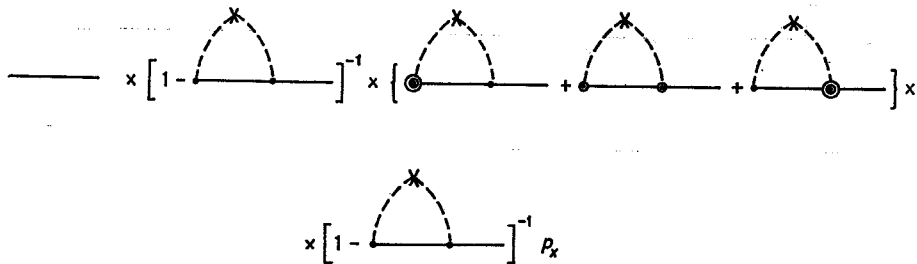


Fig. 9. The fourth-order quantum correction for the d.c. conductivity in the "Born approximation".

which is related to $i\mathcal{L}_4$ shown in Eq. (2.12) and expressed diagrammatically in the form of double circles as depicted in Fig. 8. In the Born approximation we have only to calculate the diagram shown in Fig. 9 and the result is as follows:

$$\langle \sigma_{xx}^{(4)}(z) \rangle = \hat{A} \left\{ p_x \frac{1}{z - \hat{\mathcal{O}}_0(\mathbf{p}, z)} \left[\frac{\hbar^4}{5! 2^4} \hat{\mathcal{O}}_4^{(1)}(\mathbf{p}, z) + \frac{\hbar^4}{3! 3! 2^4} \hat{\mathcal{O}}_4^{(2)}(\mathbf{p}, z) + \frac{\hbar^4}{5! 2^4} \hat{\mathcal{O}}_4^{(3)}(\mathbf{p}, z) \right] \frac{1}{z - \hat{\mathcal{O}}_0(\mathbf{p}, z)} p_x \right\}, \quad (5.11)$$

where the differential operators $\hat{\mathcal{O}}_4^{(1)}$, $\hat{\mathcal{O}}_4^{(2)}$ and $\hat{\mathcal{O}}_4^{(3)}$ are defined in Fig. 10 and take simple forms in the limit of $\omega \rightarrow 0$:*)

$$\frac{\hbar^4}{5! 2^4} \hat{\mathcal{O}}_4^{(1)} = \text{Diagram 1}$$

$$\frac{\hbar^4}{3! 3! 2^4} \hat{\mathcal{O}}_4^{(2)} = \text{Diagram 2}$$

$$\frac{\hbar^4}{5! 2^4} \hat{\mathcal{O}}_4^{(3)} = \text{Diagram 3}$$

Fig. 10. The operators $\hat{\mathcal{O}}_4^{(1)}$, $\hat{\mathcal{O}}_4^{(2)}$ and $\hat{\mathcal{O}}_4^{(3)}$.

$$\hat{\mathcal{O}}_4^{(1)}(\mathbf{p}, \omega \rightarrow 0) = \frac{\pi^2 m n_s C_T}{8} \frac{\partial^5}{\partial p_\alpha \partial p_\beta \partial p_\gamma \partial p_\xi \partial p_\eta} \frac{1}{p} T_{\alpha\beta\gamma\xi\eta\zeta}(\mathbf{p}) \frac{\partial}{\partial p_\zeta}, \quad (5.12)$$

$$\hat{\mathcal{O}}_4^{(2)}(\mathbf{p}, \omega \rightarrow 0) = \frac{\pi^2 m n_s C_T}{8} \frac{\partial^3}{\partial p_\alpha \partial p_\beta \partial p_\gamma} \frac{1}{p} T_{\alpha\beta\gamma\xi\eta\zeta}(\mathbf{p}) \frac{\partial^3}{\partial p_\xi \partial p_\eta \partial p_\zeta}, \quad (5.13)$$

$$\hat{\mathcal{O}}_4^{(3)}(\mathbf{p}, \omega \rightarrow 0) = \frac{\pi^2 m n_s C_T}{8} \frac{\partial}{\partial p_\alpha} \frac{1}{p} T_{\alpha\beta\gamma\xi\eta\zeta}(\mathbf{p}) \frac{\partial^5}{\partial p_\beta \partial p_\gamma \partial p_\xi \partial p_\eta \partial p_\zeta}, \quad (5.14)$$

where the tensor $T_{\alpha\beta\gamma\xi\eta\zeta}(\mathbf{p})$ of the sixth rank is expressed as

$$\begin{aligned} T_{\alpha\beta\gamma\xi\eta\zeta}(\mathbf{p}) = & [\alpha, \beta] [\gamma, \xi] [\eta, \zeta] + [\alpha, \gamma] [\beta, \zeta] [\xi, \eta] \\ & + [\alpha, \xi] [\beta, \eta] [\gamma, \zeta] + [\alpha, \eta] [\beta, \gamma] [\xi, \zeta] \\ & + [\alpha, \zeta] [\beta, \xi] [\gamma, \eta]. \end{aligned} \quad (5.15)$$

*) The derivation of these expressions is similar to that of $\hat{\mathcal{O}}_2^{(1)}$ and $\hat{\mathcal{O}}_2^{(2)}$.

