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Proper-Connected-Diagram Expansion of Electrical Conductivity for Electron-Impurity System†

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Abstract

The straightforward expansion of the electric conductivity σ for an electron-impurity system in powers of the impurity density n_s is known to diverge term by term. It is shown that this difficulty which arises from the average potential field of impurities, can be removed by using the expansion in terms of proper connected diagrams. This expansion, however, leads to a complicated dependence of σ on n_s. The analytical behavior of $\sigma(n_s)$ in the neighborhood of $n_s = 0$ is investigated qualitatively with the assumption that the interaction potential between electron and impurity is arbitrarily strong but has a finite range. It is found that this investigation does *not* support the argument recently advanced by several authors that $\sigma(n_s)$ should contain in its asymptotic expansion terms in the combination of n_s and $\ln n_s$. The present theory starts with Kubo's current correlation function formula for σ and proceeds with the aid of connected diagrams. It is developed for a quantum system but also applies for a classical system with few modifications in definitions.

1. *Introduction*

A system of non-interacting electrons in the potential field of impurities, characterized by (2.1), could be thought as a crude approximation to such a system as the system of conduction electrons in a semi-metal at temperatures so low that the interaction between electrons and phonons may be neglected. True, this model system is far from any real system. But, since it is one of the simplest systems which exhibit the approach to equilibrium, it has been used as a testing system when new non-equilibrium theories were developed by many authors, including Van Hove (1955, 1957) and Kohn & Luttinger (1957).

When the convergence of the density expansion of the transport coefficient

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for a more complicated imperfect gas was questioned (Kawasaki & Oppenheim, 1965; Weinstock, 1965; Kritz & Sandri, 1966; Sengers, 1966; Goldman & Frieman, 1967), the investigations of the same question for the simpler electron-impurity system were then undertaken by several authors with several methods of computation (Fixman, 1963; Van Leeuwen & Weijland, 1965; Weinstock, 1965; Kritz & Sandri, 1966; Langer & Neal, 1966; Sengers, 1966; Dorfman & Cohen, 1967; Goldman & Frieman, 1967). Although it is concluded by all that the straightforward expansion in powers of the impurity density n_s for the electrical conductivity σ has the difficulty of term-by-term divergence, the results and the proposed forms of non-power density expansion after the resummation of 'most divergent parts' are not unique. Some authors claimed to have found terms in the combination of n_s and $\ln n_s$ (Fixman, 1963; Van Leeuwen & Weijland, 1965; Langer & Neal, 1966; Murase, 1966) while others did not (Fujita, 1967a). In order to settle this controversy, we have investigated the question in further detail than hitherto attempted. It will be demonstrated in the present paper that the resummed series is unlikely to contain any logarithmic terms for small values of n_s irrespective of whether the system is quantum-mechanical or classical, and irrespective of whether the impurity potential is weak or strong. This result is in agreement with that of the earlier investigation by one of the present authors (S.F.) for the quantum-mechanical, weakly coupled system (Fujita, 1967a).

In deriving this conclusion we use Kubo's current correlation function formula (Kubo, 1957) for σ as the starting point, and the connected-diagram expansion as the analyzing tool. This expansion technique (Fujita, 1967a), developed earlier by one of the present authors (S.F.), enables one to formally expand σ in powers of n_s, the resulting expansion being found term-by-term divergent as mentioned earlier.

The cause of this divergence may be attributed to the effect of the average field of impurities. Since we calculate the current correlation function using the canonical distribution for the electrons and the appropriate distribution for the impurities, any collision process between an electron and a set of impurities should take place in the average field of other impurities. The effect of such a field, irrespective of whether the system is classical or quantum mechanical, will be to induce *perturbed* single-particle energies and *less restricted energy conservation* (collision broadening). These points will be borne out explicitly in our calculation. It is noted that the present interpretation of the cause of the divergence is different from that which is associated with the so-called recollision process and imaginary collision (Dorfman & Cohen, 1967).

The term-by-term divergence in the impurity density expansion can be eliminated by the summation of 'most divergent' parts. This was first explicitly demonstrated by Kawasaki & Oppenheim (1965) with the aid of Zwanzig's method of expansion (Zwanzig, 1963) for the case of a classical imperfect gas. The elimination of the divergence can be performed in a similar manner for the electron-impurity system. When different computational methods are used, the elimination proceeds in different ways. The results after the summation of most divergent parts were shown to be the modification in the energy denominator as seen in, for example, (3.12) of the paper by Kawasaki & Oppenheim (1965) (for the imperfect gas), (4.23) in the paper by Murase (1966) and (3.32) in the work by Fujita (1967a) (the last two for the electron-impurity system).

The discrepancies in the proposed form of the non-power density expansion i.e. the existence or non-existence of terms in the combination of n_s and $\ln n_s$, arise in essence only when the effect of this modification of the denominator on σ is estimated. A number of authors concluded the existence of the logarithmic terms by considering the case of a strong, short-range potential, such as a hard-core potential, and estimating the resulting integral in a qualitative manner (Fixman, 1963; Kawasaki & Oppenheim, 1965; Van Leeuwen & Weijland, 1965; Kritz & Sandri, 1966; Langer & Neal, 1966; Murase, 1966; Sengers, 1966; Dorfman & Cohen, 1967; Goldman & Frieman, 1967). We believe that their estimations of the integral are in error. Since the work by Murase (1966) deals with the same system and proceeds in the almost same manner as the present paper, we discuss the source of the error in this work in detail.

In Section 2, we summarize the method of connected diagrams for the calculation of the current correlation function formula for σ. This σ is expressed in terms of the solution of the transport equation (2.6) (Kohn & Luttinger, 1957; Luttinger & Kohn, 1958). The collision operator g_z and initial correlation operator $(f_z n')^{(c)}$ appearing in this equation are analyzed in Section 3 in terms of proper and improper diagrams. The results (3.2)–(3.4) are, more general than, and closely related to, the damping-theoretical expansion of the resolvent operator $[h_0 + v - z]^{-1}$ by Van Hove (1955, 1957) and others (Janner, 1962; Swenson, 1962; Mori, 1965). When these expressions (3.2)–(3.4) in place of the defining expressions of g_z and $(f_z n')^{(c)}$ in (2.7) were used to calculate σ, the difficulty of the term-by-term divergence of the impurity-density expansion mentioned earlier does not arise any more.

In Section 4 the weak-coupling and low-density approximations to (3.2)–(3.4) for g_z and $(f_z n')^{(c)}$ are described. Using the low-density limit approximation, we calculate in Section 5 the conductivity explicitly, the result being identical with that one would obtain from the Boltzmann-Bloch equation for the short-range strong interaction.

In Section 6 we investigate the behavior of σ in the neighborhood of $n_s = 0$ for the case of weak coupling. In particular we examine the possibility of the (non) existence of logarithmic terms in its impurity density expansion. The same question for the strong coupling is discussed in Section 7, with remarks on the work by Murase.

The collision operator g_z becomes diagonal in $\mathbf{k}$ in the $\mathbf{P} - \mathbf{k}$ representation when the impurity distribution is assumed to be invariant under translation. This is proved in the Appendix.

Throughout the text the units are chosen such that $\hbar = 1$.

2. *Method of Connected Diagram Analysis*†

Let us consider an electron-impurity system characterized by the time-independent Hamiltonian

$$
\begin{aligned}
H &\equiv \sum_j h^{(j)} \\
&\equiv \sum_j h_0^{(j)} + \lambda \sum_{j,\alpha} \tilde{v}_\alpha^{(j)}
\end{aligned}
\tag{2.1}
$$

where $h_0^{(j)}$ stands for the kinetic energy of the jth electron, which may contain the energy due to a constant magnetic field; $\tilde{v}_\alpha^{(j)} \equiv \tilde{v}(\mathbf{r}^{(j)} - \mathbf{R}_\alpha)$ for the potential energy due to the impurity α at $\mathbf{R}_\alpha$; λ is the coupling constant.

When the Hamiltonian is composed of single-particle energies as in (2.1), Kubo's formula (Kubo, 1957) for the electrical conductivity can be expressed in terms of a single-particle trace, denoted by tr, as

$$\sigma_{rs}(\omega) = \int_0^\infty dt \exp(-i\omega t) \lim \Omega^{-1} \frac{\partial}{\partial u_s} \operatorname{tr}\{j_r \exp(-ith)\, n' \exp(ith)\} \tag{2.2}$$

$$n' \equiv [\exp\{\beta(h - \mathbf{j}.\mathbf{u} - \zeta)\} + 1]^{-1} \tag{2.3}$$

where j_r is the r-component of the velocity operator multiplied by the electronic charge $-e$, and $\mathbf{u}$ is a c-number vector; the u_s-derivative is to be evaluated at $\mathbf{u} = 0$, and this convention will be used throughout the text. The identity between (2.2) and the standard formula in terms of current correlation function appearing in the work by Kubo (1957) can be established by simply performing the u-integration.

