

## Formal Theory of Green Functions

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The formal theory of Green functions is reviewed for many particle problems in nuclear physics or in solid state physics. In particular, one- and two-particle Green functions are discussed in detail. The Feynman amplitudes are also explained together with the effective potential and its applications. This article contains the following sections:

- §1. Preliminary remarks
- §2. Definition of Green functions
- §3. Structure of equations satisfied by Green functions
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### §1. Preliminary remarks

In classical field theories the notion of the Green function originates in considering contributions from a unit source located at a given point to the field strengths at another point. For example, consider a simple kind of scalar field, say  $\phi(x)$ , where  $x$  represents a space-time point  $\mathbf{x}$  and  $t$ . Now we suppose that the field is characterized by the field equation

$$D_x \phi(x) = J(x), \quad (1\cdot1)$$

where  $D_x$  is a linear operator and  $J(x)$  the source function of the field. Eq. (1•1) has a particular solution

$$\phi(x) = \int G(x, x') J(x') d^4 x' \quad (1.2)^*$$

under the condition that  $\phi$  vanishes as  $J$  tends to zero. One calls the kernel function  $G(x, x')$  in the right member of (1.2) the "Green function" or the "propagator". Owing to the linearity of the operator  $D_x$ , the Green function  $G(x, x')$  is independent of  $J(x)$  and consequently, is written down as follows;

$$G(x, x') = \frac{\delta\phi(x)}{\delta J(x')} \quad (1.3)$$

(About the functional derivative, see Appendix I. In particular, refer to Eq. (A.3).) From (1.1) and (1.3) we immediately obtain the equation for  $G$

$$D_x G(x, x') = \delta^{(4)}(x - x'), \quad (1.4)$$

where the formula  $\delta J(x)/\delta J(x') = \delta^{(4)}(x - x')$  has been used, and  $\delta^{(4)}(x) = \delta(x)\delta(t)$  is the four-dimensional delta function. The form of Eq. (1.4) or (1.2) permits us to interpret the Green function\*\* as contributions from a unit source. Therefore all the problems have been reduced to solving Eq. (1.4) under the appropriate boundary conditions.

In nonlinear field theories we have not so simple relations between the field and the source as in linear theories. Taking into account the condition that  $\phi$  is so chosen as to vanish when  $J$  tends to zero, the field  $\phi$  could be expanded in the Taylor type of series:

$$\begin{aligned} \phi(x) = & \int \left[ \frac{\delta\phi(x)}{\delta J(x')} \right]_{J=0} J(x') d^4 x' \\ & + \frac{1}{2!} \iint \left[ \frac{\delta^2\phi(x)}{\delta J(x')\delta J(x'')} \right]_{J=0} J(x') J(x'') d^4 x' d^4 x'' + \dots \end{aligned} \quad (1.5)$$

Thus the simple relation like (1.2) between the field and source holds only for an infinitesimally small source  $\delta J(x)$ , that is,

$$\phi(x) = \int G(x, x') \delta J(x') d^4 x', \quad (1.6)$$

where the Green function in nonlinear theories should be defined by

$$G(x, x') \equiv \lim_{J \rightarrow 0} \frac{\delta\phi(x)}{\delta J(x')} \quad (1.7)$$

In general, the Green function obeys the complicated equation

\* In what follows, we shall use the abbreviation  $d^4 x = d^3 x dt$ .

\*\* Mathematically speaking, the Green function is nothing but the elementary solution of the equation  $D_x u = 0$ .

$$\mathcal{D}_x G(x, x') = \delta^{(4)}(x - x'). \quad (1.8)$$

The operator  $\mathcal{D}_x$  is not necessarily equal to  $D_x$ , and is defined by

$$\mathcal{D}_x G(x, x') \equiv \lim_{J \rightarrow 0} \frac{\delta}{\delta J(x')} D_x[\phi] = \int \left[ \frac{\delta D_x[\phi]}{\delta \phi(x'')} \right]_{J=0} G(x'', x') d^4 x''. \quad (1.9)$$

In other words the operator  $\mathcal{D}_x$  (and then the equation of  $G$ ) cannot be constructed, unless we have the full knowledge about  $\phi$ .