Using these expressions, one may easily prove the following relation:

$$\left. \begin{aligned} \widehat{\mathcal{O}}_4^{(1)}(\mathbf{p}, \omega \rightarrow 0) p^l p_x \\ \widehat{\mathcal{O}}_4^{(2)}(\mathbf{p}, \omega \rightarrow 0) p^l p_x \end{aligned} \right\} = -\frac{5!}{4} \pi^2 m n_s C_7 l(l-2) p^{l-7} p_x, \quad (5.16)$$

$$\widehat{\mathcal{O}}_4^{(3)}(\mathbf{p}, \omega \rightarrow 0) p^l p_x = \frac{3! 3!}{2} \pi^2 m n_s C_7 l(l-2) p^{l-7} p_x, \quad (5.17)$$

which lead to the result that

$$\langle \sigma_{xz}^{(0)}(0) \rangle = 0, \quad (5.18)$$

if C_7 is finite.

§ 6. Hall conductivity

The n -th Born term in the calculation of the Hall conductivity is found to be of the form

$$\frac{1}{z^2} \left(\frac{n_s |V_k|^2}{z} \right)^n. \quad (6.1)$$

Corresponding diagrams for the classical Hall conductivity, $\langle \sigma_{yz}^{(0)}(0) \rangle$, are shown in Fig. 11, where the arrow represents the operator $-i\mathcal{L}_H$ (Eq. (2.10)). As was shown in the d.c. conductivity, the contribution from f_0 are less divergent than the Born terms. Similarly those terms, which have $-i\mathcal{L}_H$ in a manner as shown in Fig. 12, belong to non-Born terms.

From Fig. 11 one easily sees that $\langle \sigma_{yz}^{(0)}(0) \rangle$ is written as

$$\langle \sigma_{yz}^{(0)}(0) \rangle = \lim_{\omega \rightarrow 0} \widehat{A} \left\{ p_x \frac{1}{z - \widehat{\mathcal{O}}_0(\mathbf{p}, z)} (-i\mathcal{L}_H) \frac{1}{z - \widehat{\mathcal{O}}_0(\mathbf{p}, z)} p_y \right\}. \quad (6.2)$$

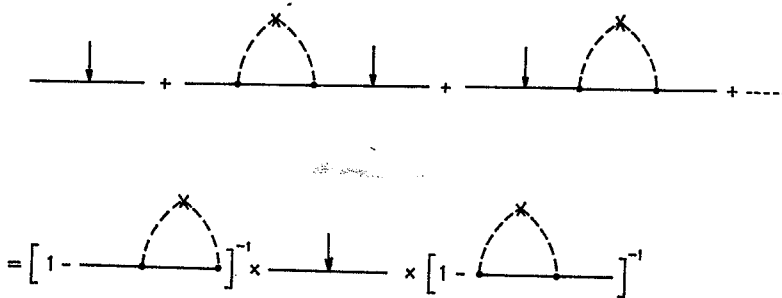


Fig. 11. The classical Hall conductivity in the "Born approximation".

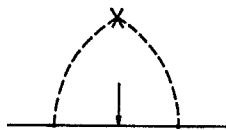


Fig. 12. Characteristic diagram for the Hall conductivity, which is neglected in the "Born approximation".

Exploiting the relations, Eq. (4.10) and

$$-i\mathcal{L}_H p^n p_v = \omega_c p^n p_x, \tag{6.3}$$

we have the following result:

$$\langle \sigma_{yx}^{(0)}(0) \rangle = \frac{ne^3}{m} \left(\frac{m}{\beta} \right)^3 \frac{315}{(2\pi^2 m n_s C_s)^2} \omega_c. \tag{6.4}$$

From Eqs. (4.11) and (6.4), one finds the classical Hall coefficient to be

$$R_H^{(0)} = -\frac{1}{nec} \frac{315\pi}{512} \simeq -\frac{1.9}{nec}. \tag{6.5}$$

Similarly the second- and fourth-order quantum corrections for the Hall conductivity, $\langle \sigma_{yx}^{(2)}(0) \rangle$ and $\langle \sigma_{yx}^{(4)}(0) \rangle$, are calculated from Figs. 13 and 14, respectively. For example, $\langle \sigma_{yx}^{(2)}(0) \rangle$ is expressed as