According to the connected diagram analysis (Fujita, 1967a) the conductivity $\sigma_{rs}(\omega)$ can be calculated alternatively by

$$\sigma_{rs}(\omega) = -i \lim_{a \to 0} \operatorname{tr}\{j_r \psi_s(-\omega + ia)\} \tag{2.4}$$

$$\psi_s(z) \equiv \frac{\partial n_z'}{\partial u_s} \equiv i \int_0^\infty dt \exp(izt) . \frac{\partial n'}{\partial u_s} \tag{2.5}$$

where the operator $\boldsymbol{\psi} \equiv (\psi_x, \psi_y, \psi_z)$ is found to satisfy the **transport equation**

$$(z - \mathscr{h}_0)\, \boldsymbol{\psi}(z) + \frac{\partial n'^{(c)}}{\partial \mathbf{u}} + \left(f_z \frac{\partial n'}{\partial \mathbf{u}}\right)^{(c)} = -g_z \boldsymbol{\psi}(z) \tag{2.6}$$

$$
\begin{aligned}
g_z &\equiv [-\lambda v + \lambda^2 v R_z^{(0)} v - \lambda^3 v R\, v_z^{(0)} . R_z^{(0)} v + \cdots]^{(c)} \\
f_z &\equiv -\lambda v R_z \\
R_z &\equiv [\mathscr{h} - z]^{-1} = R_z^{(0)} - \lambda R_z^{(0)} v R_z^{(0)} + \cdots \\
R_z^{(0)} &\equiv [\mathscr{h}_0 - z]^{-1}
\end{aligned}
\tag{2.7}
$$

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† See Fujita, S. (1967a). *Journal of Physics and Chemistry of Solids*, **28**, 615.

In these expressions, the *Liouville operators* $\mathscr{h}$, $\mathscr{h}_0$, and v, which are denoted by script letters, are defined such that

$$\mathscr{h}n' \equiv [h, n'] \equiv hn' - n'h \tag{2.8}$$

and the superscript (c) means the restriction that the product should contain no free line segments in the diagram language, e.g.

$$\begin{aligned}(vR_z^{(0)}v)^{(c)} \equiv n_s \int d^3R_\alpha \tilde{v}_\alpha R_z^{(0)} \tilde{v}_\alpha \\ + \tfrac{1}{2}n_s^2 \iint d^3R_\alpha d^3R_\beta \tilde{v}_\alpha R_z^{(0)} \tilde{v}_\beta \chi_2(\mathbf{R}_\alpha - \mathbf{R}_\beta)\end{aligned} \tag{2.9}$$

where $\chi_2(\mathbf{R}_\alpha - \mathbf{R}_\beta)$ is the two-impurity correlation function.

3. *Analysis of Collision Operator g_z and Initial Correlations Operator $(f_z n')^{(c)}$*

A connected diagram for g_z consists of potential, and correlation, bonds and non-free particle lines. A particle line is said to be *free* or *non-free* according to whether or not the diagram is broken by cutting it. Typical diagrams are shown in Fig. 1.

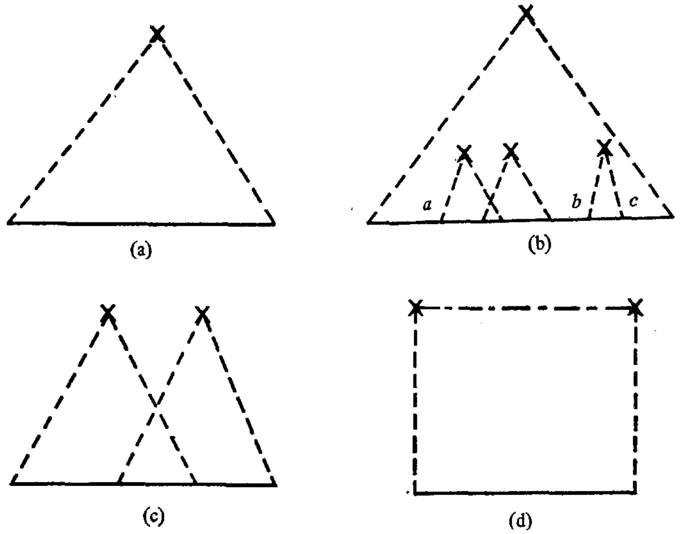

Figure 1.—Examples of connected diagrams for g_z. The improper diagram (b) which contain two inner g-parts can be uniquely reduced to the proper diagram (a). The proper diagram (c) has crossed-over potential bonds. The diagram (d) which contains an impurity correlation bond, corresponds to the second term on the right-hand-side of (2.9).

A diagram will be called an *improper* diagram if it is broken into two by simultaneously cutting two particle line segments. Otherwise, it will be called *proper*. For example, the diagram (a) in Fig. 1 is proper. The diagram

(b) is improper as it is broken into two by cutting either pair of line segments (a,b), (a,c), or (b,c). The part suspended by the pair (a,b) has the same characteristics of connectedness as the original g-part, and such a part will be called an *inner g-part*. An improper diagram can be *reduced* into a simpler one by suppressing an inner g-part with the two adjoining line segments on both sides and replacing a single line segment. When this process of reduction is continued any improper diagram will be eventually reduced to a proper one. This reduction is unique. Thus the improper diagram (b) in Fig. 1 can be reduced uniquely to the proper diagram (a). Conversely improper diagrams can be generated from proper diagrams by decorating or *dressing* the particle-line segments with inner g-parts.

Let us consider a proper diagram. Its contribution will be written as a component of

$$[-\lambda v + \lambda^2 vR_z^{(0)} v - \lambda^3 vR_z^{(0)} vR_z^{(0)} v + \cdots]^{(c,p)} \tag{3.1}$$

where the superscript p denotes the restriction that only the proper diagrams should be retained. Consider now an improper diagram which upon reduction gives rise to the proper diagram. The former can be constructed from the latter by dressing particle-line segments. By construction the sets of impurities involved in the original and in the inner g-parts are distinct from each other. The structures of all conceivable diagrams for an inner g-part are easily seen to be identical with those for the whole set of original g-parts. In the thermodynamic limit the operator for the whole set of inner g-parts will be identified with the operator g_z.

These analyses lead us to write the total contribution to g_z, which can now be obtained by considering all the proper diagrams and their associated improper diagrams, in the following form

$$g_z = [-\lambda v + \lambda^2 v\, dv - \lambda^3 v\, dv\, dv + \cdots]^{(c,p)} \tag{3.2}$$

$$d \equiv [h_0 - z - g_z]^{-1} \tag{3.3}$$

In a similar manner one can analyze the contribution to the operator $(f_z n')^{(c)}$ and obtain

$$(f_z n')^{(c)} = [-\lambda v\, dn' + \lambda^2 v\, dv\, dn' - \cdots]^{(c,p)} \tag{3.4}$$

This regrouping of diagrams is, more general than, and, closely related to, the damping theoretical expansion of the resolvent operator $[h_0 + v - z]^{-1}$ by Van Hove (1955) and others (Janner, 1962; Swenson, 1962; Mori, 1965) [see, for example, Van Hove (1955), equation (3.13)]. In our formulation the regrouping is independent of representation, while their theory intrinsically depends on the representation in which the unperturbed Hamiltonian h_0 is diagonal. The present theory has definite advantages when a system of particles, whose density is not constant, or when a system of charged particles subjected to a constant magnetic field is considered. This point has been explicitly illustrated in our earlier papers (Chen & Fujita, 1967; Fujita, 1967a). In the case where a homogeneous (constant particle-density) system subjected to no magnetic field is treated, our formulation can be *shown* to be identical with the expansion of Van Hove (1955) and others (Janner, 1962; Swenson, 1962; Mori, 1965).

The formulation developed so far does not contain any approximations (except for those which can be justified in the thermodynamic limit).

4. *Weak-Coupling and Low-Density Approximations*

In this section we shall discuss simple situations for which the operators g_z and $(f_z n')^{(c)}$ may be approximated to in terms of proper diagrams appropriately chosen.

(a) *Weak Coupling Approximation*

When the potential between electron and impurity is a small perturbation, we may describe the interaction process by choosing the simplest possible proper connected diagram shown in Fig. 2.

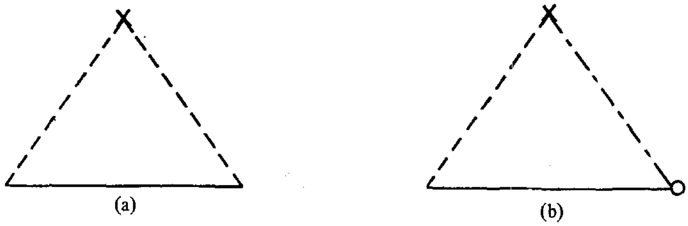

Figure 2.—The proper diagrams (a) and (b) generate the weak-coupling approximations (b, B) to $(g_z, (f_z n^1)^{(c)})$, defined in (4.1)–(4.3).

In this approximation the operators g_z and $(f_z n')^{(c)}$ will be determined by the following equations

$$g_z \to b = [\lambda^2 \, v \, d_b \, v]^{(c,p)} = \lambda^2 \sum_{\alpha} \tilde{v}_\alpha d_b \tilde{v}_\alpha \tag{4.1}$$

$$d_b \equiv [\hbar_0 - z - b]^{-1} \tag{4.2}$$

$$(f_z n')^{(c)} \to B = -[\lambda v \, d_b \, n']^{(c,p)} = -\lambda \sum_{\alpha} \tilde{v}_\alpha d_b n_\alpha' \tag{4.3}$$

where n_α' is the term of the first order in $\tilde{v}_\alpha$ in n'.

(b) *Low-density Approximation*

In the case in which electrons interact strongly with impurities one must consider contributions of arbitrarily high orders in λ. When the density of the impurities is very low, the electron will be occasionally in interaction with one impurity at one time.

