

An Expansion Theorem for the Electric Conductivity of Metals. I

—*Electric Conductivity for Longitudinal Electric Field*—

Takeo IZUYAMA

*Department of Physics, Faculty of Science
University of Tokyo, Tokyo*

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A systematic diagram representation in a composite 4-dimensional space is developed for Kubo's response function which describes the electric response currents of metals for longitudinal electric fields. Proper diagrams are defined as the Feynman type linked diagrams which cannot be decomposed into simpler diagrams connected only by one Coulomb line. The greatest care is exercised with reference to the fact that Kubo's formula for the conduction phenomena gives the transport coefficient $\chi(\mathbf{q}, \omega)$ defined as the ratio of the electric current vector to the electric displacement vector $\mathbf{D}(\mathbf{q}, \omega)$, while the electric conductivity $\sigma(\mathbf{q}, \omega)$ of a metal is defined as the electric current vector divided by the electric field vector $\mathbf{E}(\mathbf{q}, \omega)$ in the metal. Thus $\sigma(\mathbf{q}, \omega)$ is written as the product of $\chi(\mathbf{q}, \omega)$ and the dielectric constant of the metal. It is shown that, the product is reduced to a simple form. In the reduced form, $\sigma(\mathbf{q}, \omega)$ is expressed as the sum of the proper diagrams. In this expression the lowest order term in respect to the Coulomb interaction includes the usual sum on ring diagrams and, moreover, constitutes a much better approximation than the ring approximation.

§ 1. Introduction

An exact formal expression for electric conductivity in, say, a metal has been given by Kubo and Nakano.¹⁾ In their theory the electric current is interpreted as the response current for an external force which is adiabatically applied to the system and in the Taylor expansion of the response current in terms of the external force, the coefficient of the linear term which has been interpreted as the electric conductivity can be written down in an exact formal expression. The observed conductivity, however, is the quotient of the response current divided by the macroscopic electric field in the system.

This fact has been overlooked in actual calculations hitherto made theoretically on the basis of Kubo's formalism; Kubo's formula which was intended to give the coefficient of the external field has been regarded as a formula for the coefficient of the electric field. Nevertheless reasonable results have been derived through such calculations. It should be noted here that in these calculations one has completely neglected the Coulomb interaction between electrons as well as one has replaced the external field by the electric field.

The electric field in a metal is much different from the external field. A finite external field induces a large polarization of the electron cloud in a metal

and is screened almost completely by the polarization charge. Thus, the strength of the electric field in the metal is almost zero in spite of the presence of the finite external field.[†]

Several works²⁾ have recently appeared which are intended to develop a general scheme to calculate exactly the electric conductivity of a many-electron system on the basis of Kubo's formalism. In such treatments, however, one must be very careful about the difference between the two fields: One should not regard the transport coefficient given by Kubo's formula as a real conductivity of the many-electron system. Otherwise, one would obtain an absurd result, because the Coulomb interaction between electrons together with the interaction between the electron system and the external field leads to a strong screening for the field and, consequently, one would obtain a vanishing conductivity especially in the limit of infinitely long wave length of the external field.

In this paper we will develop a general scheme to calculate directly the electric conductivity of a metal without going into a calculation of the coefficient of the external field. The conventional treatment in which the external field is replaced by the electric field and the Coulomb interaction is neglected is shown to be a fairly good approximation.

In this paper the external field is taken to be a longitudinal field which may be oscillating. The electro-magnetic responses for a general electro-magnetic field will be considered in a forthcoming paper. A system composed of an electron gas and a phonon assembly is investigated here. A system which contains impurities will be treated elsewhere.

§ 2. Kubo's formalism

The electron-phonon system, whose electric properties will be investigated, is taken to be in thermal equilibrium before the application of the external field. In the equilibrium state, the system is described by the grand canonical ensemble with the following Hamiltonian:

$$H = H_0 + H', \quad (2.1)$$

$$H_0 = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} a_{\mathbf{k}}^* a_{\mathbf{k}} + \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^* b_{\mathbf{k}}, \quad (2.2)$$

$$H' = \sum_{\mathbf{k} \neq 0} \frac{4\pi e^2}{k^2} \sum_{l, m} a_{l+\mathbf{k}}^* a_l a_{m-\mathbf{k}}^* a_m + \sum_{\mathbf{k}, l} \{v(\mathbf{k}; l) a_l^* a_{l+\mathbf{k}} b_{\mathbf{k}}^* + \text{C. C.}\}, \quad (2.3)$$

$$(\hbar = 1)$$

[†] This fact was pointed out by Prof. Y. Toyozawa (private communications). A careful discussion on this problem is found in the note of S. Nakajima: *Busseiron Kenkyu* II 8 (1960), 340 (a mimeographed circular in Japanese).

where $a_{\mathbf{k}}$ is the destruction operator for an electron of momentum \mathbf{k} , $\varepsilon_{\mathbf{k}}$ denotes the energy of this electron, $b_{\mathbf{k}}$ is the destruction operator for a phonon of momentum \mathbf{k} , $\omega_{\mathbf{k}}$ denotes the frequency of the normal mode described by this phonon, and $v(\mathbf{k}; \mathbf{l})$ represents the strength of the electron-phonon interaction. In the above, we have used the assumption that the negative charge of our electron system is cancelled completely by a uniform positive charge which is not a constant but is equal to the total number of electrons multiplied by e .

The external field which is applied to the system is produced by some external charges. These external charges are placed on the two plates of a condenser between which our system is held, or they are produced in the batteries. These charges are called "true charges". The electric field produced only by the true charges is called the electric displacement $\mathbf{D}(\mathbf{x}, t)$, which is nothing but the external field. Thus, the system in the presence of the external field is described by the following Hamiltonian:

$$\mathcal{H} = H + \int \phi(\mathbf{x}, t) \mathfrak{N}(\mathbf{x}) d\mathbf{x}, \quad (2.4)$$

where

$$\mathfrak{N}(\mathbf{x}) = -e(\phi^*(\mathbf{x})\phi(\mathbf{x}) - N), \quad (2.5)$$

and

$$\mathbf{D}(\mathbf{x}, t) = -\nabla\phi(\mathbf{x}, t). \quad (2.6)$$

In the above, $\phi(\mathbf{x})$ is the quantized wave function for the electron cloud, N is the total number of electrons, and then eN is the density of the uniform positive charge; the volume of the system is taken to be unity.