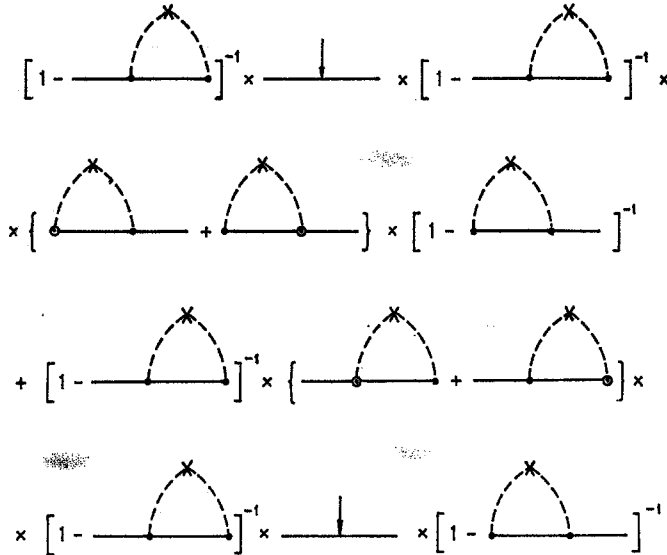


Fig. 13. The second-order quantum correction for the Hall conductivity in the "Born approximation".

$$\begin{aligned} \langle \sigma_{yx}^{(2)}(0) \rangle = & \lim_{\omega \rightarrow 0} \hat{A} \left\{ p_x \frac{1}{z - \hat{\mathcal{O}}_0(\mathbf{p}, z)} \right. \\ & \times \left[(-i\mathcal{L}_H) \frac{1}{z - \hat{\mathcal{O}}_0(\mathbf{p}, z)} \frac{\hbar^2}{3! 2^2} (\hat{\mathcal{O}}_2^{(1)}(\mathbf{p}, z) + \hat{\mathcal{O}}_2^{(2)}(\mathbf{p}, z)) \right. \\ & \left. \left. + \frac{\hbar^2}{3! 2^2} (\hat{\mathcal{O}}_2^{(1)}(\mathbf{p}, z) + \hat{\mathcal{O}}_2^{(2)}(\mathbf{p}, z)) \frac{1}{z - \hat{\mathcal{O}}_0(\mathbf{p}, z)} (-i\mathcal{L}_H) \right] \right. \\ & \left. \times \frac{1}{z - \hat{\mathcal{O}}_0(\mathbf{p}, z)} p_v \right\}, \tag{6.6} \end{aligned}$$

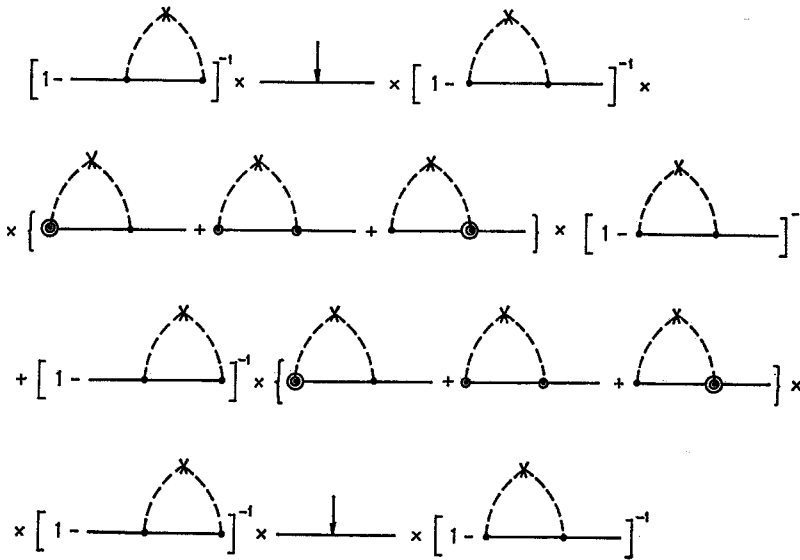


Fig. 14. The fourth-order quantum correction for the Hall conductivity in the "Born approximation".

which is shown to vanish in the same way as $\langle \sigma_{xz}^{(2)}(0) \rangle$. One can prove that $\langle \sigma_{yz}^{(2)}(0) \rangle$ also vanishes similarly.

In the case of the Hall conductivity, we have contributions from f_{2H} and f_2 (see Eq. (2.26)), which, as is easily seen, are at most of the following order:

$$\left(\frac{n_s |V_k|^2}{z}\right)^n, \quad \frac{1}{z} \left(\frac{n_s |V_k|^2}{z}\right)^n, \quad (6.7)$$

respectively, and thus less divergent in the limit of $z \rightarrow 0$ (or more accurately $\omega \rightarrow 0$) than the Born terms (Eq. (6.1)). Therefore they may be disregarded in the Born approximation.