As basic proper structures we shall choose only those diagrams for g_z and $(f_z n')^{(c)}$ in which all the potential bonds terminate at the common impurity center, as shown in Fig. 3.

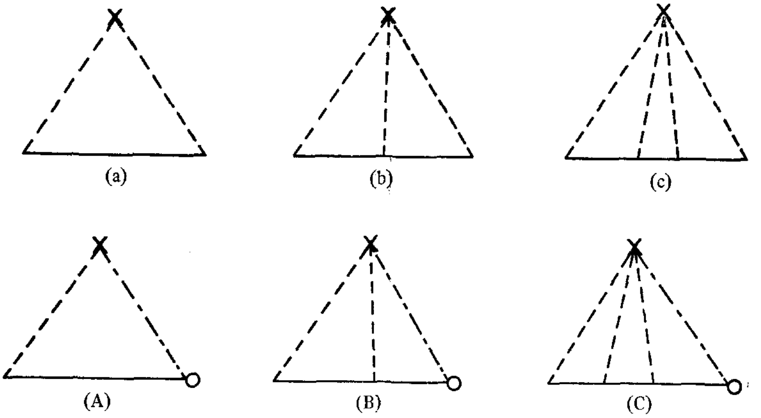

Figure 3.—These proper diagrams generate the low-density approximations (c, C) to $(g_z, (f_z n^1)^{(c)})$, defined in (4.4)–(4.8).

In this approximation the operator g_z and $(f_z n')^{(c)}$ will be given by

$$g_z \rightarrow c \equiv \sum_\alpha c_\alpha \tag{4 4}$$

$$\begin{aligned} c_\alpha &= \lambda^2 \tilde{v}_\alpha d_c \tilde{v}_\alpha - \lambda^3 \tilde{v}_\alpha d_c \tilde{v}_\alpha d_c \tilde{v}_\alpha + \cdots \\ &= \lambda^2 \tilde{v}_\alpha d_c \tilde{v}_\alpha - \lambda \tilde{v}_\alpha d_c c_\alpha \end{aligned} \tag{4.5}$$

$$d_c \equiv [\hbar_0 - z - c]^{-1} \tag{4.6}$$

$$(f_z n')^{(c)} \rightarrow C \equiv \sum_\alpha C_\alpha \tag{4.7}$$

$$\begin{aligned} C_\alpha &= -\lambda \tilde{v}_\alpha d_c n_\alpha' + \lambda^2 \tilde{v}_\alpha d_c \tilde{v}_\alpha d_c n_\alpha' \ldots \\ &= -\lambda \tilde{v}_\alpha d_c n_\alpha' - \lambda \tilde{v}_\alpha d_c C_\alpha \end{aligned} \tag{4.8}$$

The characteristics of approximations (a) and (b) is that those diagrams e.g. the diagram (c) in Fig. 1, in which potential bonds cross over one another, are not enumerated. Both of these approximations (a) and (b) will be useful in the investigation of σ at low impurity densities n_s. From the defining equations (4.1)–(4.3), the operators b and B are seen to be rather complicated functions of n_s and linearly proportional to n_s only for extremely small n_s. Therefore, the conductivity σ calculated by using the approximation (a) will depend on n_s in a complicated manner. The same conclusion may be drawn when the approximation (b) is used instead. The advantage of the use of these approximations over the straightforward expansion of g_z and $(f_z n')^{(c)}$ in (2.7) in powers of n_s lies in that the former does *not* suffer from the difficulty of the term-by-term divergence met in the latter. While there may be other ways of eliminating the divergence, we believe that the treatments by means of the approximation (a) or (b), or more generally the treatments in which approximations are made by choosing appropriate proper connected diagrams in (3.2)–(3.4), have the appeal of *self-consistency*.

5. *Calculation of Collision Term* $c\boldsymbol{\psi}$

In the following discussion we shall confine ourselves to the case in which there is no magnetic field ($\mathbf{B} = 0$) and the applied electric field is independent of time ($\omega = 0$). The momentum representation will be used and z will be set equal to ia with 'a' being an infinitesimal positive number. In the momentum representation the current density operator $\mathbf{j}$ is diagonal and thus (2.4) can be written simply as

$$\sigma = -i\frac{e}{M}\frac{1}{(2\pi)^3}\int d^3 P P_x \boldsymbol{\psi}_x(\mathbf{P}) \tag{5.1}$$

$$\boldsymbol{\psi}(P) \equiv \lim_{a\to 0}\langle\mathbf{P}|\boldsymbol{\psi}_{ia}|\mathbf{P}\rangle \tag{5.2}$$

The diagonal element $\boldsymbol{\psi}(\mathbf{P})$ satisfies the following equation

$$\frac{\partial}{\partial\mathbf{u}}\langle\mathbf{P}|n'|\mathbf{P}\rangle + \langle\mathbf{P}|\left(f_{ia}\frac{\partial n'}{\partial\mathbf{u}}\right)^{(c)}|\mathbf{P}\rangle = -[g_{ia}(\mathbf{P})]_0\,\boldsymbol{\psi}(\mathbf{P}) \tag{5.3}$$

which is obtained by taking the diagonal element of (2.6). In this equation $[g_z(\mathbf{P})]_0$ is defined by

$$\langle\mathbf{P}+\tfrac{1}{2}\mathbf{k}|g_z\boldsymbol{\psi}|\mathbf{P}-\tfrac{1}{2}\mathbf{k}\rangle = \int d^3 k'(\mathbf{k}|g_z(\mathbf{P})|\mathbf{k}')\,\boldsymbol{\psi}_{\mathbf{k}'}(\mathbf{P}) \tag{5.4}$$

$$\boldsymbol{\psi}_{\mathbf{k}'}(\mathbf{P}) \equiv \langle\mathbf{P}+\tfrac{1}{2}\mathbf{k}'|\boldsymbol{\psi}|\mathbf{P}-\tfrac{1}{2}\mathbf{k}'\rangle \tag{5.5}$$

$$(0|g_z(\mathbf{P})|\mathbf{k}) \equiv [g_z(\mathbf{P})]_0\,\delta^{(3)}(\mathbf{k}) \tag{5.6}$$

The matrix element $(\mathbf{k}|c(\mathbf{P})|\mathbf{k}')$, where $c(\mathbf{P})$ is a functional of operators $\hbar_0(\mathbf{P})$ and $v(\mathbf{P})$ can be simply calculated in the $\mathbf{P}-\mathbf{k}$ representation (Fujita, 1966) by expanding $c(\mathbf{P})$ in power series and employing the following rules:

$$(\mathbf{k}|\hbar_1\hbar_2|k') = \int d^3 k''(\mathbf{k}|\hbar_1|\mathbf{k}'')(\mathbf{k}''|\hbar_2|\mathbf{k}') \tag{5.7}$$

$$\begin{gathered}(\mathbf{k}|\hbar(\mathbf{P})|\mathbf{k}') \equiv \eta^{\mathbf{k}'}h_{\mathbf{k}-\mathbf{k}'}(\mathbf{P})\,\eta^{-\mathbf{k}} - \eta^{-\mathbf{k}'}h_{\mathbf{k}-\mathbf{k}'}(\mathbf{P})\,\eta^{\mathbf{k}}\\ (\mathbf{k}|1|\mathbf{k}') \equiv \delta^{(3)}(\mathbf{k}-\mathbf{k}')\end{gathered} \tag{5.8}$$

where $\eta^{\pm\mathbf{k}}$ is the displacement operator acting on a function ϕ of $\mathbf{P}$ such that

$$\eta^{\pm\mathbf{k}}\phi(\mathbf{P}) = \phi(\mathbf{P}\pm\tfrac{1}{2}\mathbf{k})\,\eta^{\pm\mathbf{k}} \tag{5.9}$$

The explicit forms of matrix elements $(\mathbf{k}|\hbar_0(\mathbf{P})|\mathbf{k}')$ and $(\mathbf{k}|v(\mathbf{P})|\mathbf{k}')$ are derived, for example, by Fujita [1966, equation (5.7.13)]

$$\begin{gathered}(\mathbf{k}|\hbar_0(\mathbf{P})|\mathbf{k}') = M^{-1}\,\mathbf{P}.\mathbf{k}\,\delta^{(3)}(\mathbf{k}-\mathbf{k}')\\ (\mathbf{k}|v(\mathbf{P})|\mathbf{k}') = \sum_{\alpha}\tilde{v}_{\alpha}(\mathbf{k}-\mathbf{k}')(\eta^{\mathbf{k}'-\mathbf{k}} - \eta^{-\mathbf{k}'+\mathbf{k}})\end{gathered} \tag{5.10}$$

The property that $g_z(\mathbf{P})$ is diagonal in $\mathbf{k}$ arises from the definition of connected g-part and the assumption of translation-invariant distribution of impurities. This property is proved in the Appendix.

From the defining expression (4.4), the operator c is proportional to the impurity density n_s in the vicinity of $n_s = 0$. Therefore for very small n_s, the operator d_c may be approximated to by $R_z^{(0)}$:

$$d_c \to R_z^{(0)} \equiv [\hbar_0 - z]^{-1} \tag{5.11}$$

and c_α will be approximated to by $c_\alpha^{(0)}$

$$\begin{aligned} c_\alpha \to c_\alpha^{(0)} &\equiv \lambda^2 \tilde{v}_\alpha R_z^{(0)} \tilde{v}_\alpha - \lambda^3 \tilde{v}_\alpha R_z^{(0)} \tilde{v}_\alpha R_z^{(0)} \tilde{v}_\alpha + \cdots \\ &= \lambda^2 \tilde{v}_\alpha R_z^{(0)} \tilde{v}_\alpha - \lambda \tilde{v}_\alpha R_z^{(0)} c_\alpha^{(0)} \end{aligned} \tag{5.12}$$

The interaction process which will be described by $c^{(0)} \equiv \sum_\alpha c_\alpha^{(0)}$ is clearly a one-impurity process.