The density matrix $\rho(t)$ describing our system obeys the following equation of motion,

$$i\dot{\rho}(t) = [\mathcal{H}, \rho(t)].$$

Further, writing $\rho(t)$ as

$$\rho(t) = \rho + \Delta\rho(t),$$

where ρ represents the equilibrium density matrix for the grand canonical ensemble, we must impose on $\Delta\rho(t)$ the following boundary condition

$$\begin{aligned} \Delta\rho(t) &\xrightarrow{t \rightarrow -\infty} 0 \\ \left(\phi(\mathbf{x}, t) \right) &\xrightarrow{t \rightarrow -\infty} 0, \end{aligned}$$

due to the assumption mentioned previously. Then we get in the linear approximation,

$$\Delta\rho(t) = \frac{1}{i} \int_{-\infty}^t dt' \int d\mathbf{x}' \phi(\mathbf{x}', t') e^{iH(t'-t)} [\mathfrak{N}(\mathbf{x}'), \rho] e^{-iH(t'-t)}. \quad (2.7)$$

Now, the current operator is denoted by

$$\mathfrak{J}(\mathbf{x}) = \frac{e}{2im} \left\{ \psi^*(\mathbf{x}) (\nabla \psi(\mathbf{x})) - (\nabla \psi^*(\mathbf{x})) \psi(\mathbf{x}) \right\}. \quad (2.8)$$

Then the observed current is given by

$$\mathbf{J}(\mathbf{x}, t) = \text{Tr} \{ \rho(t) \mathfrak{J}(\mathbf{x}) \} = \text{Tr} \{ \Delta \rho(t) \mathfrak{J}(\mathbf{x}) \}.$$

Inserting Eq. (2.7) into the above expression, we get

$$\mathbf{J}(\mathbf{x}, t) = \frac{1}{i} \int_{-\infty}^t dt' \int d\mathbf{x}' \phi(\mathbf{x}', t') \langle [\mathfrak{J}(\mathbf{x}, t-t'), \mathfrak{N}(\mathbf{x}')] \rangle, \quad (2.9)$$

where

$$\langle \mathfrak{N} \rangle \equiv \text{Tr} \{ \rho \mathfrak{N} \},$$

and

$$\mathfrak{J}(\mathbf{x}, t) \equiv e^{iHt} \mathfrak{J}(\mathbf{x}) e^{-iHt}.$$

If we define

$$\mathfrak{N}(\mathbf{x}, t) \equiv e^{iHt} \mathfrak{N}(\mathbf{x}) e^{-iHt}, \quad (2.10)$$

it can be easily seen that the equation of continuity is satisfied by $\mathfrak{N}(\mathbf{x}, t)$ and $\mathfrak{J}(\mathbf{x}, t)$ given in Eqs. (2.10) and (2.8) respectively. The Fourier transform of the spatial component of this continuity equation is written as

$$\dot{\mathfrak{N}}(\mathbf{q}, t) = -i\mathbf{q} \cdot \mathfrak{J}(\mathbf{q}, t). \quad (2.11)$$

If the applied field is periodic, i.e.,

$$\phi(\mathbf{x}, t) = e^{i\mathbf{q} \cdot \mathbf{x} + i\omega t} \phi(\mathbf{q}, \omega),^\dagger \quad (2.12)$$

then

$$\mathbf{J}(\mathbf{x}, t) = e^{i\mathbf{q} \cdot \mathbf{x} + i\omega t} \mathbf{J}(\mathbf{q}, \omega),$$

and Eq. (2.9) is expressed as

$$\mathbf{J}(\mathbf{q}, \omega) = \frac{1}{i} \int_0^\infty dt e^{-i\omega t} \langle [\mathfrak{J}(\mathbf{q}, t), \mathfrak{N}(-\mathbf{q})] \rangle \phi(\mathbf{q}, \omega). \quad (2.13)$$

Noting that $\mathbf{J}(\mathbf{q}, \omega)$ is parallel to \mathbf{q} and

$$\mathbf{D}(\mathbf{q}, \omega) = -i\mathbf{q}\phi(\mathbf{q}, \omega)$$

and inserting Eq. (2.11) into Eq. (2.13), we obtain

$$\mathbf{J}(\mathbf{q}, \omega) = \chi(\mathbf{q}, \omega) \mathbf{D}(\mathbf{q}, \omega), \quad (2.14)$$

where³⁾

[†] The convergence factor is omitted here. It will be omitted sometimes in order to save notations.

$$\begin{aligned}\chi(\mathbf{q}, \omega) &= \lim_{\delta \rightarrow +0} \frac{i}{q^2} \int_0^{\infty} dt e^{-i\omega t - \delta t} \langle [\dot{\mathfrak{N}}(\mathbf{q}, t), \mathfrak{N}(-\mathbf{q})] \rangle \\ &= \lim_{\delta \rightarrow +0} \frac{\omega}{q^2} \int_0^{\infty} dt e^{-i\omega t - \delta t} \langle [\mathfrak{N}(-\mathbf{q}), \mathfrak{N}(\mathbf{q}, t)] \rangle.\end{aligned}\quad (2.15)$$

In the above we have used the following fact,

$$[\mathfrak{N}(\mathbf{q}), \mathfrak{N}(-\mathbf{q})] = 0.$$

It should be noted that the usual expression (2.15) is a formula for the transport coefficient χ defined by Eq. (2.14) and does not give the conductivity in itself.

Now, the dielectric constant is defined by

$$\mathbf{D}(\mathbf{q}, \omega) = \epsilon(\mathbf{q}, \omega) \mathbf{E}(\mathbf{q}, \omega), \quad (2.16)$$

where \mathbf{E} is the macroscopic electric field in the metal. Then, the conductivity σ , which is defined by

$$\mathbf{J}(\mathbf{q}, \omega) = \sigma(\mathbf{q}, \omega) \mathbf{E}(\mathbf{q}, \omega), \quad (2.17)$$

is expressed as

$$\sigma(\mathbf{q}, \omega) = \epsilon(\mathbf{q}, \omega) \chi(\mathbf{q}, \omega). \quad (2.18)$$

As we shall see in the next section,

$$\epsilon(\mathbf{q}, \omega) = \left[1 - \frac{4\pi}{i\omega} \chi(\mathbf{q}, \omega) \right]^{-1}, \quad (2.19)$$

and therefore we get the relation

$$\sigma(\mathbf{q}, \omega) = \frac{\chi(\mathbf{q}, \omega)}{1 - (4\pi/i\omega)\chi(\mathbf{q}, \omega)}. \quad (2.20)$$

§ 3. Dielectric constant

Eq. (2.19) is easily verified, if we are allowed to use the phenomenological relation

$$\mathbf{D} = \mathbf{E} + 4\pi\mathbf{P}, \quad \mathbf{J} = \dot{\mathbf{P}}.$$

However, it may be inadequate to make use of the phenomenological equation without any proof. Then we shall prove Eq. (2.19) on the basis of the fundamental equations by means of Kubo's linear approximation.