§ 7. Comparison with the kinetic theory

The kinetic theory for the present system is developed by starting with the following Hamiltonian:

$$\mathcal{H} = \sum_{\mathbf{p}} \epsilon_{\mathbf{p}} c_{\mathbf{p}}^{\dagger} c_{\mathbf{p}} + \sum_{\mathbf{p}} \sum_{\mathbf{k}} \sum_{\mathbf{i}} V_{\mathbf{k}} e^{-i\mathbf{k} \cdot \mathbf{R}_{\mathbf{i}}} c_{\mathbf{p}+\hbar\mathbf{k}}^{\dagger} c_{\mathbf{p}}, \quad (7.1)$$

where $c_{\mathbf{p}}, c_{\mathbf{p}}^{\dagger}$ and $\epsilon_{\mathbf{p}}$ are the annihilation and creation operators and the energy of a free electron with a momentum \mathbf{p} , respectively. According to the time-dependent perturbation theory, one has an equation for the evolution of the distribution function $f(\mathbf{p}, t)$ of an electron with a momentum \mathbf{p} ,^{4),5)} such as

$$\frac{\partial}{\partial t} f(\mathbf{p}, t) = -n_s \int d^3k \frac{2\pi}{\hbar} |V_{\mathbf{k}}|^2 \{f(\mathbf{p}, t) [1 - f(\mathbf{p} + \hbar\mathbf{k}, t)]$$

$$-f(\mathbf{p} + \hbar\mathbf{k}, t) [1 - f(\mathbf{p}, t)] \} \delta(\varepsilon_{\mathbf{p} + \hbar\mathbf{k}} - \varepsilon_{\mathbf{p}}), \tag{7.2}$$

where the transition probability is obtained within the usual quantum mechanical Born approximation and averaged over the random configurations of impurities.

The r.h.s. of Eq. (7.2) can be written in the form of a differential operator as follows:

$$\frac{\partial}{\partial t} f(\mathbf{p}, t) = \hat{Q}(\mathbf{p}) f(\mathbf{p}, t), \tag{7.3}$$

$$\hat{Q}(\mathbf{p}) \equiv \frac{4\pi n_i}{\hbar^2} \int d^3k |V_{\mathbf{k}}|^2 e^{\hbar/2 \cdot \mathbf{k} \cdot \partial/\partial \mathbf{p}} \delta\left(\frac{\mathbf{p} \cdot \mathbf{k}}{m}\right) \sinh\left(\frac{\hbar}{2} \mathbf{k} \cdot \frac{\partial}{\partial \mathbf{p}}\right). \tag{7.4}$$

If we expand the expression of the operator $\hat{Q}(\mathbf{p})$ in the power of \hbar , then we obtain the same operators as shown in the previous sections:

$$\begin{aligned} \hat{Q}(\mathbf{p}) = & \hat{\mathcal{O}}_0(\mathbf{p}, \omega \rightarrow 0) \\ & + \frac{\hbar^2}{3! 2^2} [\hat{\mathcal{O}}_2^{(1)}(\mathbf{p}, \omega \rightarrow 0) + \hat{\mathcal{O}}_2^{(2)}(\mathbf{p}, \omega \rightarrow 0)] \\ & + \left(\frac{\hbar}{2}\right)^4 \left[\frac{1}{5!} \hat{\mathcal{O}}_4^{(1)}(\mathbf{p}, \omega \rightarrow 0) + \frac{1}{3! 3!} \hat{\mathcal{O}}_4^{(2)}(\mathbf{p}, \omega \rightarrow 0) \right. \\ & \left. + \frac{1}{5!} \hat{\mathcal{O}}_4^{(3)}(\mathbf{p}, \omega \rightarrow 0) \right] + O(\hbar^6). \end{aligned} \tag{7.5}$$

We have assumed that C_5 and C_7 which are included in $\hat{\mathcal{O}}_2$'s and $\hat{\mathcal{O}}_4$'s respectively are well-defined, i.e., that the \mathbf{k} -integrations giving C_5 and C_7 are convergent. The higher-order terms are also easily seen to be equivalent to those obtained from the Wigner representation method. Hence, if one accomplishes the \mathbf{k} -integral before summing up the power series with respect to \hbar , one will have C_{2n+3} as the coefficient of \hbar^{2n} , and therefore it is necessary that C_{2n+3} 's for $n=0$ to l are well-defined, in order for the expansion of the form as Eq. (7.5) to be possible up to the order of \hbar^{2l} . When the \mathbf{k} -integrations determining C_{2n+3} 's for $n \geq l+1$ are divergent, the summation of the power series for $n \geq l+1$ should be taken before the \mathbf{k} -integration. This situation will be discussed later. Before it, we show that the conductivity calculated from Eqs. (7.3) to (7.5) is equal to the one obtained previously. Using (7.3), we have an expression for the conductivity $\sigma_{xx}(z)$:

$$\sigma_{xx}(z) = -\frac{ne^2}{m} \int d^3p p_x \frac{1}{z - \hat{Q}(\mathbf{p})} \frac{\partial}{\partial p_x} f_{\text{eq}}(\mathbf{p}), \tag{7.6}$$

where f_{eq} is the normalized equilibrium distribution function. We assume f_{eq} to be Maxwellian and expand the resolvent $(z - \hat{Q}(\mathbf{p}))^{-1}$ in the power of \hbar . Then, making use of the relations (4.10), (5.7), (5.8), (5.12), (5.13) and (5.14), we find that the second- and fourth-order terms in \hbar vanish and that the conductivity

is written as

$$\sigma_{xx}(z) = \frac{ne^2}{m} \frac{\beta}{m} \int d^3p \frac{1}{z + (2\pi^2 mn_s/p^3) C_3} p_x^2 f_{eq}(\mathbf{p}) + O(\hbar^6). \quad (7.7)$$

In the limit of $\omega \rightarrow 0$, this expression is the same as that obtained in previous sections.