For short-range forces the term $[c^{(0)}(\mathbf{P})]_0 \psi(\mathbf{P})$, which is the low-density limit approximation to the term on the r.h.s. (right-hand side) of (5.3), can be evaluated as follows (Fujita, 1967b).

Let us consider the following simple situation. At the initial time $t = 0$ non-interacting particles are distributed uniformly in space and a fixed scattering center with the potential $\tilde{v}$ of short range r_0 is located at the origin $\mathbf{r} = 0$. Because of this potential the momentum distribution function $n(\mathbf{P}, t)$, whose initial condition is given arbitrarily, will change with time t. By elementary considerations, the changing part in n for $t \gg \tau_d$ (duration of scattering) $\approx r_0/(PM^{-1})$ will be given by

$$n(\mathbf{P}, t) - n(\mathbf{P}, 0) = t \iint d\phi\, d\theta \sin\theta \frac{P}{M} I(\mathbf{P}, \theta)\, [n(\mathbf{P}', 0) - n(\mathbf{P}, 0)], \quad t \gg \tau_d \tag{5.13}$$

where $I(P, \theta)$ is the differential cross section for the elastic scattering $(\mathbf{P} \to \mathbf{P}')$; θ and ϕ are respectively the scattering and azimuthal angles. Such increments could be made to occur uniformly in space if scattering centers were distributed uniformly throughout the space. In this case, the term on the r.h.s. of (5.13) should be multiplied by the impurity density n_s, thus obtaining

$$n(\mathbf{P}, t) - n(\mathbf{P}, 0) = t\Gamma n(\mathbf{P}, 0) \tag{5.14}$$

$$\Gamma n(\mathbf{P}, 0) \equiv n_s \iint d\phi\, d\theta \sin\theta \frac{P}{M} I(P, \theta)\, [n(\mathbf{P}', 0) - n(\mathbf{P}, 0)], \qquad t \gg \tau_d \tag{5.15}$$

On the other hand, the formal solution to the Liouville equation

$$i\frac{\partial n}{\partial t} = (\hbar_0 + \lambda v)\, n \tag{5.16}$$

for the present system is given by

$$n(\mathbf{P}, t) = [\exp\{-it(\hbar_0 + \lambda v)\}]_0\, n(\mathbf{P}, 0) \tag{5.17}$$

$$(0|\exp[-it(\hbar_0 + \lambda v)]|\mathbf{k}) \equiv \delta^{(3)}(\mathbf{k})\, [\exp\{-it(\hbar_0 + \lambda v)\}]_0 \tag{5.18}$$

The asymptotic behavior of $n(\mathbf{P}, t)$ can be simply handled in the Laplace space. The Laplace transform of $n(t)$ is defined by

$$n_z(\mathbf{P}) \equiv i \int_0^\infty dt \exp(izt)\, n(\mathbf{P}, t) \tag{5.19}$$

By taking the Laplace transform of (5.14) one obtains

$$n_z(\mathbf{P}) + \frac{n(\mathbf{P}, 0)}{z} = -i\frac{\Gamma}{z^2} n(\mathbf{P}, 0) \tag{5.20}$$

This equation implies that $-i\Gamma n$ is precisely given by the coefficient of z^{-2} in the Laurent expansion of n_z.

The Laplace transform of (5.17) yields

$$n_z(\mathbf{P}) = \left[\frac{1}{\hbar_0 + \lambda v - z}\right]_0 n(\mathbf{P}, 0) = [R_z]_0\, n(\mathbf{P}, 0) \tag{5.21}$$

By expanding R_z in powers of λ as in (2.7), and noticing that

$$(0|\hbar_0(\mathbf{P})|\mathbf{k}) = \delta^{(3)}(\mathbf{k})\, M^{-1}\, \mathbf{P}\,.\,\mathbf{k} = 0 \tag{5.22}$$

we obtain

$$[R_z]_0\, n(\mathbf{P}, 0) = \left\{-\frac{1}{z} + \frac{1}{z^2}[-\lambda v + \lambda^2\, v R_z^{(0)}\, v - \lambda^3\, v R_z^{(0)}\, v R_z^{(0)}\, v + \cdots]_0\right\} n(\mathbf{P}, 0)$$

$$\equiv -\frac{1}{z} n(\mathbf{P}, 0) + \frac{1}{z^2}[c_z^{(0)}]_0\, n(\mathbf{P}, 0) \tag{5.23}$$

By assuming that $[c_z^{(0)}]_0 n(\mathbf{P}, 0)$ is analytic in the neighborhood of the origin $z = 0$, we thus find

$$[c_{ia}^{(0)}]_0\, n(\mathbf{P}, 0) = -i\Gamma n(\mathbf{P}, 0) \tag{5.24}$$

In (5.3) the second term on the l.h.s. (left-hand side) is proportional to at least the first power of the impurity density n_s and can be neglected in comparison with the first term in the low-density limit. In this limit the latter is given by

$$\frac{\partial}{\partial u_x}\langle\mathbf{P}|n'|\mathbf{P}\rangle = \frac{e}{M} P_x \frac{df}{d\varepsilon_{\mathbf{P}}} \tag{5.25}$$

$$f(\varepsilon_{\mathbf{P}}) \equiv [\exp\{\beta(\varepsilon_{\mathbf{P}} - \zeta)\} + 1]^{-1} \tag{5.26}$$

where ζ is the Fermi energy.

From (5.3), (5.12), (5.24), and (5.25), one obtains

$$\frac{e}{M} P_x \frac{df}{d\varepsilon_{\mathbf{P}}} = -i\Gamma\psi_x(\mathbf{P}) \tag{5.27}$$

From the symmetry consideration, the solution $\psi_x(\mathbf{P})$ to the transport equation (5.27) is expected to be of the form

$$\psi_x(\mathbf{P}) = P_x \phi(|\mathbf{P}|) \tag{5.28}$$

Then, by considering the angular integration with the choice of the x-direction as the polar axis, one can show that

$$\begin{aligned} \Gamma\psi_x(\mathbf{P}) &= n_s(P/M) \iint d\phi\, d\theta \sin\theta I(P,\theta)\,[P_x' \phi(\varepsilon_{\mathbf{P}}) - P_x \phi(\varepsilon_{\mathbf{P}})] \\ &= -\tau_f^{-1}(\mathbf{P})\, P_x \phi(\varepsilon_{\mathbf{P}}) = -\tau_f^{-1}(\mathbf{P})\, \psi_x(\mathbf{P}) \end{aligned} \tag{5.29}$$

$$\tau_f^{-1}(\mathbf{P}) \equiv (2\pi)^3 n_s(P/M) \iint d\phi\, d\theta \sin\theta I(P,\theta)\,(1-\cos\theta) \geqq 0 \tag{5.30}$$

From (5.27) and (5.29) one obtains

$$\psi_x(\mathbf{P}) = -i\tau(\mathbf{P}) \frac{e}{M} P_x \frac{df}{d\varepsilon_{\mathbf{P}}} \tag{5.31}$$

By substituting this expression for $\psi_x(\mathbf{P})$ into (5.1) one finds for the conductivity σ:

$$\sigma = -\frac{(e)^2}{M} \frac{1}{(2\pi)^3} \int d^3P P_x^2 \tau(\mathbf{P}) \frac{df}{d\varepsilon_{\mathbf{P}}} \tag{5.32}$$

This is a familiar result in agreement with the traditional Boltzmann-Bloch treatment of the electrical conductivity for the electron-impurity system.

It is noted that the calculation of σ in classical mechanics proceeds in much the same way. The starting formulas (5.1)–(5.3) retain the same form except that $\langle \mathbf{P}|\psi_z|\mathbf{P}\rangle$ and $\langle \mathbf{P}|n'|\mathbf{P}\rangle$ are now to be redefined as classical momentum distribution functions, and the Liouville operators in $\mathbf{P}-\mathbf{k}$ representation are replaced with the corresponding classical Liouville operators in wave-vector representation:

$$h \equiv h_0 + \lambda v \tag{5.33}$$

$$\begin{aligned} (\mathbf{k}|h_0(\mathbf{P})|\mathbf{k}') &= M^{-1}\, \mathbf{P}.\mathbf{k}\, \delta^{(3)}(\mathbf{k}-\mathbf{k}') \\ (\mathbf{k}|v(\mathbf{P})|\mathbf{k}') &= -v(\mathbf{k}-\mathbf{k}')\,(\mathbf{k}-\mathbf{k}')\cdot\frac{\partial}{\partial \mathbf{P}} \end{aligned} \tag{5.34}$$

The relations (5.15) and (5.24), where the differential cross section $I(\mathbf{P},\theta)$ must now be calculated classical mechanically, can be established with the identical argument. The use of these relations and the consideration of the classical statistics yields for σ the expression identical in form with (5.32), where $f(\mathbf{P})$ is now replaced with the Boltzmann distribution function $f(\mathbf{P}) = \exp[-\beta(\varepsilon_{\mathbf{P}} - \zeta)]$.