The electric field $\hat{\mathbf{E}}(\mathbf{x}, t)$ produced by the matter field as well as the external field is expressed as an operator, and the macroscopic electric field $\mathbf{E}(\mathbf{x}, t)$ is given by

$$\mathbf{E}(\mathbf{x}, t) = \text{Tr} \{ \rho(t) \hat{\mathbf{E}}(\mathbf{x}, t) \}. \quad (3.1)$$

This may be written as

$$\varphi(\mathbf{x}, t) = \text{Tr} \{ \rho(t) \hat{\varphi}(\mathbf{x}, t) \}, \quad (3.2)$$

where

$$\hat{\mathbf{E}}(\mathbf{x}, t) = -\nabla \hat{\varphi}(\mathbf{x}, t)$$

and

$$\mathbf{E}(\mathbf{x}, t) = -\nabla \varphi(\mathbf{x}, t).$$

Let us denote the free charge, the true charge and the polarization charge by \mathfrak{N}_f , \mathfrak{N}_r and \mathfrak{N} , respectively. Then

$$\text{div} \hat{\mathbf{E}}(\mathbf{x}, t) = 4\pi \mathfrak{N}_f(\mathbf{x}, t) = 4\pi \mathfrak{N}_r(\mathbf{x}, t) + 4\pi \mathfrak{N}(\mathbf{x}, t) = \text{div} \mathbf{D}(\mathbf{x}, t) + 4\pi \mathfrak{N}(\mathbf{x}, t).$$

Therefore,

$$\hat{\varphi}(\mathbf{x}, t) = \phi(\mathbf{x}, t) + \int \frac{d\mathbf{x}'}{|\mathbf{x} - \mathbf{x}'|} \mathfrak{N}(\mathbf{x}'). \quad (3.3)$$

Substituting Eq. (3.3) in Eq. (3.2), we get

$$\varphi(\mathbf{x}, t) = \phi(\mathbf{x}, t) + \int \frac{d\mathbf{x}'}{|\mathbf{x} - \mathbf{x}'|} \text{Tr} \{ \rho \mathfrak{N}(\mathbf{x}') \} + \int \frac{d\mathbf{x}'}{|\mathbf{x} - \mathbf{x}'|} \text{Tr} \{ \Delta \rho(t) \mathfrak{N}(\mathbf{x}') \}. \quad (3.4)$$

It is easily shown that Fourier coefficients of the second term in the right-hand side of Eq. (3.4) vanish, so far as macroscopic phenomena are concerned.[†] Therefore, inserting Eq. (2.7) into Eq. (3.4), we obtain

$$\begin{aligned} \varphi(\mathbf{x}, t) = & \phi(\mathbf{x}, t) + \frac{1}{i} \int_{-\infty}^t dt'' \int d\mathbf{x}' \int d\mathbf{x}'' \frac{1}{|\mathbf{x} - \mathbf{x}'|} \\ & \times \langle [\mathfrak{N}(\mathbf{x}', t - t''), \mathfrak{N}(\mathbf{x}'')] \rangle \phi(\mathbf{x}'', t''). \end{aligned} \quad (3.5)$$

The Fourier transform of this is

$$\varphi(\mathbf{q}, \omega) = \phi(\mathbf{q}, \omega) + \frac{4\pi}{iq^2} \int_0^{\infty} d\tau e^{-i\omega\tau} \langle [\mathfrak{N}(\mathbf{q}, \tau), \mathfrak{N}(-\mathbf{q})] \rangle \phi(\mathbf{q}, \omega). \quad (3.6)$$

Now, the dielectric constant has been defined by Eq. (2.16) or

$$\epsilon(\mathbf{q}, \omega) \varphi(\mathbf{q}, \omega) = \phi(\mathbf{q}, \omega).$$

Therefore, we obtain from Eq. (3.6)

$$\epsilon(\mathbf{q}, \omega) = \left[1 + \frac{4\pi}{iq^2} \int_0^{\infty} dt e^{-i\omega t} \langle [\mathfrak{N}(\mathbf{q}, t), \mathfrak{N}(-\mathbf{q})] \rangle \right]^{-1}.$$

Thus, Eq. (2.19) has been verified.

[†] If microscopic phenomena are concerned, on the other hand, it is necessary to consider Fourier components whose wave vectors are comparable to reciprocal lattice vectors in magnitude. The Fourier component of the second term whose wave vector is equal to a reciprocal lattice vector does not vanish.

§ 4. Diagram representation

Here we shall develop a diagram representation of the expression for χ given by Eq. (2.15), by making use of the technique developed by C. Bloch et C. de Dominicis⁴⁾ (hereafter referred to as BDD) in the statistical mechanics of equilibrium states.

The following functions are introduced at first:

$$F(\mathbf{l}, \mathbf{k}|0^+, it) \equiv \langle \alpha_l^{-q} e^{iHt} \alpha_k^q e^{-iHt} \rangle = \frac{1}{Z} \text{Tr} \{ e^{-\beta(H-\mu N)} \alpha_l^{-q} e^{iHt} \alpha_k^q e^{-iHt} \}, \quad (4.1)$$

$$F(\mathbf{l}, \mathbf{k}|0^-, it) \equiv \langle e^{iHt} \alpha_k^q e^{-iHt} \alpha_l^{-q} \rangle = \frac{1}{Z} \text{Tr} \{ e^{-\beta(H-\mu N)} e^{iHt} \alpha_k^q e^{-iHt} \alpha_l^{-q} \}, \quad (4.2)$$

where Z is the grand partition function and

$$\alpha_k^q \equiv a_{k+q}^* a_k. \quad (4.3)$$

Thus,

$$\langle [\mathfrak{R}(-\mathbf{q}), \mathfrak{R}(\mathbf{q}, t)] \rangle = e^2 \sum_{\mathbf{k}, \mathbf{l}} \{ F(\mathbf{l}, \mathbf{k}|0^+, it) - F(\mathbf{l}, \mathbf{k}|0^-, it) \}. \quad (4.4)$$

Next the following notations are introduced:

$$\left. \begin{aligned} \alpha_k^q(u) &\equiv \alpha_k^q e^{u(\varepsilon_k + q - \varepsilon_{k'})} = a_{k+q}^* a_k e^{u(\varepsilon_k + q - \varepsilon_{k'})}, \\ b_k^*(u) &\equiv b_k^* e^{u\omega_k}, \\ b_k(u) &\equiv b_k e^{-u\omega_k}, \end{aligned} \right\} \quad (4.5)$$

and

$$\begin{aligned} H'(u) &\equiv e^{uH_0} H' e^{-uH_0} = \sum_{\mathbf{k} \neq 0} \frac{4\pi e^2}{k^2} \sum_{\mathbf{l}, \mathbf{m}} \alpha_l^{\mathbf{k}}(u) \alpha_m^{-\mathbf{k}}(u) \\ &+ \sum_{\mathbf{k} \neq 0} \sum_{\mathbf{l}} \{ v(\mathbf{k} : \mathbf{l}) \alpha_{\mathbf{l}+\mathbf{k}}^{-\mathbf{k}}(u) b_{\mathbf{k}}^*(u) + v^*(\mathbf{k} : \mathbf{l}) \alpha_{\mathbf{l}}^{\mathbf{k}}(u) b_{\mathbf{k}}(u) \}. \end{aligned} \quad (4.6)$$