§ 8. On the validity of the \hbar -expansion

According to Eqs. (7.5) and (7.6), we may say that after summing up terms of all orders in \hbar in the Born approximation, we obtain an expression for the static conductivity:

$$\sigma_{xx}(0) = \frac{ne^2}{m} \frac{\beta}{m} \lim_{\omega \rightarrow 0} \int d^3p p_x \frac{1}{\omega - \hat{Q}(\mathbf{p})} p_x f_{eq}. \quad (8.1)$$

In the case of spherically symmetric potential, the operator $\hat{Q}(\mathbf{p})$ has a desirable property as

$$\hat{Q}(\mathbf{p}) p_\nu \phi(\mathbf{p}) = -\psi(\mathbf{p}) p_\nu \phi(\mathbf{p}), \quad (8.2)$$

where $\nu = x, y$ or z , $\phi(\mathbf{p})$ is an arbitrary function of p ($= |\mathbf{p}|$), and

$$\psi(\mathbf{p}) = \frac{2\pi^2 m}{p^3} \int_0^{2p/\hbar} dk k^3 |V_k|^2. \quad (8.3)$$

Using Eq. (8.2), we can replace the operator $\hat{Q}(\mathbf{p})$ in Eq. (8.1) by $-\psi(\mathbf{p})$. Thus we obtain an expression for the static conductivity:

$$\sigma_{xx}(0) = \frac{ne^2}{m} \frac{\beta}{m} \int d^3p p_x^2 \psi(\mathbf{p})^{-1} f_{eq}. \quad (8.4)$$

Now that the complete form of the static conductivity is given, we can discuss the validity of the \hbar -expansion. In order to clarify the discussion, we shall present here two cases,

1) The case in which the Fourier component of the potential has the following form:

$$V_k = V_0 \frac{\kappa^{2m-3}}{(k^2 + \kappa^2)^m} \quad (8.5)$$

corresponding to

$$\begin{aligned} V(\mathbf{r}) &= \frac{(2\pi)^3}{(2\pi)^{3/2}} \frac{V_0}{\kappa r} \frac{1}{(m-1)!} \left[\frac{d^{m-1}}{dx^{m-1}} \frac{x e^{i\kappa r x}}{(x+i)^m} \right]_{x=t} \\ &\simeq \frac{\pi^2 V_0}{(2\pi)^{3/2} (m-1)!} \left(\frac{\kappa r}{2} \right)^{m-2} e^{-\kappa r}. \quad (r \rightarrow \infty) \end{aligned} \quad (8.6)$$

For $m \geq 2$, C_3 is finite and therefore the classical limit exists. However, because

C_{2n+3} 's for $n \geq 2m - 2$ are infinite, we must sum up all terms of $4(m-1)$ -th and higher order in \hbar before the \mathbf{k} -integration. It is easy to see that if $V_{\mathbf{k}}$ has such a form as Eq. (8.5), $\psi(\mathbf{p})$ has no terms of the order of \hbar^{2n} where $1 \leq n \leq 2m - 3$. This situation is physically clear because the large value of m corresponds to the long-range interaction (see Eq. (8.6)), where the effect of the momentum-coordinate commutation is of higher order.

As a more explicit illustration, we discuss the case of $m = 2$, where we have

$$\psi(\mathbf{p}) = \frac{2\pi^2 m n_s}{p^3} \left\{ \frac{1}{12\kappa^2} - \frac{\kappa^2}{12} \frac{3(2\mathbf{p}/\hbar)^2 + \kappa^2}{[(2\mathbf{p}/\hbar)^2 + \kappa^2]^3} \right\}, \tag{8.7}$$

which can be expanded in powers of \hbar as

$$\psi(\mathbf{p}) = \frac{2\pi^2 m n_s}{p^3} \left\{ \frac{1}{12\kappa^2} - \frac{1}{4} \frac{\hbar^4 \kappa^2}{(2\mathbf{p})^4} + \dots \right\}. \tag{8.8}$$

In this expression, it should be noticed that there is no term of the second order in \hbar . This corresponds to the finiteness of C_5 , while the finite value of the fourth-order term in $\psi(\mathbf{p})$ is related to the divergence of C_7 .