6. *Non-Power Impurity-Density Expansion. Case of Weak Coupling*

In this section we shall investigate the behavior of the conductivity σ in the neighborhood of $n_s = 0$ for the weak coupling case. In particular we examine the possibility of the existence of logarithmic terms in its impurity density expansion.

As we discussed in Section 4, the collision operator g_z will be then approximated to by b. In the $\mathbf{P}-\mathbf{k}$ representation the integral equation (4.1) satisfied by b is written as

$$\begin{aligned}(0|b|\mathbf{k}') &= \lambda^2 \sum_{\alpha} \iint d^3k_1\, d^3k_2 (0|\tilde{v}_\alpha|\mathbf{k}_1)(\mathbf{k}_1|d_b|\mathbf{k}_2)(\mathbf{k}_2|\tilde{v}_\alpha|\mathbf{k}') \\ &= (2\pi)^3 n_s \lambda^2 \int d^3k |\tilde{v}(\mathbf{k})|^2 (\eta^{\mathbf{k}} - \eta^{-\mathbf{k}})\{M^{-1}\mathbf{P}.\mathbf{k} \\ &\qquad - [b(\mathbf{P})]_{\mathbf{k}} - ia\}^{-1} (\eta^{-\mathbf{k}} - \eta^{\mathbf{k}})\, \delta^{(3)}(\mathbf{k}') \\ &\equiv [b(\mathbf{P})]_0\, \delta^{(3)}(\mathbf{k}') \end{aligned} \tag{6.1}$$

$$(\mathbf{k}|b|\mathbf{k}') \equiv [b(\mathbf{P})]_{\mathbf{k}}\, \delta^{(3)}(\mathbf{k}-\mathbf{k}') \tag{6.2}$$

where the diagonal property of the collision operator is used. See (A.1) in Appendix.

Applying the operator $[b(\mathbf{P})]_0$ on $\boldsymbol{\psi}(\mathbf{P})$ one obtains

$$\begin{aligned}[b(\mathbf{P})]_0\, \boldsymbol{\psi}(\mathbf{P}) = (2\pi)^3 n_s \lambda^2 \int d^3k |\tilde{v}(\mathbf{k})|^2 \{&(\varepsilon_{\mathbf{P}+\mathbf{k}} - \varepsilon_{\mathbf{P}} - [b(\mathbf{P}+\tfrac{1}{2}\mathbf{k})]_{\mathbf{k}} - ia)^{-1} \\ &- (\varepsilon_{\mathbf{P}+\mathbf{k}} - \varepsilon_{\mathbf{P}} + [b(\mathbf{P}+\tfrac{1}{2}\mathbf{k})]_{-\mathbf{k}} + ia)^{-1}\} \times \\ &\times [\boldsymbol{\psi}(\mathbf{P}) - \boldsymbol{\psi}(\mathbf{P}+\mathbf{k})] \end{aligned} \tag{6.3}$$

For very small values of n_s, b is linearly proportional to n_s. If the b-terms in the energy denominators are neglected, the collision term $[b(P)]_0\, \boldsymbol{\psi}_x(\mathbf{P})$ is given by

$$\begin{aligned}[b(\mathbf{P})]_0\, \boldsymbol{\psi}_x(\mathbf{P}) &\to [b^{(0)}(\mathbf{P})]_0\, \boldsymbol{\psi}_x(\mathbf{P}) \\ &= (2\pi)^3 n_s \lambda^2 \int d^3k |\tilde{v}(\mathbf{k})|^2 (2\pi i)\, \delta(\varepsilon_{\mathbf{P}+\mathbf{k}} - \varepsilon_{\mathbf{P}}) \times \\ &\qquad \times [\psi_x(\mathbf{P}) - \psi_x(\mathbf{P}+\mathbf{k})] \end{aligned} \tag{6.4}$$

According to the analysis in Section 5, the last expression can be written as

$$[b^{(0)}(\mathbf{P})]_0\, \psi_x(\mathbf{P}) = i\tau_f^{-1}(\mathbf{P})\, \psi_x(\mathbf{P}) \equiv i\omega_f^{(0)}\, \psi_x(\mathbf{P}) \tag{6.5}$$

where the collision frequency $\omega_f^{(0)}$ is given in the form of (5.30) with the cross-section $I(\mathbf{P},\theta)$ being evaluated to the second order in λ.

For small values of k, the self-consistent field correction $[b(\mathbf{P}+\frac{1}{2}\mathbf{k})]_{\pm\mathbf{k}}$ to the energy denominator will have the behavior of the form

$$[b(\mathbf{P}+\tfrac{1}{2}\mathbf{k})]_{\pm\mathbf{k}} = [b(\mathbf{P})]_0 + \Delta b_{\pm} \tag{6.6}$$

where $\Delta b^{\pm}$ are known to vanish as $k \to 0$ [see (6.13) and (6.14)].

For very small n_s, (6.6) may be approximated by

$$[b(\mathbf{P}+\tfrac{1}{2}\mathbf{k})]_{\pm\mathbf{k}} \approx [b^{(0)}(\mathbf{P})]_0 + \Delta b_{\pm}^{(0)} \tag{6.7}$$

where both terms on the r.g.s. are linear in n_s. Substituting (6.7) into (6.3), one obtains

$$[b(\mathbf{P})]_0 \psi_x(\mathbf{P}) = (2\pi)^3 n_s \lambda^2 \int d^3k |\tilde{v}(\mathbf{k})|^2 \{(\varepsilon_{\mathbf{P+k}} - \varepsilon_{\mathbf{P}} - [b^{(0)}(\mathbf{P})]_0 - \Delta b_+^{(0)})^{-1} \\ - (\varepsilon_{\mathbf{P+k}} - \varepsilon_{\mathbf{P}} + [b^{(0)}(\mathbf{P})]_0 + \Delta b_-^{(0)})^{-1}\} \times \\ \times [\psi_x(\mathbf{P}) - \psi_x(\mathbf{P+k})] \tag{6.8}$$

By using this form of collision term we may calculate the conductivity σ through (5.1) and (5.3). The calculation equivalent to this was explicitly carried out in the previous paper (Fujita, 1967a). It is found there that within this approximation no logarithmic terms arise in the impurity density expansion of σ.

In order to further investigate the possibility of the existence of logarithmic terms, we shall adopt (6.6) in place of its low-density limit approximation (6.7). Substitution of (6.6) into (6.3) yields

$$[b(\mathbf{P})]_0 \psi_x(\mathbf{P}) = (2\pi)^3 n_s \lambda^2 \int d^3k |\tilde{v}(\mathbf{k})|^2 \{(\varepsilon_{\mathbf{P+k}} - \varepsilon_{\mathbf{P}} - [b(\mathbf{P})]_0 - \Delta b_+)^{-1} \\ - (\varepsilon_{\mathbf{P+k}} - \varepsilon_{\mathbf{P}} + [b(\mathbf{P})]_0 + \Delta b_-)^{-1}\} \times \\ \times [\psi_x(\mathbf{P}) - \psi_x(\mathbf{P+k})] \tag{6.9}$$

For small n_s, the term on the l.h.s. may be approximated to by

$$[b(\mathbf{P})]_0 \psi_x(\mathbf{P}) = i\omega_f \psi_x(\mathbf{P}) \tag{6.10}$$

$$\omega_f \to \omega_f^{(0)} \equiv \tau_f^{-1} \qquad \text{as} \qquad n_s \to 0 \tag{6.11}$$

Since both ω_f and $\psi_x(\mathbf{P})$ are real numbers (6.10) implies that $[b(\mathbf{P})]_0 \psi_x(\mathbf{P})$ should be a pure imaginary number. This can be seen as follows: $vn' = vn' - n'v$ (n' a density operator). Taking Hermitian adjoints, one obtains $(vn')^\dagger = -vn'$. Similarly $(\hbar_0 n')^\dagger = -\hbar_0 n'$. Therefore $\{[v(\hbar_0 - ia)^{-1} v]^{(c)} n'\}^\dagger = -[v(\hbar_0 - ia)^{-1} v]^{(c)} n'$. More generally, $(g_{ia} n')^\dagger = -g_{ia} n'$. This means that the diagonal elements of $g_{ia} n'$ are pure imaginary numbers.