Then

$$\left. \begin{aligned} e^{-\beta H} &= e^{-\beta H_0} \cdot e^{-\int_0^\beta du H'(u)}, \\ e^{iHt} &= e^{-i \int_t^0 du H'(iu)} \cdot e^{iH_0 t}, \\ e^{-iHt} &= e^{-iH_0 t} \cdot e^{-i \int_0^t du H'(iu)}. \end{aligned} \right\} \quad (4.7)$$

where we denote by $e_{(+)}$ and $e_{(-)}$ the ordered exponentials

$$e_{(+)}^{\int_a^b du \mathfrak{A}(u)} \equiv 1 + \sum_{n=1}^{\infty} \int_a^b du_1 \int_a^{u_1} du_2 \cdots \int_a^{u_{n-1}} du_n \mathfrak{A}(u_1) \mathfrak{A}(u_2) \cdots \mathfrak{A}(u_n)$$

and

$$e^{\int_b^a du \mathfrak{A}(u)} \equiv 1 + \sum_{n=1}^{\infty} \int_b^{u_1} du_1 \int_b^{u_2} du_2 \cdots \int_b^{u_{n-1}} du_n \cdot \mathfrak{A}(u_1) \mathfrak{A}(u_2) \cdots \mathfrak{A}(u_n)$$

($a < b$),

for any operator $\mathfrak{A}(u)$. Substituting Eq. (4.7) into Eqs. (4.1) and (4.2), we obtain, respectively,

$$F(\mathbf{l}, \mathbf{k}|0^+, it) = \frac{Z_0}{Z} \langle e^{-\int_0^\beta du H'(u)} \cdot \alpha_l^{-q} \cdot e^{-i \int_t^0 du H'(iu)} \cdot \alpha_k^q(it) \cdot e^{-i \int_0^t du H'(iu)} \rangle_0, \quad (4.1')$$

and

$$F(\mathbf{l}, \mathbf{k}|0^-, it) = \frac{Z_0}{Z} \langle e^{-\int_0^\beta du H'(u)} \cdot e^{-i \int_t^0 du H'(iu)} \cdot \alpha_k^q(it) \cdot e^{-i \int_0^t du H'(iu)} \cdot \alpha_l^{-q} \rangle_0. \quad (4.2')$$

In the above,

$$\langle \mathfrak{A} \rangle_0 \equiv \text{Tr} \rho_0 \mathfrak{A},$$

where

$$\rho_0 \equiv Z_0^{-1} e^{-\beta(H_0 - \mu N)}$$

is the grand canonical density matrix for the unperturbed system, whose grand partition function is denoted by Z_0 .

In order to describe the "time-ordered" expansion in Eqs. (4.1') and (4.2'), we here introduce a composite 4-dimensional space as shown in Fig. 1. The abscissa of this figure represents the 3-dimensional configuration space. A path $L(t)$ is taken along the vertical axis. This path is composed of the following three parts. The first part which is denoted by $[[0^-, it]]$ is composed of the imaginary numbers ranging from zero to it . An imaginary number $i\tau$ ($0 \leq \tau < t$) is represented by $i\tau^-$ on this part. The second part which is denoted by $[[it, 0^+]]$ is the reflection of $[[0^-, it]]$ with respect to the point it . An imaginary number $i\tau$ ($0 \leq \tau < t$) is represented by $i\tau^+$ on $[[it, 0^+]]$. The last part which is denoted by $[[0^+, \beta]]$ corresponds to an interval $[0, \beta]$ composed of real numbers.

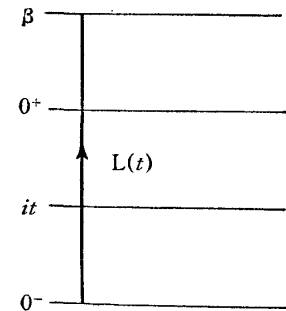


Fig. 1.

Referring to the path $L(t)$, we may write Eqs. (4.1') and (4.2') as

$$F(\mathbf{l}, \mathbf{k}|0^\pm, it) = \frac{Z_0}{Z} \langle P[e^{-\int_{L(t)} du H'(u)} \cdot \alpha_l^{-q}(0^\pm) \cdot \alpha_k^q(it)] \rangle_0, \quad (4.8)$$

where P represents Dyson's chronological ordering on the path $L(t)$, and $\int_{L(t)} du$ is the path integral along this path.

According to BDD, the contraction between two operators a and a' is defined as

$$a' a^* = \langle a a' \rangle_0.$$

In the evaluation of Eq. (4.8), we are met by the statistical average of a product

of some creation and annihilation operators. The average is taken in the unperturbed system, where the density matrix can be written as

$$\rho_0 = \prod \left(\frac{e^{\beta(\mu - \epsilon_k) a_k^* a_k}}{1 + e^{\beta(\mu - \epsilon_k)}} \right) \prod \left((1 - e^{-\beta \omega_k}) e^{-\beta \omega_k b_k^* b_k} \right).$$

Therefore, according to BDD, the statistical average of the product of the operators under consideration can be decomposed into a unique sum of all possible sets of the complete contractions one can indicate.

The contractions which do not vanish are classified into the following four types :

$$a_k \cdot a_k^* = f_k^{(+)} \equiv \frac{1}{1 + e^{\beta(\mu - \epsilon_k)}},$$

$$a_k^* \cdot a_k = f_k^{(-)} \equiv \frac{1}{1 + e^{\beta(\epsilon_k - \mu)}},$$

$$b_k \cdot b_k^* = g_k^{(+)} \equiv \frac{1}{1 - e^{-\beta \omega_k}},$$

$$b_k^* \cdot b_k = g_k^{(-)} \equiv \frac{1}{e^{\beta \omega_k} - 1}.$$

With use of the notations of BDD, we represent $a_k(u) \cdot a_k^*(u')$ and $a_k^*(u) \cdot a_k(u')$ by the respective arrows shown in Fig. 2.1 and Fig. 2.2, and $b_k(u) \cdot b_k^*(u')$ and $b_k^*(u) \cdot b_k(u')$ by the "dotted" arrows shown in Fig. 3.1 and Fig. 3.2, respectively.

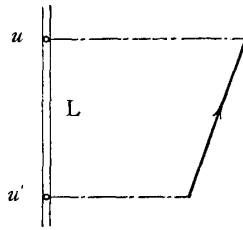


Fig. 2.1.

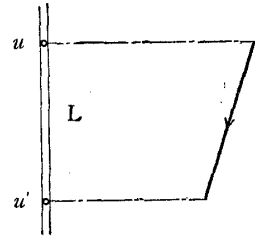


Fig. 2.2.

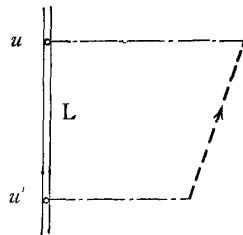


Fig. 3.1.