Moreover we must see in more detail the expanded form of $\psi(\mathbf{p})$. The higher-order terms contain higher power of the inverse of \mathbf{p} , which give rise to the divergence of the \mathbf{p} -integration. From Eq. (8.3) we can write as

$$\psi^{-1}(\mathbf{p}) = p^3 g\left(\frac{\hbar}{p}\right). \tag{8.9}$$

Hence the conductivity $\sigma_{xx}(0)$ is expressed as

$$\sigma_{xx}(0) = \frac{ne^2}{m} \frac{\beta}{m} \int d^3 p p_x^2 p^3 g\left(\frac{\hbar}{p}\right) f_{eq}, \tag{8.10}$$

which clearly shows that the contributions higher than \hbar^6 are divergent when \mathbf{p} -integrated separately. Thus those terms higher than \hbar^6 may not be written in the form of the power series. In fact, if we calculate the conductivity without expanding $\psi(\mathbf{p})$ in the power of \hbar in the example treated above (i.e., the case of $m = 2$), we have such a non-analytic contribution as $\hbar^3 \log \hbar$ in addition to the zeroth, fourth- and sixth-order terms in \hbar .

II) The case in which the Fourier component of the potential has the following form:

$$V_{\mathbf{k}} = V_0 e^{-(\mathbf{k}/\kappa)^\alpha} \quad (\alpha > 0) \tag{8.11}$$

corresponding to the potential function as

$$V(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} 8\pi V_0 \frac{\kappa^3}{[1 + (\kappa r)^2]^2}, \quad (\alpha = 1) \tag{8.12}$$

$$V(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} \frac{V_0}{2} (\sqrt{\pi} \kappa)^3 \exp\left[-\frac{1}{4} (\kappa r)^2\right], \quad (\alpha = 2) \text{ etc.} \tag{8.13}$$

In this case, one has finite C 's:

$$C_{2n+3} = V_0^2 \frac{1}{\alpha} 2^{-(1/\alpha)(2n+4)} \kappa^{2n+4} \Gamma\left(\frac{1}{\alpha}(2n+4)\right), \quad (8.14)$$

which will lead to the vanishing of all the terms except for the zeroth order one. However, this does not mean that $\psi(p)$ is independent of \hbar . In order to see it, we calculate $\psi(p)$ using Eq. (8.11) and obtain the following expressions:

$$\psi(p) \begin{cases} = \frac{2\pi^2 m n_s V_0^2 \kappa^4}{p^3} \left\{ 1 - e^{-2p/\hbar\kappa} \left[\left(\frac{2p}{\hbar\kappa}\right)^3 + 3\left(\frac{2p}{\hbar\kappa}\right)^2 + 6\left(\frac{2p}{\hbar\kappa}\right) + 6 \right] \right\}, & (\alpha=1) \\ = \frac{2\pi^2 m n_s V_0^2 \kappa^4}{p^3} \frac{1}{2} \left\{ 1 - e^{-(2p/\hbar\kappa)^2} - \left(\frac{2p}{\hbar\kappa}\right)^2 e^{-(2p/\hbar\kappa)^2} \right\}, & (\alpha=2) \text{ etc.}, \end{cases} \quad (8.15)$$

$$(8.16)$$

which are essentially singular functions of \hbar .

The finiteness of C_{2n+3} 's shown in Eq. (8.14), which might lead to the wrong conclusion that $\psi(p)$ should be independent of \hbar , is related to the following relation:

$$\lim_{\hbar \rightarrow 0} \frac{\partial^n \psi(p)}{\partial \hbar^n} = 0 \quad \text{for } n=1, 2, \dots \quad (8.17)$$

The expansion of the collision operator $\hat{Q}(p)$ in the power of \hbar , which leads to the form $\sim C_{2n+3} \hbar^{2n}$, gives no definite information about the analyticity of $\psi(p)$ as a function of \hbar .

§ 9. Concluding remarks

Using the Wigner representation, we have expanded the d.c. and Hall conductivities of an electron-impurity system in powers of \hbar and shown that the second- and fourth-order terms do not appear within the Born approximation if the expansion is reasonable. Here the Born approximation means that we calculate the conductivities to the lowest order with respect to the impurity-potential strength, and it tends to the quantum mechanical Born approximation when we sum up all order terms in \hbar that are of the same order with respect to the impurity-potential strength (see § 7). One may easily check the validity condition for this approximation by estimating the neglected diagrams such as Figs. 1 (b) to (e) in the classical limit. The order-of-magnitude estimation shows that the following conditions are necessary for the diagrams of the types of Figs. 1 (b) and (c) to be negligible, respectively, compared with the contribution from Fig. 2:

$$\frac{m^2 n_s}{p^4} \int_0^\infty dk k^2 |V_k|^2 \ll 1, \quad (9.1)$$

$$\frac{m}{p^2} \int_0^\infty dk k^2 |V_k| \ll 1. \quad (9.2)$$

One finds that, if these conditions are satisfied, one may also neglect those diagrams of the types of Figs. 1 (d) and (e). Since $p^2/2m \sim k_B T$ in the Boltzmann statistics, the conditions will be satisfied in the low-impurity density limit if the potential is small compared with $k_B T$ and the k -integrations are convergent.