In the same approximation the operators $[b(\mathbf{P})]_0$ and $\Delta b^\pm$ in the energy denominator will be replaced by numbers $i\omega_f$ and $\Delta\varepsilon^\pm$ respectively, where $\Delta\varepsilon^\pm$ are proportional to n_s at least linearly and tend to zero as $k \to 0$. The use of this approximation in (6.9) yields the following integral equation for ω_f:

$$i\omega_f = (2\pi)^3 n_s \lambda^2 \int d^3k |\tilde{v}(\mathbf{k})|^2 \{(\varepsilon_{\mathbf{P+k}} - \varepsilon_{\mathbf{P}} - \Delta\varepsilon_+ - i\omega_f)^{-1} \\ - (\varepsilon_{\mathbf{P+k}} - \varepsilon_{\mathbf{P}} + \Delta\varepsilon_- + i\omega_f)^{-1}\} \tag{6.12}$$

According to the previous analysis (Fujita, 1967a), the energy corrections $\Delta\varepsilon^\pm$ are given, to the first order in n_s, by

$$\Delta\varepsilon_+ = \Delta\varepsilon_{\mathbf{P+k}} - \Delta\varepsilon_{\mathbf{P}} = -\Delta\varepsilon \tag{6.13}$$

$$\Delta\varepsilon_{\mathbf{P}} \equiv (2\pi)^3 n_s \lambda^2 \int d^3k\,|\tilde{v}(\mathbf{k})|^2\, \mathscr{P}\frac{1}{\varepsilon_{\mathbf{P}+\mathbf{k}} - \varepsilon_{\mathbf{P}}} \tag{6.14}$$

where the symbol $\mathscr{P}$ means that Cauchy's principal value should be taken upon the integration across the pole. Using this approximation one obtains from (6.12)

$$\omega_f = 2(2\pi)^3 n_s \lambda^2 \int d^3k\,|\tilde{v}(\mathbf{k})|^2 \frac{\omega_f}{(\varepsilon'_{\mathbf{P}+\mathbf{k}} - \varepsilon_{\mathbf{P}}')^2 + \omega_f^{\,2}} \tag{6.15}$$

$$\varepsilon_{\mathbf{P}}' \equiv \varepsilon_{\mathbf{P}} + \Delta\varepsilon_{\mathbf{P}} \tag{6.16}$$

In this equation ω_f and $\varepsilon_{\mathbf{P}}'$ may be referred to respectively as the *renormalized* collision frequency and the *perturbed* single-particle energy corresponding to the momentum **P** of the electron.

Let us now examine the low-density behavior of ω_f. As $\mathbf{k} \to 0$,

$$E \equiv \varepsilon'_{\mathbf{P}+\mathbf{k}} - \varepsilon_{\mathbf{P}}' \to 0 \tag{6.17}$$

and $\omega_f \to \omega_f^{(0)}$. Since the collision frequency ω_f is proportional to n_s for small n_s, we may introduce x such that

$$\omega_f \equiv n_s x(n_s) \tag{6.18}$$

When the integration variable **k** is changed to E (and angular variables), the important values of the integrand will be roughly between $-\omega_d$ and ω_d because of the short-range nature of the potential, where ω_d is the inverse of the average duration of collision τ_d. In view of these considerations we may roughly estimate the integral in (6.15) by

$$n_s x = \omega_1 \int_{-\omega_d}^{\omega_d} dE \frac{n_s x}{E^2 + (n_s x)^2}$$

$$= 2\omega_1 \tan^{-1}\frac{\omega_d}{n_s x} \tag{6.19}$$

where the quantity ω_1 of the dimension of a frequency is introduced by the dimensional consideration. One can determine ω_1 by considering the low-density limit of (6.19):

$$\lim_{n_s\to 0} \omega_f = \omega_f^{(0)} \equiv n_s x_0 = 2\omega_1\left(\frac{\pi}{2}\right) \tag{6.20}$$

From the last two equations one obtains

$$\tan\left[\frac{\pi}{2}\frac{x(n_s)}{x_0}\right] = \frac{\omega_d}{n_s x(n_s)} \tag{6.21}$$

This transcendental equation for $x(n_s)$ determines the behavior of $x(n_s)$ for small n_s and for $0 < x \leqq x_0$. Although this behavior is rather complicated, it *does* allow an approximate solution of the form

$$x = x_0 - \frac{2}{\pi}\frac{n_s x_0^{\,2}}{\omega_d} + \cdots \tag{6.22}$$

for very small n_s, which is verified by simple substitution. Therefore, we see from (6.22) that the correction of the self-consistent field to the pure one-impurity collision process should give rise to a contribution whose order of magnitude is smaller by the ratio of the duration of collision τ_d to the mean free time τ_f than the Boltzmann-Bloch collision frequency $\omega_f^{(0)}$. Also, we note that in the present estimation of (6.15) no correction in the form of logarithmic terms in n_s are expected.

The actual behavior of $\omega_f = n_s x(n_s)$ near $n_s = 0$ certainly depends on the impurity potential. However, the qualitative n_s-dependence is unlikely to depend very much on an approximation such as (6.19). In fact, it is easy to show that an equation of the same form as (6.21) is obtained directly from (6.15) by assuming that

$$\begin{aligned} |v(k)|^2 &= \text{constant for } k \leqq k_0 \equiv 1/R \\ &= 0 \qquad\qquad \text{for } k \geqq k_0 \end{aligned} \tag{6.23}$$

$$\omega_d \equiv P k_0 / M \tag{6.24}$$

and by retaining terms of important orders. Also, see the calculation in the next section.

7. *Non-Power Impurity Density Expansion. Case of Strong Coupling*

In the case of strong coupling, the (even simplest) low-density limit of the collision operator, $c_z^{(0)}$ with $z = -\omega + ia$, is given by the infinite power series of λ or equivalently by the solution of the algebraic equation (5.12). Therefore, it is in general difficult to obtain the collision term in a closed form except for special cases. One of the exceptional cases is that which we calculated in Section 5. In fact, we saw there that the low-density limit of the collision term for $z = ia$ can be expressed in terms of the differential cross-section $I(P, \theta)$. This result can be alternatively expressed in terms of the transition matrix, defined by

$$\begin{gathered} T_{12}(\varepsilon_0) = \lambda \tilde{v}_{12} - \lambda \int d^3 p_3\, \tilde{v}_{13} [\varepsilon_3 - \varepsilon_0 - ia]^{-1}\, T_{32}(\varepsilon_0) \\ T_{12} \equiv \langle \mathbf{p}_1 | T | \mathbf{p}_2 \rangle, \qquad \tilde{v}_{12} \equiv \langle \mathbf{p}_1 | \tilde{v} | \mathbf{p}_2 \rangle \end{gathered} \tag{7.1}$$

as

$$\begin{aligned} [c^{(0)}]_0\, \psi_x(\mathbf{P}, 0) &= i 2 (2\pi)^3 n_s \int d^3 k\, |T_{\mathbf{P},\,\mathbf{P}+\mathbf{k}}(\varepsilon_{\mathbf{P}})|^2 \times \\ &\qquad \times \operatorname{Im} [\varepsilon_{\mathbf{P}+\mathbf{k}} - \varepsilon_{\mathbf{P}} - ia]^{-1} [1 - \cos(\mathbf{P}, \mathbf{P}+\mathbf{k})]\, \psi_x \\ &\equiv -i \tau_f(\mathbf{P})^{-1}\, \psi_x(\mathbf{P}) \equiv i \omega_f^{(0)}\, \psi_x(\mathbf{P}) \end{aligned} \tag{7.2}$$

where the symbol Im means the imaginary part. It is stressed that this expression is identical in form with the weak-coupling limit (6.4) except for the fact that the elements of T-matrix now enters in place of those of v-matrix.

The evaluation of the T-matrix elements or equivalently that of the differential cross-section $I(P, \theta)$ generally require large amount of labor in either quantum or classical mechanics. Therefore, the quantitative treatment of the strong coupling case is difficult.

In order to more closely investigate the low-density behavior of the collision term, we must solve the equations (4.4)–(4.6) for $c(\mathbf{P})$ with $z = ia$. This makes the quantitative treatment even more difficult. In the following, therefore, we shall discuss the case qualitatively by using the analogy between the weak and strong couplings.

Let us postulate, as we did for $b(\mathbf{P})$ in (6.6), that

$$[c(\mathbf{P})]_0 \, \psi_x(\mathbf{P}) = i\omega_f \, \psi_x(\mathbf{P}) \tag{7.3}$$

with the number ω_f approaching $\omega_f^{(0)}$ in the low-density limit:

$$\omega_f \to \omega_f^{(0)} \qquad \text{as} \qquad n_s \to 0 \tag{7.4}$$

In view of the said analogy the equation to be solved for ω_f will be similar to (6.12) and will be written as

$$\omega_f(\varepsilon_{\mathbf{P}}') = (2\pi)^3 n_s \int d^3 k |T'_{\mathbf{P},\, \mathbf{P}+\mathbf{k}}(\varepsilon_{\mathbf{P}}')|^2 \times \operatorname{Im}\, [\varepsilon'_{\mathbf{P}+\mathbf{k}} - \varepsilon_{\mathbf{P}}' - i\omega_f(\varepsilon_{\mathbf{P}}')]^{-1} \tag{7.5}$$

$$T'_{12}(\varepsilon') \equiv \lambda \tilde{v}_{12} - \lambda \int d^3 p_3 \, \tilde{v}_{13} [\varepsilon_3' - \varepsilon' - i\omega_f(\varepsilon')] \, T'_{32}(\varepsilon') \tag{7.6}$$

In these equations $\varepsilon' \equiv \varepsilon_{\mathbf{P}}'$ is the perturbed energy and is given to the first order in n_s by

$$\varepsilon_{\mathbf{P}}' = \varepsilon_{\mathbf{P}} + (2\pi)^3 n_s \int d^3 k |T_{\mathbf{P},\, \mathbf{P}+\mathbf{k}}(\varepsilon_{\mathbf{P}})|^2 \, \mathscr{P} \frac{1}{\varepsilon_{\mathbf{P}+\mathbf{k}} - \varepsilon_{\mathbf{P}}} \tag{7.7}$$

When the potential v has a short range, the general argument would ensure that the square of the T'-matrix element effectively cut off the E-integral for $|E| \equiv |\varepsilon'_{\mathbf{P}+\mathbf{k}} - \varepsilon_{\mathbf{P}}'| > \omega_d$. Because of this property, we can study the qualitative behavior of ω_f in the neighborhood of $n_s = 0$ in the same way as in the case of weak coupling, and can draw the same conclusion with respect to the improbability of obtaining the correction involving $\ln n_s$.