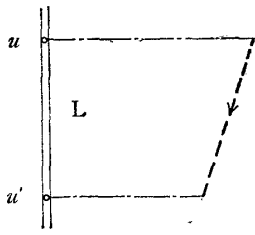


Fig. 3.2.

The Coulomb interaction

$$\frac{4\pi e^2}{q^2} a_{l+k}^* a_l a_{m-k}^* a_m$$

is written as in Fig. 4. The electron-phonon interactions

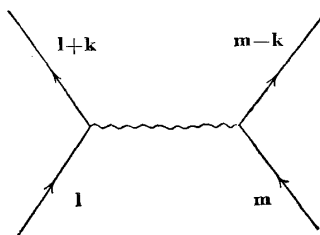


Fig. 4.

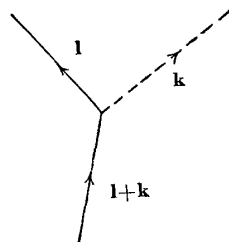


Fig. 5.

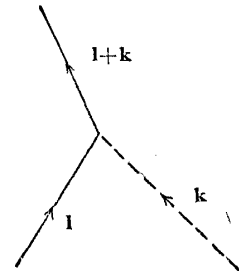


Fig. 6.

$$v(\mathbf{k} : \mathbf{l}) a_l^* a_{l+k} b_k^*$$

and

$$v^*(\mathbf{k} : \mathbf{l}) a_{l+k}^* a_l b_k$$

are expressed as in Fig. 5 and Fig. 6, respectively.

Thus, $F(\mathbf{l}, \mathbf{k} | 0^\pm, it)$ given by Eq. (4.8) can be expressed as a unique sum of Feynman diagrams in the composite 4-dimensional space. The rule for calculating the contribution of each diagram to the F-function is similar to the rule given by BDD, except that the path of the u -integration is now $L(t)$ instead of the interval $[0, \beta]$.

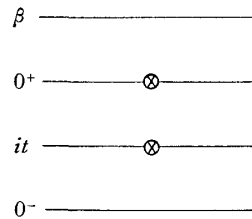


Fig. 7.

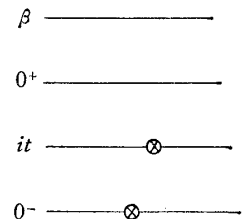


Fig. 8.

§ 5. Elimination of disconnected diagrams

A diagram which falls into two or more unconnected parts is said to be a disconnected diagram, and otherwise it is called connected. A disconnected diagram has such a form as shown in Fig. 9. There are no diagrams like that in Fig. 10.

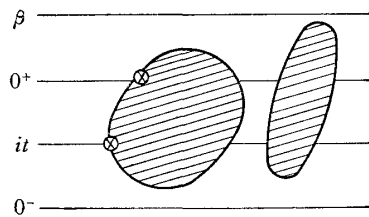


Fig. 9.

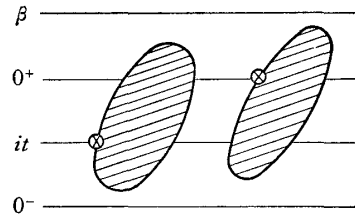
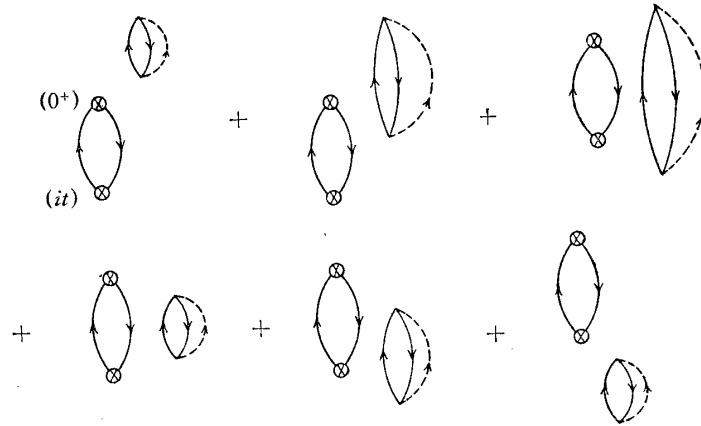


Fig. 10.

Let us consider a disconnected diagram. Its connected part, i.e., the part connected to the \otimes vertices, is indicated as Γ_1 , and its disconnected part composed of one or more unconnected parts which do not contain the \otimes vertex is denoted by Γ_2 . Retaining the order[†] of vertices of Γ_1 and that of Γ_2 , respectively, we shall change the order between the vertices of Γ_1 and those of Γ_2 . Then we obtain a family of diagrams. We shall consider the contribution of all the diagrams belonging to this family. For example,

[†] The order of vertices on the path L is simply called the order from now on.



The contribution of the above sum is equal to the product of “the contribution of $\begin{matrix} \circ \\ \updownarrow \\ \circ \end{matrix}$ (Γ_1) to the F-function” and “the contribution of $\begin{matrix} \circ \\ \updownarrow \\ \circ \end{matrix}$ (Γ_2) to $\langle P[e^{-\int_L du H'(u)}] \rangle^0$ ”. Accordingly, we get

$$F(\mathbf{l}, \mathbf{k}|0^\pm, it) = \frac{Z_0}{Z} \langle P[e^{-\int_L du H'(u)} \cdot \alpha_k^q(it) \alpha_l^{-q}(0^\pm)] \rangle_C^0 \langle P[e^{-\int_L du H'(u)}] \rangle^0, \quad (5.1)$$

where the suffix C indicates the sum of all connected diagrams. Further,

$$\frac{Z_0}{Z} \langle P[e^{-\int_L du H'(u)}] \rangle = \frac{Z_0}{Z} \langle e^{-\int_0^\beta du H'(u)} \rangle^0 = \frac{1}{Z} \text{Tr} e^{-\beta(H - \mu N)} = 1.$$

Inserting this into Eq. (5.1), we obtain

$$F(\mathbf{l}, \mathbf{k}|0^\pm, it) = \langle P[e^{-\int_L du H'(u)} \cdot \alpha_k^q(it) \cdot \alpha_l^{-q}(0^\pm)] \rangle_C^0. \quad (5.2)$$

§ 6. Definitions and lemmas

(Definition)

For two arbitrary points ξ and η on $L(t)$, we define

$$\begin{aligned} F_t(\mathbf{l}, \mathbf{k}|\xi, \eta) &\equiv \frac{Z_0}{Z} \langle P[e^{-\int_{L(t)} du H'(u)} \cdot \alpha_l^{-q}(\xi) \alpha_k^q(\eta)] \rangle^0 \\ &= \langle P[e^{-\int_{L(t)} du H'(u)} \alpha_l^{-q}(\xi) \alpha_k^q(\eta)] \rangle_C^0. \end{aligned} \quad (6.1)$$