In the case of the screened Coulomb potential, the condition (9.2) cannot be satisfied because of the divergence of the k -integral at the upper limit, which seems to be attributed to the divergence of the potential at the origin. The integral defining C_3 is divergent for the same reason, so the classical limit cannot be discussed within the Born approximation. This difficulty will be avoided in two ways, i.e., by the use of the quantum Born approximation or by the summation of all the diagrams of the type of Fig. 1 (c). The answer to the former case is given by Eq. (8.3), which shows that the divergence of the k -integral at the upper limit is saved by the momentum-coordinate uncertainty, i.e., that, because of the uncertainty, an electron does not feel directly the infinite potential at the positions of impurities. The answer to the latter case has not yet been obtained at present, however we may expect that, if we use the bare Coulomb potential instead of the screened one, we shall have an expression equivalent to Rutherford's formula^{*)} as a result of the summation of all the diagrams of the type of Fig. 1 (c).

The examples used in the previous section can satisfy the conditions (9.1) and (9.2). Examining the validity of the Born approximation in each order of \hbar ,^{**)} one easily sees that the condition for \hbar -expansion to be possible is the sufficient one for the Born approximation to be valid.

As was shown in the previous section, the vanishing of the second- and fourth-order terms does not necessarily mean that the quantum corrections begin from the higher-order term. It includes the case where $\hbar=0$ is the essential singularity, depending upon the explicit form of the impurity potential. However, we may conclude from the examples of the previous section that the quantum corrections are negligible if the coordinate uncertainty corresponding to the momentum p , \hbar/p , is much less than the potential range κ^{-1} . Moreover Eqs. (8.7), (8.15) and (8.16) show that the quantum effect acts to increase the conductivity, at least within the quantum Born approximation.

In the Wigner representation, the expansion in powers of \hbar means that the conductivities are expanded in powers of $\hbar k/p$ before k - and p -integrations. If the coefficients are divergent when integrated, one must sum up the power series with respect to \hbar before the integrations.

When the impurity potential is anisotropic, the quantum corrections of the second- and fourth-order seem not to vanish in the Born approximation even if C_5 and C_7 are well defined. However, it is not known at present how this fact

^{*)} By the way, the equivalence between Rutherford's formula and the quantum Born approximation seems to be accidental.

^{**)} The conditions (9.1) and (9.2) are the ones in the zeroth order of \hbar .

is related to the analyticity of $\psi(\mathbf{p})$. Moreover, in this case, the operator $\widehat{\mathcal{O}}_0(\mathbf{p}, \omega \rightarrow 0)$ does not satisfy such a simple relation as Eq. (4.12), so even the classical limit $\sigma_{xx}^{(0)}$ is difficult to be calculated. The case of an anisotropic potential is now under investigation.

According to Kubo,¹⁾ f_{2H} is a very important term which gives the Landau diamagnetism of conduction electrons. However, we have shown that the contributions of f_{2H} and f_2 to the conductivities are not included in the Born approximation. It is clear from the result of §7 that they are also not included in the quantum Born approximation. Hence, it seems natural that these contributions do not appear in the usual naive theory of the Hall conductivity. If one wants to discuss the contributions f_{2H} and f_2 , one must calculate at the same time the contributions from some diagrams similar to those in Figs. 1 (b) to (e) which are neglected in the Born approximation.

The effect of the Fermi statistics is left for the future work.

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Appendix A

We show the derivation of the expression (4.6).

Defining a tensor of the second rank as

$$I_{\alpha\beta}(\mathbf{p}, \omega) = \int d^3k |V_{\mathbf{k}}|^2 \frac{k_\alpha k_\beta}{z - i \cdot (\mathbf{p} \cdot \mathbf{k}/m)}, \quad (z = i\omega + 0) \quad (\text{A} \cdot 1)$$

we have

$$\widehat{\mathcal{O}}_0(\mathbf{p}, z) = n_s \frac{\partial}{\partial p_\alpha} I_{\alpha\beta}(\mathbf{p}, \omega) \frac{\partial}{\partial p_\beta}. \quad (\text{A} \cdot 2)$$

The tensor $I_{\alpha\beta}(\mathbf{p}, \omega)$ has a symmetry such as

$$I_{\alpha\beta}(\mathbf{p}, \omega) = A(\mathbf{p}, \omega) \delta_{\alpha\beta} + B(\mathbf{p}, \omega) p_\alpha p_\beta. \quad (\text{A} \cdot 3)$$

It is easily seen that

$$A(\mathbf{p}, \omega) = \frac{2\pi n_s^2 \omega}{ip^2} \int_0^\infty dk k^2 |V_{\mathbf{k}}|^2 \\ + \frac{\pi m}{ip} \int_0^\infty dk k^3 |V_{\mathbf{k}}|^2 \left[\left(\frac{m\omega}{pk} \right)^2 - 1 \right] \ln \left| \frac{m\omega - pk}{m\omega + pk} \right|$$

$$+ \frac{\pi^2 m}{p} \int_{m\omega/p}^{\infty} dk k^3 |V_k|^2 \left[1 - \left(\frac{m\omega}{pk} \right)^2 \right] \quad (\text{A} \cdot 4)$$

and a similar expression is obtained for $B(p, \omega)$. In the limit of $\omega \rightarrow 0$, $I_{\alpha\beta}$ becomes

$$I_{\alpha\beta}(p, \omega \rightarrow 0) = \pi^2 m C_s \frac{1}{p} \left(\delta_{\alpha\beta} - \frac{p_\alpha p_\beta}{p^2} \right), \quad (\text{A} \cdot 5)$$

which leads to the expression of the differential operator $\widehat{\mathcal{O}}_0(p, \omega \rightarrow 0)$ shown in Eq. (4.6).