The foregoing argument should also apply for the classical mechanical system although the square of T-matrix element should be replaced with a kind of cross section, which has the property of cutting off the contribution due to excessively large energy transfer.

In the article published by Murase (1966), the same problem was investigated starting from the expression equivalent to (5.1) and (5.3), and using the same connected diagram expansion. Analyzing the most divergent parts in terms of the diagrams, he found that the term-by-term divergence can be eliminated by summing the infinite series of R-type diagrams, which is a subclass of those included in the defining equations

(4.4)–(4.6) for c in our case. He also found [Murase, 1966, equation (4.23)] that the resummation leads to the modification in the propagator

$$\frac{1}{M^{-1}\mathbf{P}.\mathbf{k}-ia} \to \frac{1}{M^{-1}\mathbf{P}.\mathbf{k}-in_s\omega_f^{(0)}(\mathbf{P})} \tag{7.8}$$

(Change of notations: $v \to M^{-1}\mathbf{P}$, $\gamma(\mathbf{P}) \to \omega_f^{(0)}$.)

This is in qualitative agreement with our treatment if the higher-order effects as well as the change in the single-particle energy were neglected in our equation (7.5).

In estimating the effect of this modification on the conductivity σ for a *two*-dimensional system he proceeded to use the following equations [Murase, 1966, equation (4.24)],

$$\begin{aligned} n_s \operatorname{Im} \int d^2k S_z &\equiv \operatorname{Im} \int d^2k \left[\frac{1}{M^{-1}\mathbf{P}.\mathbf{k}-ia} - \frac{1}{M^{-1}\mathbf{P}.\mathbf{k}-ia+[c^{(0)}(\mathbf{P})]_{\mathbf{k}}}\right] \\ &\sim \omega_f^{(0)} \int_0^{M\omega_f^{(0)}/P} dkk \frac{1}{M^{-2}P^2k^2+n_s{}^2[\omega_f^{(0)}]^2} \\ &\sim \omega_f^{(0)} \frac{M^2}{P^2}(-\ln n_s) \end{aligned} \tag{7.9}$$

We believe that the step of approximation in going from the second to third member cannot be justified. If this step were made with due care, no logarithmic terms should have appeared in his treatment.

This can be seen by explicitly carrying out the integration indicated. Let us first note that the integrand in (7.9) should be multiplied by the factor $|T_{\mathbf{P},\mathbf{P}+\mathbf{k}}(\varepsilon_{\mathbf{P}})|^2$ as in (7.5), in order to really estimate the correction to the density expansion. Then, the first term in the second member of (7.9) yields

$$(2\pi)^2 n_s \operatorname{Im} \int d^2k \frac{1}{M^{-1}\mathbf{P}.\mathbf{k}-ia} |T_{\mathbf{P},\mathbf{P}+\mathbf{k}}(\varepsilon_{\mathbf{P}})|^2 \equiv \omega_f^{(0)} \tag{7.10}$$

where the term on the r.h.s. is the collision frequency in the low-impurity-density limit in two-dimensional problem. As we have analyzed before and in agreement with Murase's arguments, the operator $[c^{(0)}(\mathbf{P})]_{\mathbf{k}}$ appearing in the second member of (7.9) can be replaced with the numerical factor $-i\omega_f^{(0)}$ in our qualitative estimate. Thus, we must deal with the integral

$$\begin{aligned} I_2 &\equiv (2\pi)^2 n_s \operatorname{Im} \int d^2k |T_{\mathbf{P},\mathbf{P}+\mathbf{k}}|^2 \frac{1}{M^{-1}\mathbf{P}.\mathbf{k}-ia-i\omega_f^{(0)}} \\ &= (2\pi)^2 n_s \omega_f^{(0)} \int_0^\infty dkk \int_0^{2\pi} d\theta |T_{\mathbf{P},\mathbf{P}+\mathbf{k}}|^2 \frac{1}{(M^{-1}Pk\cos\theta)^2+(\omega_f^{(0)})^2} \end{aligned} \tag{7.11}$$

where we have introduced the plane polar coordinate (k, θ) with the polar axis pointing along the direction of the vector $\mathbf{P}$. If one neglects the angular dependence of $|T_{\mathbf{P},\mathbf{P}+\mathbf{k}}|^2$, the integration with respect to the angle θ can be carried out simply, yielding

$$I_2 = (2\pi)^2 n_s \int_0^\infty dkk|T_{\mathbf{P},\mathbf{P}+\mathbf{k}}|^2 \frac{2\pi}{\sqrt{[M^{-2}P^2k^2 + (\omega_f^{(0)})^2]}} \tag{7.12}$$

Note that this form is very different to the third member of (7.9). The integral in (7.12) can be estimated by noticing the fact that the factor $|T_{\mathbf{P},\mathbf{P}+\mathbf{k}}|^2$ falls off rapidly for the values of k greater than the inverse of the range R of force.

Thus, by assuming that

$$\begin{aligned} |T|^2 &= K \qquad \text{for } k < 0 \\ &= 0 \qquad \text{for } k > k_0 \equiv \frac{1}{R} \end{aligned} \tag{7.13}$$

we obtain from (7.12) that

$$I_2 = (2\pi)^3 n_s KM^2P^{-2}\{\sqrt{[M^{-2}P^2k_0{}^2 + (\omega_f^{(0)})^2]} - \omega_f^{(0)}\} \tag{7.14}$$

With the assumption (7.13), the collision frequency $\omega_f^{(0)}$ can be calculated as

$$\omega_f^{(0)} = (2\pi)^3 n_s KMP^{-1}k_0 \tag{7.15}$$

Using this relation, we can rewrite (7.14) in the form

$$I_2 = \omega_f^{(0)}\{\sqrt{[1 + (\omega_f^{(0)})^2/\omega_d{}^2]} - \omega_f^{(0)}/\omega_d\} \tag{7.16}$$

with $\omega_d \equiv M^{-1}Pk_0$ denoting the inverse of collision duration. The last expression means that the correction is of the order of $\omega_f^{(0)}/\omega_d$ in qualitative agreement with the conclusion stated in the last part of Section 6.

The present estimation has a further difference from Murase's work in that the cut-off $k_0 \equiv 1/R$ in the k-integral is provided by that property of $|T|^2$ arising from the finite-range nature of the interaction potential in our calculation whereas the cut-off $M\omega_f^{(0)}/P$ appearing in (7.9) is related to the collision frequency $\omega_f^{(0)}$ and thus distinct from k_0. Although this difference does not affect the (non) existence of a logarithmic term, it is emphasized that our cut-off k_0 is *built in* within the formulation whereas the cut-off $M\omega_f^{(0)}/P$ was introduced *extraneously* by using the collision time arguments (Kawasaki & Oppenheim, 1965) or phase volume arguments (Weinstock, 1965; Kritz & Sandri, 1966; Senger, 1966; Goldman & Frieman, 1967).

The extension of the calculation to the three-dimensional case can be carried out in a similar manner. In place of I_2 in (7.11) one deals with

$$\begin{aligned} I_3 &= (2\pi)^3 n_s \int d^3k|T_{\mathbf{P},\mathbf{P}+\mathbf{k}}|^2 \operatorname{Im}[M^{-1}\mathbf{P}.\mathbf{k} - ia - i\omega_f^{(0)}]^{-1} \\ &= (2\pi)^4 n_s \omega_f^{(0)} \int_0^\infty dkk^2 \int_{-1}^{+1} d(\cos\theta)\,|T_{\mathbf{P},\mathbf{P}+\mathbf{k}}|^2\,[(M^{-1}Pk\cos\theta)^2 + (\omega_f^{(0)})^2]^{-1} \end{aligned} \tag{7.17}$$

The angular integration yields

$$I_3 = (2\pi)^4 n_s \int_0^\infty dk k^2 |T_{\mathbf{P},\mathbf{P}+\mathbf{k}}|^2 (2MP^{-1} k^{-1}) \tan^{-1}(M^{-1} Pk/\omega_f^{(0)}) \tag{7.18}$$

By using the simplifying assumption of the same form as (7.13), one obtains

$$\begin{aligned} I_3 &= (2\pi)^4 n_s KMP^{-1} k_0{}^2 \left[\tan^{-1}(\omega_d/\omega_f^{(0)}) - \frac{\omega_f^{(0)}}{\omega_d} \right. \\ &\quad \left. + \left(\frac{\omega_f^{(0)}}{\omega_d}\right)^2 \tan^{-1}(\omega_d/\omega_f^{(0)} \right] \\ &= \omega_f^{(0)} \left[1 - \frac{2}{\pi} \frac{\omega_f^{(0)}}{\omega_d} + \left(\frac{\omega_f^{(0)}}{\omega_d}\right)^2 + \cdots \right] \end{aligned} \tag{7.19}$$

$$\begin{aligned} \omega_f^{(0)} &= (2\pi)^3 n_s \int d^3 k |T_{\mathbf{P},\mathbf{P}+\mathbf{k}}|^2 \operatorname{Im} [M^{-1} \mathbf{P}.\mathbf{k} - ia]^{-1} \\ &= (2\pi)^4 n_s KMP^{-1} k_0{}^2 (\pi/2) \end{aligned} \tag{7.20}$$

The expression (7.19) is in complete agreement with the conclusion obtained in Section 6.