(Corollary)

$$F_t(\mathbf{l}, \mathbf{k}|0^\pm, it) = F(\mathbf{l}, \mathbf{k}|0^\pm, it).$$

(Lemma 1)

- i) $F_t(\mathbf{l}, \mathbf{k}|0^+, i\tau^+) = F_t(\mathbf{l}, \mathbf{k}|0^+, i\tau^-) = F(\mathbf{l}, \mathbf{k}|0^+, i\tau).$
- ii) $F_t(\mathbf{l}, \mathbf{k}|0^-, i\tau^+) = F_t(\mathbf{l}, \mathbf{k}|0^-, i\tau^-) = F(\mathbf{l}, \mathbf{k}|0^-, i\tau).$

$$(0 < \tau < t)$$

[Proof]

$$\begin{aligned} F_t(\mathbf{l}, \mathbf{k}|0^+, i\tau^+) &= \frac{Z_0}{Z} \langle e^{-\int_0^\beta du H'(u)} \alpha_l^{-q} e^{-i\int_\tau^0 du H'(iu)} \alpha_k^q(i\tau) \\ &\quad \times e^{-i\int_t^\tau du H'(iu)} \cdot e^{-i\int_0^t du H'(iu)} \rangle_0 \\ &= \frac{Z_0}{Z} \langle e^{-\int_0^\beta du H'(u)} \cdot \alpha_l^{-q} \cdot e^{-i\int_\tau^0 du H'(iu)} \alpha_k^q(i\tau) e^{-i\int_0^\tau du H'(iu)} \rangle_0 \\ &= F(\mathbf{l}, \mathbf{k}|0^+, i\tau). \end{aligned}$$

The remaining relations can be proved quite in the same way.
(Lemma 2)

$$F_t(\mathbf{l}, \mathbf{k}|0^-, \hat{\xi}) = F_t(\mathbf{l}, \mathbf{k}|0^+, \hat{\xi})$$

for $\hat{\xi} \in [[0^+, \beta]]$.

[Proof]

This is a straightforward consequence of the identity

$$e^{-i\int_t^0 du H'(iu)} e^{-i\int_0^t du H'(iu)} = 1.$$

(Lemma 3)

$$\begin{aligned} F_t(\mathbf{l}, \mathbf{k}|i\tau^-, it) &= F(\mathbf{l}, \mathbf{k}|0^-, i(t-\tau)), \\ F_t(\mathbf{l}, \mathbf{k}|i\tau^+, it) &= F(\mathbf{l}, \mathbf{k}|0^+, i(t-\tau)). \end{aligned}$$

[Proof]

$$\begin{aligned} F_t(\mathbf{l}, \mathbf{k}|i\tau^-, it) &= \frac{1}{Z} \text{Tr} \{ e^{-\beta(H-\mu N)} \cdot e^{iHt} \cdot \alpha_k^q \cdot e^{-iH(t-\tau)} \cdot \alpha_l^{-q} \cdot e^{-iH\tau} \} \\ &= \frac{1}{Z} \text{Tr} \{ e^{-\beta(H-\mu N)} \cdot e^{iH(t-\tau)} \cdot \alpha_k^q \cdot e^{-iH(t-\tau)} \cdot \alpha_l^{-q} \} = F(\mathbf{l}, \mathbf{k}|0^-, i(t-\tau)). \end{aligned}$$

The other part of this lemma can also be proved in the same way.

(Definition)

A connected diagram is called improper whenever it can be made to fall into two parts by eliminating a single Coulomb line. A connected diagram which is not improper is called proper: A proper diagram can never be transformed into a disconnected diagram by cutting a single Coulomb line.

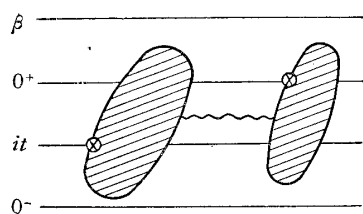


Fig. 11.

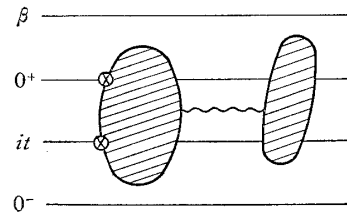


Fig. 12.

An improper diagram has such a form as shown in Fig. 11. There are no diagrams like that in Fig. 12. Examples of proper and improper diagrams are given in Fig. 13.

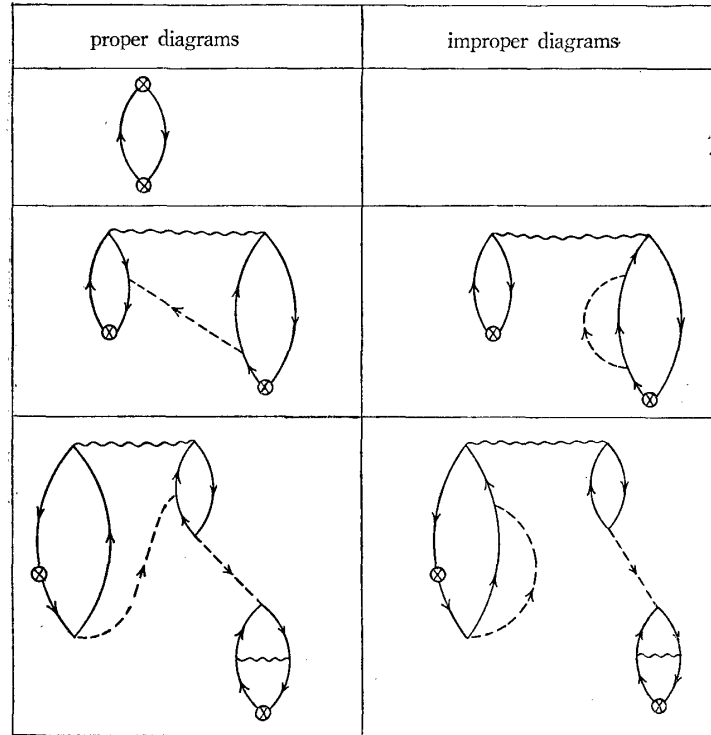


Fig. 13.

(Definition)

We shall define the following function of ξ and η on $L(t)$

$$\Delta_t(\mathbf{l}, \mathbf{k} | \xi, \eta) \equiv \langle P[e^{-\int_{L(t)} du H^I(u)} \cdot \alpha_l^{-q}(\xi) \cdot \alpha_k^q(\eta)] \rangle_{proper}^0, \quad (6.2)$$

where the suffix "proper" indicates that the expression is a sum of proper diagrams. In the following the suffix "t" of Δ_t shall be omitted in the case

$$\Delta_t(\mathbf{l}, \mathbf{k} | 0^\pm, it) = \Delta(\mathbf{l}, \mathbf{k} | 0^\pm, it). \quad (6.3)$$

(Lemma 1')

- i) $\Delta(\mathbf{l}, \mathbf{k} | 0^+, i\tau^+) = \Delta(\mathbf{l}, \mathbf{k} | 0^+, i\tau^-) = \Delta(\mathbf{l}, \mathbf{k} | 0^+, i\tau)$.
- ii) $\Delta(\mathbf{l}, \mathbf{k} | 0^-, i\tau^+) = \Delta(\mathbf{l}, \mathbf{k} | 0^-, i\tau^-) = \Delta(\mathbf{l}, \mathbf{k} | 0^-, i\tau)$.