We can also introduce in a natural way the Green function method into second-quantized theories of many-particle systems or into quantum field theories. The field is described by the operator function  $\phi(x)$  obeying the following type of equation:

$$D_x \phi(x) = J(x), \quad (1.10)$$

where  $D_x$  is a linear or nonlinear operator and  $J(x)$  a  $c$ -number function representing an external source distribution. In order to introduce the ( $c$ -number) Green function in a way analogous to that in classical theories, we must prepare the expectation value  $\langle \phi(x) \rangle$  of the field operator  $\phi(x)$ . To do this, we first consider the expectation value of an operator, say  $Q$ , which is defined by

$$\langle Q \rangle \equiv \langle m | Q | m \rangle, \quad (1.11a)$$

$|m\rangle$  being the state of the medium. When the medium is in a mixed state described by a density matrix  $\rho$ , (1.11a) must be replaced with

$$\langle Q \rangle \equiv \text{Tr}\{\rho Q\} / \text{Tr}\{\rho\}, \quad (1.11b)$$

where

$$\rho \equiv \sum_m |m\rangle w_m \langle m|, \quad (1.12)$$

$w_m$  being the weight factor of a state  $|m\rangle$  in the mixed state of the medium. In practical cases we often choose, as the state  $|m\rangle$ , an eigenstate of the total Hamiltonian of the system. However, since eigenstates of the total Hamiltonian are not stationary in the presence of the time-dependent external field or source, specification of states by them becomes not to be meaningful. Thus it is required to modify the definition (1.11a) or (1.11b) (and (1.12)) in the presence of the time-dependent external source. To do this, we have only to design the external source in such a way that it is independent of time at the beginning and at the end of the process. Consequently the eigenstates,  $|m_I\rangle$  at the beginning and  $|m_F\rangle$  at the end, of the total Hamiltonian may be utilized for the purpose of specification of states. Assuming\* that  $|m_F\rangle$  approaches to  $|m_I\rangle$  as

\* If the state  $|m\rangle$  is the non-degenerate ground state of the medium, this assumption is valid. Otherwise, this may mean that one must select an appropriate class of variations for the external sources. And see 3).

the external source tends to zero, we may generalize the definition (1.11a) or (1.11b) as follows;

$$\langle Q \rangle \equiv \langle m_F | Q | m_I \rangle / \langle m_F | m_I \rangle \quad (1.11a')$$

$$\text{or} \quad \equiv \text{Tr} \{ \rho Q \} / \text{Tr} \{ \rho \}, \quad (1.11b')$$

where

$$\rho \equiv \sum_m | m_I \rangle w_m \langle m_F |. \quad (1.12')$$

Owing to the definition (1.11a) or (1.11b), we can now consider the expectation value  $\langle \phi(x) \rangle$  of the second-quantized field operator  $\phi(x)$ . The function  $\langle \phi(x) \rangle$  has a non-vanishing value only in the presence of the external source, because, when  $J=0$ , the operator  $\phi(x)$  has an effect of decreasing the particle number by one\* and then  $\langle m | \phi | m \rangle = 0$ . Hence the function  $\langle \phi(x) \rangle$  could be expanded in the same type of series as (1.5), that is,

$$\begin{aligned} \langle \phi(x) \rangle &= \int \left[ \frac{\delta \langle \phi(x) \rangle}{\delta J(x')} \right]_{J=0} J(x') d^4 x' \\ &+ \frac{1}{2!} \iint \left[ \frac{\delta^2 \langle \phi(x) \rangle}{\delta J(x') \delta J(x'')} \right]_{J=0} J(x') J(x'') d^4 x' d^4 x'' + \dots \end{aligned} \quad (1.13)$$

In linear cases the right member of (1.13) vanishes except the first term. In general, we can write the formula

$$\langle \phi(x) \rangle = \int G(x, x') \delta J(x') d^4 x' \quad (1.14)$$

only for an infinitesimally small source  $\delta J(x)$ . Here the function defined by

$$G(x, x') \equiv \lim_{J \rightarrow 0} \frac{\delta \langle \phi(x) \rangle}{\delta J(x')} \quad (1.15)$$

is to be regarded as the Green function in second-quantized theories of many-particle systems.