Appendix B

The operators $\widehat{\mathcal{O}}_2^{(1)}(p, \omega \rightarrow 0)$ and $\widehat{\mathcal{O}}_2^{(2)}(p, \omega \rightarrow 0)$.

Using the following tensor of the fourth rank

$$J_{\alpha\beta\tau\xi}(p, \omega) = \int d^3k |V_k|^2 \frac{k_\alpha k_\beta k_\tau k_\xi}{z - i \cdot (p \cdot k/m)}, \quad (\text{B} \cdot 1)$$

one may write

$$\widehat{\mathcal{O}}_2^{(1)}(p, z) = -n_s \frac{\partial^3}{\partial p_\alpha \partial p_\beta \partial p_\tau} J_{\alpha\beta\tau\xi}(p, \omega) \frac{\partial}{\partial p_\xi} \quad (\text{B} \cdot 2)$$

and

$$\widehat{\mathcal{O}}_2^{(2)}(p, z) = -n_s \frac{\partial}{\partial p_\alpha} J_{\alpha\beta\tau\xi}(p, \omega) \frac{\partial^3}{\partial p_\beta \partial p_\tau \partial p_\xi}. \quad (\text{B} \cdot 3)$$

The tensor $J_{\alpha\beta\tau\xi}(p, \omega)$ has a symmetry such as

$$\begin{aligned} J_{\alpha\beta\tau\xi}(p, \omega) = & A(p, \omega) [\delta_{\alpha\beta} \delta_{\tau\xi} + \delta_{\alpha\tau} \delta_{\beta\xi} + \delta_{\alpha\xi} \delta_{\beta\tau}] \\ & + B(p, \omega) [\delta_{\alpha\beta} p_\tau p_\xi + \delta_{\alpha\tau} p_\beta p_\xi + \delta_{\alpha\xi} p_\beta p_\tau \\ & + \delta_{\tau\xi} p_\alpha p_\beta + \delta_{\beta\xi} p_\alpha p_\tau + \delta_{\beta\tau} p_\alpha p_\xi] + C(p, \omega) p_\alpha p_\beta p_\tau p_\xi. \end{aligned} \quad (\text{B} \cdot 4)$$

The explicit forms of $A(p, \omega)$, $B(p, \omega)$ and $C(p, \omega)$ are easily obtained, for example,

$$\begin{aligned} A(p, \omega) = & \frac{\pi^2 m}{4p} \int_{m\omega/p}^{\infty} dk k^5 |V_k|^2 \left[1 - \left(\frac{m\omega}{pk} \right)^2 \right]^2 \\ & - \frac{\pi m}{4pi} \int_0^{\infty} dk k^5 |V_k|^2 \left[1 - \left(\frac{m\omega}{pk} \right)^2 \right]^2 \ln \left| \frac{m\omega - pk}{m\omega + pk} \right| \\ & + \frac{\pi m}{4pi} \int_0^{\infty} dk k^5 |V_k|^2 \left[\frac{10}{3} \left(\frac{m\omega}{pk} \right) - 2 \left(\frac{m\omega}{pk} \right)^3 \right]. \end{aligned} \quad (\text{B} \cdot 5)$$

In the limit of $\omega \rightarrow 0$, we have

$$A(p, \omega \rightarrow 0) = \frac{\pi^2 m}{4p} C_s. \quad (\text{B} \cdot 6)$$

Similarly

$$B(p, \omega \rightarrow 0) = -\frac{\pi^2 m}{4p^3} C_5, \quad (\text{B}\cdot 7)$$

$$C(p, \omega \rightarrow 0) = \frac{\pi^2 m}{4p^5} C_5. \quad (\text{B}\cdot 8)$$

These results lead to a simpler expression for the tensor $J_{\alpha\beta\gamma\xi}(p, \omega \rightarrow 0)$:

$$J_{\alpha\beta\gamma\xi}(p, \omega \rightarrow 0) = \frac{\pi^2 m}{4} C_5 \frac{1}{p} \{ [\alpha, \beta] [\gamma, \xi] + [\alpha, \gamma] [\beta, \xi] + [\alpha, \xi] [\beta, \gamma] \}, \quad (\text{B}\cdot 9)$$

where $[\alpha, \beta]$ is defined by Eq. (4.7). This expression, as well as Eq. (A.5), is obtainable by a rotation in the \mathbf{k} -space, which makes z -axis coincide with the direction of \mathbf{p} .

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