[Proof]

$$\Delta(\mathbf{l}, \mathbf{k} | 0^+, i\tau^+) = \langle e^{-\int_{(+)}^{\beta} du H^I(u)} \alpha_l^{-q} e^{-i \int_{(-)}^0 du H^I(iu)} \alpha_k^q(i\tau) P[e^{-\int_{[[0^-, i\tau^+]]} du H^I(u)}] \rangle_{proper}^0.$$

In the above expression,

$$P[e^{-\int_{[[0^-, i\tau^+]]} du H'(u)}] \sim e_{(-)}^{-i \int_t^\tau du H'(iu)} \cdot e_{(+)}^{-i \int_0^t du H'(iu)}$$

is shown to be reduced to

$$e_{(+)}^{-i \int_0^\tau du H'(iu)}$$

This is a consequence of the following fact: The contribution of each diagram which has one or more vertices (except \otimes) lying in the interval $[[i\tau^-, i\tau^+]]$ vanishes after the integration over u . Thus, it is proved that

$$\Delta_t(\mathbf{l}, \mathbf{k}|0^+, i\tau^+) = \Delta(\mathbf{l}, \mathbf{k}|0^+, i\tau).$$

The remaining relations of this lemma are proved quite similarly. (Lemma 2')

$$\Delta_t(\mathbf{l}, \mathbf{k}|0^+, \xi) = \Delta_t(\mathbf{l}, \mathbf{k}|0^-, \xi),$$

for $\xi \in [[0^+, \beta]]$.

[Proof]

$$\Delta_t(\mathbf{l}, \mathbf{k}|0^+, \xi) = \langle e_{(+)}^{-\int_\xi^\beta du H'(u)} \cdot \alpha_k^q(\xi) \cdot e_{(+)}^{-\int_0^\xi du H'(u)} \cdot \alpha_l^{-q} P[e^{-\int_{[[0^-, 0^+]]} du H'(u)}] \rangle_{proper}^0.$$

In the above expression,

$$P[e^{-\int_{[[0^-, 0^+]]} du H'(u)}] \sim e_{(-)}^{-i \int_t^0 du H'(iu)} \cdot e_{(+)}^{-i \int_0^t du H'(iu)}$$

is reduced to 1. This is a special case of the fact mentioned in the proof of (Lemma 1'). Thus, we obtain

$$\Delta_t(\mathbf{l}, \mathbf{k}|0^+, \xi) = \langle e_{(+)}^{-\int_\xi^\beta du H'(u)} \cdot \alpha_k^q(\xi) \cdot e_{(+)}^{-\int_0^\xi du H'(u)} \cdot \alpha_l^{-q} \rangle_{proper}^0.$$

It can be shown in the same manner that $\Delta_t(\mathbf{l}, \mathbf{k}|0^-, \xi)$ is reduced to the right-hand side of the above equation.

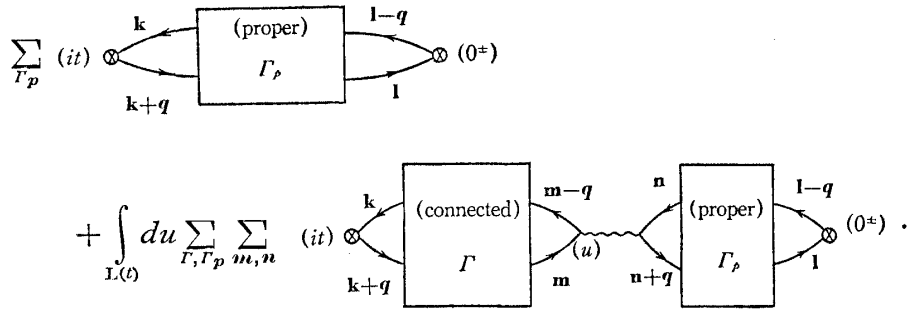
§ 7. Elimination of improper diagrams

Inserting Eq. (2.15) into Eq. (2.20) and using Eq. (4.4), we obtain

$$\sigma(\mathbf{q}, \omega) = \frac{\left(\frac{e^2 \omega}{q^2}\right) \sum_{\mathbf{k}, \mathbf{l}} \int_0^\infty dt \cdot e^{-i\omega t} \{F(\mathbf{l}, \mathbf{k}|0^+, it) - F(\mathbf{l}, \mathbf{k}|0^-, it)\}}{1 + i \left(\frac{4\pi e^2}{q^2}\right) \sum_{\mathbf{k}, \mathbf{l}} \int_0^\infty dt \cdot e^{-i\omega t} \{F(\mathbf{l}, \mathbf{k}|0^+, it) - F(\mathbf{l}, \mathbf{k}|0^-, it)\}} \quad (7.1)$$

It will be shown in the forthcoming discussion that this expression for σ can be reduced to a simple form.

According to Eq. (5.2), $F(\mathbf{l}, \mathbf{k}|0^\pm, it)$ can be expressed as follows:



This expression indicates that the F-function satisfies the following integral equation :

$$\begin{aligned}
 F(\mathbf{l}, \mathbf{k}|0^\pm, it) &= \Delta(\mathbf{l}, \mathbf{k}|0^\pm, it) \\
 &\quad - \left(\frac{4\pi e^2}{q^2}\right) \int_{L(t)} du \sum_{m,n} \Delta_t(\mathbf{l}, \mathbf{n}|0^\pm, u) F_t(\mathbf{m}, \mathbf{k}|u, it). \tag{7.2}
 \end{aligned}$$

The minus sign in front of the last term has its origin in the minus sign found in the exponential function on the right-hand side of Eq. (5.2).