The above function  $G(x, x')$  is called the one-particle Green function which describes one-particle (or one-hole) propagations in a medium. To describe two or more particle propagations, we would necessitate the two- or many-particle Green function which will be defined in the next section.

In interacting systems the Green functions obey the very complicated equations, in which the operators may not be constructed unless the problem is completely solved. Nevertheless, it is known that the Green function method is very useful for the purpose of approximate calculations

\* Strictly speaking,  $\phi$  should change the difference between numbers of particles and holes by one.

or general discussions of some physical quantities. The purpose of this article is to study the structures of the Green functions and the equations satisfied by them, and to explain their applications to some many-particle problems.

The Green function method has originally been introduced by Feynman<sup>1)</sup> and Schwinger<sup>2)</sup> into quantum field theories, and has been developed by many authors.

## §2. Definition of Green functions

For the moment let us consider the system composed of two kinds of particles, one being bosons and the other fermions, and denote the boson field by  $\phi(x)$  and the fermion field by  $\psi(x)$ , respectively. For simplicity  $\phi(x)$  is a real scalar field, namely, it describes neutral particles without spin. The Lagrangian density of the system is a function of the field operators and their derivatives with respect to space and time variables. In order to introduce artificially the external sources,  $J(x)$  for bosons and  $\eta(x)$  for fermions, one must add the extra term

$$-\phi(x)J(x) - \sum_{\alpha} \psi_{\alpha}^{*}(x)\eta_{\alpha}(x) - \sum_{\alpha} \eta_{\alpha}^{*}(x)\psi_{\alpha}(x) \quad (2.1)$$

to the Lagrangian density. The subscript  $\alpha$  stands for the spinor index. Here it is noted that  $\eta(x)$  is only a  $c$ -number function which is anti-commutable with other spinors. Following discussions given in the previous section, we may define the one-boson Green function  $K(x, x')$  and the one-fermion Green function  $G(x, x')$  by

$$K(x, x') \equiv \lim_{J, \eta \rightarrow 0} \frac{\delta \langle \phi(x) \rangle}{\delta J(x')},$$

$$G_{\alpha\beta}(x, x') \equiv \lim_{J, \eta \rightarrow 0} \frac{\delta \langle \psi_{\alpha}(x) \rangle}{\delta \eta_{\beta}(x')}, \quad (2.2)$$

respectively. By making use of the formulas prepared in Appendix II, the functional derivatives in (2.2) become

$$\frac{\delta \langle \phi(x) \rangle}{\delta J(x')} = \frac{1}{i\hbar} \{ \langle T(\phi(x)\phi(x')) \rangle - \langle \phi(x) \rangle \langle \phi(x') \rangle \},$$

$$\frac{\delta \langle \psi_{\alpha}(x) \rangle}{\delta \eta_{\beta}(x')} = \frac{1}{i\hbar} \{ \langle T(\psi_{\alpha}(x)\psi_{\beta}^{*}(x')) \rangle - \langle \psi_{\alpha}(x) \rangle \langle \psi_{\beta}^{*}(x') \rangle \},$$

which yield the explicit definitions

$$K(x, x') = \frac{1}{i\hbar} \langle T(\phi(x)\phi(x')) \rangle,$$

$$G_{\alpha\beta}(x, x') = \frac{1}{i\hbar} \langle T(\psi_\alpha(x)\psi_\beta^*(x')) \rangle. \quad (2.3)$$

Here the symbol  $\langle \dots \rangle$  must be equated to (1.11a) or (1.11b).