8. *Concluding Remarks*

The term-by-term divergence in the straightforward impurity density (n_s) expansion of the conductivity σ can be completely eliminated by introducing the expansion of σ in terms of proper connected diagrams. The divergence is thought to arise from the fact that any interaction process between the electron and a set of impurities should take place in the average field of other impurities, and all the impurities should be treated self-consistently in the statistical mechanical theory of transport coefficients. This treatment automatically induces the perturbed single-particle energy and the collision broadening effects. Unlike the connected-diagram expansion the new expansion does not yield the straightforward expansion of $\sigma(n_s)$ in powers of n_s. The qualitative investigation of the analytical behavior of $\sigma(n_s)$ near the origin does not support the existence of logarithmic terms, much publicized in the recent literature (Fixman, 1963; Kawasaki & Oppenheim, 1965; Van Leeuwen & Weijland, 1965; Kritz & Sandri, 1966; Langer & Neal, 1966; Murase, 1966; Sengers, 1966; Dorfman & Cohen, 1967; Goldman & Frieman, 1967). The analytical behavior of $\sigma(n_s)$ is in general very complicated but does allow an asymptotic expansion in powers of the ratio of the collision frequency $\omega_f^{(0)}$ to the inverse of collision duration ω_d, $\omega_f^{(0)}/\omega_d \propto n_s$, for the simple model discussed in the present paper.

The method of the expansion in terms of proper connected diagrams can be generalized for a more complicated many-body systems such as an imperfect gas. By means of this generalization, we can remove the term-by-term divergence of the density expansion of a transport coefficient and discuss the analytical behavior of the density expansion. This topic will be reported in a separate paper (Fujita, 1967c).

Appendix

In this appendix we wish to prove the property that

$$(\mathbf{k}|g_z|\mathbf{k}') = \delta^{(3)}(\mathbf{k}-\mathbf{k}')\,[g_z]_{\mathbf{k}} \tag{A.1}$$

on the condition that the impurity distribution is invariant under translation. The k-particle impurity distribution function $n_s(\mathbf{R}_1, \mathbf{R}_2, \ldots, \mathbf{R}_k)$ is called translation-invariant if

$$n_s(\mathbf{R}_1+\mathbf{R}, \mathbf{R}_2+\mathbf{R}, \ldots, \mathbf{R}_k+\mathbf{R}) = n_s(\mathbf{R}_1, \mathbf{R}_2, \ldots, \mathbf{R}_k) \tag{A.2}$$

for an arbitrary constant vector $\mathbf{R}$.

Let us first consider the simple diagram (a) in Fig. 1. In the $\mathbf{P}-\mathbf{k}$ representation its contribution is written as

$$\begin{aligned}(\mathbf{k}|g_z^{(a)}|\mathbf{k}') &\equiv \lambda^2 \sum_\alpha (\mathbf{k}|\tilde{v}_\alpha[\hbar_0 - z]^{-1}\,\tilde{v}_\alpha|\mathbf{k}') \\ &= \lambda^2 \sum_\alpha \int d^3k_1 (\mathbf{k}|\tilde{v}_\alpha|\mathbf{k}_1)\,[M^{-1}\mathbf{P}.\mathbf{k}_1 - z]^{-1}\,(\mathbf{k}_1|\tilde{v}_\alpha|\mathbf{k}') \\ &= \lambda^2 \sum_\alpha \int d^3k_1\, \tilde{v}(\mathbf{k}-\mathbf{k}_1)\exp[-i(\mathbf{k}-\mathbf{k}_1).\mathbf{R}_\alpha] \times \\ &\qquad \times (\eta^{\mathbf{k}_1-\mathbf{k}} - \eta^{-\mathbf{k}_1+\mathbf{k}})\,[M^{-1}\mathbf{P}.\mathbf{k}_1 - z]^{-1} \times \\ &\qquad \times \tilde{v}(\mathbf{k}_1-\mathbf{k}')\exp[-i(\mathbf{k}_1-\mathbf{k}').\mathbf{R}_\alpha]\,(\eta^{\mathbf{k}'-\mathbf{k}_1} - \eta^{-\mathbf{k}'+\mathbf{k}_1})\end{aligned} \tag{A.3}$$

where

$$\tilde{v}(\mathbf{k}-\mathbf{k}') \equiv (2\pi)^{-3} \int d^3r\,\tilde{v}(\mathbf{r})\exp[-i(\mathbf{k}-\mathbf{k}').\mathbf{r}] \tag{A.4}$$

By the assumption of translation-invariant distribution of impurities, the summation with respect to α can be replaced by the integration:

$$\sum_\alpha \rightarrow n_s \int d^3R_\alpha \tag{A.5}$$

and the third member of (A.3) yields the delta-function

$$n_s \int d^3R_\alpha \exp[-i(\mathbf{k}-\mathbf{k}_1).\mathbf{R}_\alpha - i(\mathbf{k}_1-\mathbf{k}').\mathbf{R}_\alpha] = (2\pi)^3 n_s \delta^{(3)}(\mathbf{k}-\mathbf{k}') \tag{A.6}$$

Thus one sees that the matrix $(\mathbf{k}|g_z^{(a)}|\mathbf{k}')$ is diagonal in $\mathbf{k}$.

Such a diagonal property is easily verified for general one-impurity diagrams such as the diagram (b) in Fig. 3 by noticing

$$\begin{aligned}&\lambda^l \sum_\alpha (k|\tilde{v}_\alpha R_z^{(0)}\,\tilde{v}_\alpha \ldots \tilde{v}_\alpha|\mathbf{k}') \\ &\quad \propto \sum_\alpha \int \cdots \int d^3k_1 \ldots d^3k_{l-1} \exp\{-i[(\mathbf{k}-\mathbf{k}_1) + (\mathbf{k}_1-\mathbf{k}_2) + \cdots \\ &\qquad + (\mathbf{k}_{l-1}-\mathbf{k}')].\mathbf{R}_\alpha\} \\ &\quad \propto n_s \int d^3R \exp[-i(\mathbf{k}-\mathbf{k}').\mathbf{R}_\alpha] \\ &\quad = (2\pi)^3 n_s \delta^{(3)}(\mathbf{k}-\mathbf{k}')\end{aligned} \tag{A.7}$$

The equation (A.7) gives rise to the property that the vector sum of those momenta absorbed by the impurity center is equal to zero.

We now consider the diagram (d) in Fig. 1 which contains a correlation bond between the two impurity centers. Its contribution is given by

$$g_z^{(d)} \equiv \tfrac{1}{2}\lambda^2 \sum_{\alpha,\beta} \tilde{v}_\alpha[\mathscr{h}_0 - z]^{-1}\, \tilde{v}_\beta\, \chi_2(\mathbf{R}_\alpha, \mathbf{R}_\beta) \tag{A.8}$$

From the assumption of translation-invariant distribution of impurities, the two-impurity correlation function $\chi_2(\mathbf{R}_\alpha, \mathbf{R}_\beta)$ depends only on the difference $\mathbf{R}_\alpha - \mathbf{R}_\beta$:

$$\chi_2(\mathbf{R}_\alpha, \mathbf{R}_\beta) = \chi(\mathbf{R}_\alpha - \mathbf{R}_\beta) \tag{A.9}$$

By writing the Fourier transform of $\chi(\mathbf{R}_\alpha - \mathbf{R}_\beta)$ as

$$\chi_\mathbf{q} = \int d^3 R \exp(-i\mathbf{q}.\mathbf{R})\, \chi(\mathbf{R})$$

$$\chi(\mathbf{R}) = \frac{1}{(2\pi)^3} \int d^3\mathbf{q} \exp(i\mathbf{q}.\mathbf{R})\, \chi_\mathbf{q} \tag{A.10}$$

and examining the exponential factors containing the impurity coordinates in the $\mathbf{k} - \mathbf{k}'$ element of $g_z^{(d)}$, one sees that the element contains in its integrand:

$$\begin{aligned} n_s^2 \iint d^3 R_\alpha\, d^3 R_\beta &\exp[-i(\mathbf{k} - \mathbf{k}_1).\mathbf{R}_\alpha] \times \\ &\times \exp[-i(\mathbf{k}_1 - \mathbf{k}').\mathbf{R}_\beta] \exp[i\mathbf{q}.(\mathbf{R}_\alpha - \mathbf{R}_\beta)] \\ = (2\pi)^6 n_s^2\, &\delta^{(3)}(\mathbf{k} - \mathbf{k}_1 + \mathbf{q})\, \delta^{(3)}(\mathbf{k}_1 - \mathbf{k}' + \mathbf{q}) \\ = (2\pi)^6 n_s^2\, &\delta^{(3)}(\mathbf{k} - \mathbf{k}_1 + \mathbf{q})\, \delta^{(3)}(\mathbf{k} - \mathbf{k}') \end{aligned} \tag{A.11}$$

The presence of the factor $\delta^{(3)}(\mathbf{k} - \mathbf{k}')$ here implies that $(\mathbf{k}|g_z^{(d)}|\mathbf{k}')$ is diagonal and that the net momentum absorbed by the pair of correlated impurities is equal to zero. In a similar manner one can show that the net momentum absorbed by the set of any number of correlated impurity centers vanishes.

A general diagram for g_z may contain arbitrary numbers of correlated and/or uncorrelated impurity centers. The net momentum absorbed by all the impurity centers is clearly the sum of those momenta absorbed by each set of correlated impurity centers and each uncorrelated impurity center. Since the latter momenta are separately equal to zero, so is the net momentum. This establishes the desired property (A.1).

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