From the integral equation Eq. (7.2) we get

$$\begin{aligned}
 F(\mathbf{l}, \mathbf{k}|0^+, it) - F(\mathbf{l}, \mathbf{k}|0^-, it) &= \Delta(\mathbf{l}, \mathbf{k}|0^+, it) - \Delta(\mathbf{l}, \mathbf{k}|0^-, it) \\
 &\quad - \left(\frac{4\pi e^2}{q^2}\right) \sum_{m,n} \int_{L(t)} du \{ \Delta_t(\mathbf{l}, \mathbf{n}|0^+, u) - \Delta_t(\mathbf{l}, \mathbf{n}|0^-, u) \} F_t(\mathbf{m}, \mathbf{k}|u, it).
 \end{aligned}$$

Based upon Lemma 2' the above path integral can be rewritten as

$$\begin{aligned}
 &\int_{L(t)} du \{ \Delta_t(\mathbf{l}, \mathbf{n}|0^+, u) - \Delta_t(\mathbf{l}, \mathbf{n}|0^-, u) \} \cdot F_t(\mathbf{m}, \mathbf{k}|u, it) \\
 &= i \int_0^t d\tau \{ \Delta_t(\mathbf{l}, \mathbf{n}|0^+, i\tau^-) - \Delta_t(\mathbf{l}, \mathbf{n}|0^-, i\tau^-) \} \cdot F_t(\mathbf{m}, \mathbf{k}|i\tau^-, it) \\
 &\quad - i \int_0^t d\tau \{ \Delta_t(\mathbf{l}, \mathbf{n}|0^+, i\tau^+) - \Delta_t(\mathbf{l}, \mathbf{n}|0^-, i\tau^+) \} \cdot F_t(\mathbf{m}, \mathbf{k}|i\tau^+, it).
 \end{aligned}$$

This is further reduced to

$$\begin{aligned}
 &i \int_0^t d\tau \{ \Delta(\mathbf{l}, \mathbf{n}|0^+, i\tau) - \Delta(\mathbf{l}, \mathbf{n}|0^-, i\tau) \} \\
 &\quad \times \{ F(\mathbf{m}, \mathbf{k}|0^-, i(t-\tau)) - F(\mathbf{m}, \mathbf{k}|0^+, i(t-\tau)) \},
 \end{aligned}$$

by means of Lemma 1' and Lemma 3. Consequently, we obtain

$$\begin{aligned}
 F(\mathbf{l}, \mathbf{k}|0^+, it) - F(\mathbf{l}, \mathbf{k}|0^-, it) &= \Delta(\mathbf{l}, \mathbf{k}|0^+, it) - \Delta(\mathbf{l}, \mathbf{k}|0^-, it) \\
 &\quad + i \left(\frac{4\pi e^2}{q^2}\right) \sum_{m,n} \int_0^t d\tau \{ \Delta(\mathbf{l}, \mathbf{n}|0^+, i\tau) - \Delta(\mathbf{l}, \mathbf{n}|0^-, i\tau) \}
 \end{aligned}$$

$$\times \{F(\mathbf{m}, \mathbf{k}|0^+, i(t-\tau)) - F(\mathbf{m}, \mathbf{k}|0^-, i(t-\tau))\}.$$

This equation is substituted in the numerator of the expression (7.1) for σ , where the following calculation is performed:

$$\begin{aligned} & \sum_{\mathbf{k}, \mathbf{l}} \int_0^\infty dt e^{-i\omega t} \{F(\mathbf{l}, \mathbf{k}|0^+, it) - F(\mathbf{l}, \mathbf{k}|0^-, it)\} \\ &= \sum_{\mathbf{k}, \mathbf{l}} \int_0^\infty dt e^{-i\omega t} \{\Delta(\mathbf{l}, \mathbf{k}|0^+, it) - \Delta(\mathbf{l}, \mathbf{k}|0^-, it)\} \\ &+ i \left(\frac{4\pi e^2}{q^2} \right) \sum_{\mathbf{k}, \mathbf{l}, \mathbf{m}, \mathbf{n}} \int_0^\infty dt \int_0^t d\tau \{\Delta(\mathbf{l}, \mathbf{n}|0^+, i\tau) - \Delta(\mathbf{l}, \mathbf{n}|0^-, i\tau)\} e^{-i\omega\tau} \\ &\times \{F(\mathbf{m}, \mathbf{k}|0^+, i(t-\tau)) - F(\mathbf{m}, \mathbf{k}|0^-, i(t-\tau))\} e^{-i\omega(t-\tau)} \\ &= \left[\sum_{\mathbf{k}, \mathbf{l}} \int_0^\infty d\tau e^{-i\omega\tau} \{\Delta(\mathbf{l}, \mathbf{k}|0^+, i\tau) - \Delta(\mathbf{l}, \mathbf{k}|0^-, i\tau)\} \right] \\ &\times \left[1 + i \left(\frac{4\pi e^2}{q^2} \right) \sum_{\mathbf{m}, \mathbf{n}} \int_0^\infty dt e^{-i\omega t} \{F(\mathbf{m}, \mathbf{n}|0^+, it) - F(\mathbf{m}, \mathbf{n}|0^-, it)\} \right]. \end{aligned}$$

Therefore, we get

$$\sigma(\mathbf{q}, \omega) = \lim_{\delta \rightarrow +0} \left(\frac{e^2 \omega}{q^2} \right) \sum_{\mathbf{k}, \mathbf{l}} \int_0^\infty dt e^{-i\omega t - \delta t} \{\Delta(\mathbf{l}, \mathbf{k}|0^+, it) - \Delta(\mathbf{l}, \mathbf{k}|0^-, it)\}. \quad (7.3)$$

This may be written symbolically as

$$\sigma(\mathbf{q}, \omega) = \lim_{\delta \rightarrow +0} \frac{\omega}{q^2} \int_0^\infty dt e^{-i\omega t - \delta t} \langle [\mathcal{N}(-\mathbf{q}), \mathcal{N}(\mathbf{q}, t)] \rangle_{proper}.$$

§ 8. Discussions

The conventional calculation by means of Kubo's formalism, in which \mathbf{D} is replaced by \mathbf{E} and the Coulomb interaction is neglected, corresponds to the lowest order term of Eq. (7.3) with respect to the Coulomb interaction, if the chemical potential μ is replaced by μ^0 , the chemical potential of the unperturbed system. This term includes all possible diagrams whose structure is shown in Fig. 14. Therefore, it includes all the ring diagrams in Gell-Mann and Brueckner's sense⁵⁾ and, moreover, constitutes the best approximation as for the effective field which polarizes the electrons giving a net electric current.

The correction terms to the simple conventional calculation, other than the correction to the chemical potential μ^0 , must be afforded by proper diagrams

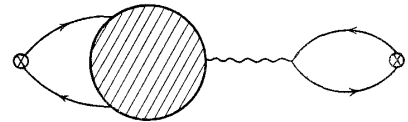


Fig. 14.

corresponding to the following processes. i) The polarized electron and the hole, whose current is measured as a component of the net current, collide with each other or with the electrons constituting the medium. ii) One or more phonons produced by the electric polarization due to the electric field take part in polarizing the "auf" electron whose current is observed.

The introduction of the unknown chemical potential would be a calculational disadvantage of our proper diagram expansion. It will be removed⁶⁾ in our future paper.

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Note added in proof: A diagram expansion given recently by Konstantinov and Perel (reference 2)) seems to be essentially equivalent to that given in § 4 of the present work. The diagram representation presented here is more convenient, because it is more closely related to the Feynman-Goldstone's one.

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