Now we briefly explain a physical content of the Green function. For example, consider the one-fermion Green function defined in a pure state of the medium, that is,

$$G(x, x') = \frac{1}{i\hbar} \langle m | T(\psi(x)\psi^*(x')) | m \rangle. \quad (2.4)^*$$

The expression for  $t > t'$ ,  $G(x, t; x', t') = (i\hbar)^{-1} \langle m | \psi(x, t)\psi^*(x', t') | m \rangle$ , may permit us to interpret the Green function as the amplitude for propagation from  $x'$  to  $x$  of a particle. On the contrary, the Green function for  $t < t'$  may be explained as the amplitude for propagation from  $x$  to  $x'$  of a hole. In interacting system, however, such an interpretation could be justified only for the asymptotic behaviors. Nevertheless, the above interpretation is frequently used with understanding that it is only a crude interpretation. With similarly crude interpretations, therefore, we may define the two- and many-particle Green functions by the analogous expressions

$$\left. \begin{aligned} G_{\text{II}}(x_1, x_2; x'_1, x'_2) &\equiv \lim_{J, \eta \rightarrow 0} \frac{\delta^2 \langle T(\psi(x_1)\psi(x_2)) \rangle}{\delta\eta(x'_1)\delta\eta(x'_2)} \\ &= (i\hbar)^{-2} \langle T(\psi(x_1)\psi(x_2)\psi^*(x'_2)\psi^*(x'_1)) \rangle \\ G_{\text{III}}(x_1, x_2, x_3; x'_1, x'_2, x'_3) &\equiv \lim_{J, \eta \rightarrow 0} \frac{\delta^3 \langle T(\psi(x_1)\psi(x_2)\psi(x_3)) \rangle}{\delta\eta(x'_1)\delta\eta(x'_2)\delta\eta(x'_3)} \\ &= (i\hbar)^{-3} \langle T(\psi(x_1)\psi(x_2)\psi(x_3)\psi^*(x'_3)\psi^*(x'_2)\psi^*(x'_1)) \rangle, \end{aligned} \right\} (2.5)$$

and

$$\left. \begin{aligned} K_{\text{II}}(x_1, x_2; x'_1, x'_2) &\equiv \lim_{J, \eta \rightarrow 0} \frac{\delta^2 \langle T(\phi(x_1)\phi(x_2)) \rangle}{\delta J(x'_1)\delta J(x'_2)} \\ &= (i\hbar)^{-2} \langle T(\phi(x_1)\phi(x_2)\phi(x'_1)\phi(x'_2)) \rangle. \end{aligned} \right\}$$

In §5 and §6 readers will find more detailed discussions on the relationships between the Green functions and some important quantities.

In practical cases we often deal with particles moving in the medium which is in the ground state or in thermal equilibrium with temperature  $T = (1/\beta)$ . The former case is concerned with some nuclear problems or problems of matter near zero degree in absolute temperature. The latter is used for some finite temperature problems, in which the Green function

\* Here we have suppressed the spinor indices. In what follows we shall not write them explicitly.

$$G(\mathbf{x}, \mathbf{x}') = (i\hbar)^{-1} \text{Tr} \{ e^{-\beta H} T(\psi(\mathbf{x})\psi^*(\mathbf{x}')) \} / \text{Tr} \{ e^{-\beta H} \} \quad (2\cdot6)^*$$

is called the *time-temperature* Green function. If  $t$  and  $t'$  are replaced in (2·6) by  $i\beta$  and  $i\beta'$ , we obtain the temperature Green function which was first introduced by Matsubara.<sup>6)</sup> The temperature Green functions are extensively used in statistical mechanics.

Next, we shall explain a qualitative relation between the space-time variation of the Green function and the uniformity of the medium. Differentiating the Green function with respect to  $\mathbf{x}$ , one gets

$$\nabla G(\mathbf{x}, t; \mathbf{x}', t') = -\nabla' G(\mathbf{x}, t; \mathbf{x}', t') + \hbar^{-2} \langle [T(\psi(\mathbf{x}, t)\psi^*(\mathbf{x}', t')), P] \rangle. \quad (2\cdot7)$$

Here we have used the equation

$$\nabla \psi(\mathbf{x}, t) = \frac{i}{\hbar} [P, \psi(\mathbf{x}, t)], \quad (2\cdot8)$$

$P$  being the total momentum operator

$$P \equiv \int \psi^*(\mathbf{x}, t) \frac{\hbar}{i} \nabla \psi(\mathbf{x}, t) d^3\mathbf{x}. \quad (2\cdot9)$$

If the state  $|m\rangle$  is an eigenstate of  $P$  or the density matrix  $\rho$  is commutable with  $P$ , in other words, if the medium is uniform in space, the last term in the right-hand side of (2·7) vanishes and the function  $G$  satisfies the equation

$$(\nabla + \nabla') G(\mathbf{x}, t; \mathbf{x}', t') = 0. \quad (2\cdot10)$$

Eq. (2·10) means that  $G$  is a function depending only on the difference  $\mathbf{x} - \mathbf{x}'$  with respect to the spatial coordinates, that is to say, a uniform function irrelevant to the origin of the coordinate system. Concerning the problems for finite nuclei or surface of solid, the medium is not uniform and consequently,  $G$  is not uniform function satisfying Eq. (2·10). Similarly we can regard  $G$  as uniform with respect to the time coordinate, when and only when the state  $|m\rangle$  is an eigenstate of the total Hamiltonian or the density matrix  $\rho$  is commutable with the total Hamiltonian. If the medium is uniform in space and time,  $G(\mathbf{x}, \mathbf{x}')$  is written down as a function of  $\mathbf{x} - \mathbf{x}'$  and  $t - t'$ .

In the presence of time- and space-dependent external sources or fields, the Green functions and other quantities are not uniform in time and space.

Finally it is noted that, by intervention of the spinor sources, the

\*  $H$  is often replaced with  $H - \mu N$ , where  $\mu$  is the chemical potential and  $N$  the operator corresponding to the number of particles.

calculations become considerably troublesome due to the strange properties of  $\eta$  or  $\eta^*$ . Therefore it is desired to calculate the Green functions or other important quantities without resort to  $\eta$  or  $\eta^*$ . For this purpose, (as will be seen in the next section) we have only to introduce the additional term  $-\psi^*(x)\psi(x)\varphi(x)$ , into the Lagrangian density, where  $\varphi(x)$  is a real and scalar external field.

### §3. Structure of equations satisfied by Green functions

In the present section the equations of the Green functions will be derived from their definitions and the fundamental equation. The structures of the Green functions will be suggested by investigating the equations, on which one can proceed to calculate the perturbation series of the Green functions. For the practical purpose we shall restrict ourselves to systems described by the Lagrangian density

$$L \equiv i\hbar\psi^*(x)\frac{\partial\psi(x)}{\partial t} - \frac{\hbar^2}{2m}\nabla\psi^*(x)\cdot\nabla\psi(x) - \frac{1}{2}\int\psi^*(x)\psi^*(x')U(x-x')\psi(x')\psi(x)d^4x', \quad (3\cdot1)$$

where  $\psi(x)$  is a spinor field of fermions and  $U(x-x') \equiv V(x-x')\delta(t-t')$ ,  $V(x-x')$  being the potential for the two-particle interaction. Moreover it is assumed that  $U(x-x')$  is a symmetric function of  $x$  and  $x'$ . The Lagrangian density (3.1) yields the Hamiltonian

$$H = \int\psi^*(x)\left[-\frac{\hbar^2}{2m}\nabla^2\right]\psi(x)d^3x + \frac{1}{2}\iint\psi^*(x)\psi^*(x')U(x-x')\psi(x')\psi(x)d^4xd^3x' \quad (3\cdot2)$$

and the field equation

$$i\hbar\frac{\partial}{\partial t}\psi(x) = \left[-\frac{\hbar^2}{2m}\nabla^2 + \int\psi^*(x')U(x-x')\psi(x')d^4x'\right]\psi(x). \quad (3\cdot3)$$

For the sake of mathematical convenience mentioned at the end of the last section, we introduce a  $c$ -number external field  $\varphi(x)$  by adding the term

$$-\psi^*(x)\psi(x)\varphi(x) \quad (3\cdot4)$$

to the Lagrangian density. This results in the modification

$$-\frac{\hbar^2}{2m}\nabla^2 \rightarrow -\frac{\hbar^2}{2m}\nabla^2 + \varphi(x)$$



in (3.2) and (3.3). Thus  $\psi(x)$  obeys the equation

$$i\hbar \frac{\partial}{\partial t} \psi(x) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + \varphi(x) + \int \psi^*(x') U(x-x') \psi(x') d^4x' \right] \psi(x). \quad (3.5)$$

Following discussions in Appendix II, we can utilize the formula

$$i\hbar \frac{\delta}{\delta \varphi(x)} \langle Q \rangle = \langle T \{ Q \psi^*(x) \psi(x) \} \rangle - \langle Q \rangle \langle \psi^*(x) \psi(x) \rangle. \quad (3.6)$$

Differentiating (2.3) with respect to  $t$ , we get

$$\frac{\partial}{\partial t} G(x, x') = (i\hbar)^{-1} \delta^{(4)}(x-x') + (i\hbar)^{-1} \langle T \left\{ \frac{\partial \psi(x)}{\partial t} \psi^*(x') \right\} \rangle, \quad (3.7)$$

where the delta function comes from the jump of  $G$  at its discontinuous point  $t=t'$ . Substituting (3.3) into (3.7), one immediately obtains the equation

$$\begin{aligned} \left[ i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 \right] G(x, x') &= \delta^{(4)}(x-x') \\ &+ (i\hbar)^{-1} \int d^4x'' U(x-x'') \langle T(\psi^*(x'') \psi(x'') \psi(x) \psi^*(x')) \rangle \end{aligned}$$

for the one-particle Green function. The last term of the right member can be written in terms of the two-particle Green function, that is

$$\begin{aligned} \left[ i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 \right] G(x, x') &= \delta^{(4)}(x-x') \\ &- i\hbar \int d^4x'' U(x-x'') G_{\text{II}}(x, x''; x', x''). \end{aligned} \quad (3.8)$$

Thus the one-particle Green function is coupled with the two-particle Green function. Similarly the equation of  $G_{\text{II}}$  includes the one-particle Green function  $G$  and the three-particle Green function  $G_{\text{III}}$ . In general, the equation of the  $N$ -particle Green function  $G_N$  is participated with the  $(N \pm 1)$ -particle Green function. Hence we have arrived at the set of simultaneous equations for an infinite number of Green functions,  $G, G_{\text{II}}, G_{\text{III}}, \dots$  as follows; besides (3.8),

$$\begin{aligned} \left[ i\hbar \frac{\partial}{\partial t_1} + \frac{\hbar^2}{2m} \nabla_1^2 \right] G_N(x_1, \dots, x_N; x'_1, \dots, x'_N) \\ + i\hbar \int d^4x_{N+1} U(x_1 - x_{N+1}) G_{N+1}(x_1, \dots, x_{N+1}; x'_1, \dots, x'_{N+1}) \\ = \sum_{i=1}^N \delta^{(4)}(x_1 - x'_i) (-1)^{i-1} G_{N-1}(x_2, \dots, x_N; x'_1 \dots x'_{i-1}, x'_{i+1} \dots x'_N) \\ (N \geq 2). \end{aligned} \quad (3.9)$$

We may as well obtain, in a compact form, the equation to be satisfied by the one-particle Green function alone, by eliminating other Green functions. This procedure may be achieved by means of functional differentiation with respect to  $\varphi(x)$  introduced at the beginning of the present section. In the following subsections, we shall investigate the structures of the equations satisfied by the one-particle Green function and by the two-particle Green function.

### 3.1 One-particle Green function

Denote the Green function in the external field  $\varphi$  by  $G_\varphi$ .  $G_\varphi$  obeys the equation

$$\left[ i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 - \varphi(x) \right] G_\varphi(x, x') = \delta^{(4)}(x - x') \\ + (i\hbar)^{-1} \int d^4x'' U(x - x'') \langle T(\psi^*(x'') \psi(x'') \psi(x) \psi^*(x')) \rangle.$$

Using (3.6), we can rewrite the last term of the right member as follows;

$$(i\hbar)^{-1} \int d^4x'' U(x - x'') \langle T(\psi^*(x'') \psi(x'') \psi(x) \psi^*(x')) \rangle \\ = \bar{V}_\varphi(x) G_\varphi(x, x') + i\hbar \int d^4x'' U(x - x'') \frac{\delta}{\delta\varphi(x'')} G_\varphi(x, x'),$$

where we have used the abbreviation

$$\bar{V}_\varphi(x) \equiv \int d^4x'' U(x - x'') \langle \psi^*(x'') \psi(x'') \rangle \\ = -i\hbar \int d^4x'' U(x - x'') \text{tr} G_\varphi(x'', t''; x'', t'' + 0), \quad (3.10)$$

where tr stands for the trace on spinor indices. Hence the equation for  $G_\varphi$  becomes

$$\left[ i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 - \varphi(x) - \bar{V}_\varphi(x) \right. \\ \left. - i\hbar \int d^4x'' U(x - x'') \frac{\delta}{\delta\varphi(x'')} \right] G_\varphi(x, x') = \delta^{(4)}(x - x'). \quad (3.11)$$

This includes only the one-particle Green function. Here it must be remembered that the function  $\varphi(x)$  is to be put equal to zero everywhere after all calculations have been completed. The function defined by

$$\bar{V}(x) \equiv \lim_{\varphi \rightarrow 0} \bar{V}_\varphi(x) = \int \langle m | \psi^*(x'', t) \psi(x'', t) | m \rangle V(x - x'') d^3x'' \\ \text{or} \quad = \int \frac{\text{Tr} \{ \rho \psi^*(x'', t) \psi(x'', t) \}}{\text{Tr} \{ \rho \}} V(x - x'') d^3x'' \quad (3.12)$$

is interpreted as the *static average potential* for a particle moving in the medium. Since the state  $|m\rangle$  is an eigenstate of  $H$  or is commutable with  $H$ , the function  $\bar{V}(\mathbf{x})$  is independent of time. On the other hand  $\bar{V}(\mathbf{x})$  is naturally reduced to a constant independent of  $\mathbf{x}$  if  $G$  is uniform in space, in other words, if the medium is in an eigenstate of the total momentum operator  $\mathbf{P}$  or in a mixed state described by  $\rho$  commutable with  $\mathbf{P}$ . The dependence of  $\bar{V}(\mathbf{x})$  on space coordinates is a reflection of the non-uniformity of the medium. Moreover it is easy to see that  $\bar{V}(\mathbf{x})$  is a real function.

The last term\* of the left member in (3.11), after the limit  $\varphi \rightarrow 0$ , represents the *exchange effects* between the particle in consideration and the medium particles or among the medium particles and the *pair-excitation effects* of the medium caused by motions of the particle, because the operation  $\delta/\delta\varphi(x)$  means the creation of a particle-hole pair at  $x$ . Such a term is to be regarded as the result of elimination of many-particle Green functions in the set of equations, in which their participation means all possible exchanges among particles and all possible excitations of the medium. The situation (or effect of  $\delta/\delta\varphi$ ) is well visualized by introducing the graphical method developed in quantum field theory.

In order to introduce the graphical method analogous to relativistic vacuum field theories, it is of essential importance to utilize extensively the fact that the annihilation operator  $\psi$  can be interpreted as a creation operator of a hole in the medium when applied to the state vector of the medium. This resembles the creation operator for anti-particles in relativistic vacuum field theory. However, there is an essential difference between relativistic vacuum field theory and the present theory. In the present theory  $\psi$  cannot always be interpreted as a creation operator of a hole, because the medium has only a finite number of degrees of freedom. Hence it must be understood that the complete parallelism between both theories holds if we discard the terms vanishing at the limit of infinite freedom of the medium.

For the purpose of formulating the graphical method, we first assume the existence of the inverse function  $G_\varphi^{-1}(x, x')$  satisfying the relations

$$\begin{aligned} \int G_\varphi^{-1}(x, x'') G_\varphi(x'', x') d^4x'' &= \delta^{(4)}(x - x'), \\ \int G_\varphi(x, x'') G_\varphi^{-1}(x'', x') d^4x'' &= \delta^{(4)}(x - x'). \end{aligned} \quad (3.13)$$

\* It may be worth while to remark that the Green function is free from divergences because the functional differentiation occurs only in the integral with the kernel  $U(x-x')$ . In contrast with this, the equation of the Green function contains the corresponding term  $\lim_{\varphi \rightarrow 0} (\delta/\delta\varphi(x)) G_\varphi(x, x')$  in some cases of divergent field theories.

In other words, the inverse function  $G_\varphi^{-1}$  is nothing but the operator applied to  $G_\varphi$ , although it must be written as an integral operator. Now define the quantities  $\langle\varphi(x)\rangle$  and  $\Delta_\varphi(x, x')$  by

$$\begin{aligned}\langle\varphi(x)\rangle &\equiv \varphi(x) + \bar{V}_\varphi(x) - \bar{V}(x), \\ \Delta_\varphi(x, x') &\equiv \int d^4x'' U(x-x'') \frac{\delta\langle\varphi(x'')\rangle}{\delta\varphi(x'')}.\end{aligned}\quad (3\cdot14)$$

Then Eq. (3\cdot11) becomes

$$\begin{aligned}\left[ i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 - \bar{V}(x) - \langle\varphi(x)\rangle \right. \\ \left. - i\hbar \int d^4x'' \Delta_\varphi(x, x'') \frac{\delta}{\delta\langle\varphi(x'')\rangle} \right] G_\varphi(x, x') = \delta^{(4)}(x-x').\end{aligned}\quad (3\cdot15)$$

The functions  $\langle\varphi(x)\rangle$  and  $\Delta_\varphi(x, x')$  are respectively regarded as the external field and the two-particle potential modified by interaction with the medium. Differentiating one of (3\cdot13) with respect to  $\langle\varphi(x)\rangle$ , we immediately obtain the formula

$$\frac{\delta G_\varphi(x, x')}{\delta\langle\varphi(x'')\rangle} = - \iint G_\varphi(x, \xi) \frac{\delta G_\varphi^{-1}(\xi, \zeta)}{\delta\langle\varphi(x'')\rangle} G_\varphi(\zeta, x') d^4\xi d^4\zeta.\quad (3\cdot16)$$

Replacing the functional derivative in (3\cdot15) with (3\cdot16), one can find the explicit form of the integral operator  $G_\varphi^{-1}$  as follows;

$$G_\varphi^{-1}(x, x') = \left[ i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 - \bar{V}(x) - \langle\varphi(x)\rangle \right] \delta^{(4)}(x-x') - \Pi_\varphi(x, x'),\quad (3\cdot17)$$

where we have used the abbreviation

$$\Pi_\varphi(x, x') \equiv i\hbar \iint d^4x'' d^4\xi \Delta_\varphi(x, x'') G_\varphi(x, \xi) \Gamma_\varphi(\xi, x'; x''),\quad (3\cdot18)$$

$\Gamma_\varphi$  being defined by

$$\Gamma_\varphi(\xi, \zeta; x'') \equiv - \frac{\delta G_\varphi^{-1}(\xi, \zeta)}{\delta\langle\varphi(x'')\rangle}.\quad (3\cdot19)$$

Here let us define the quantity  $\Sigma_\varphi$  by

$$\Sigma_\varphi(x, x') \equiv \bar{V}(x) \delta^{(4)}(x-x') + \Pi_\varphi(x, x').\quad (3\cdot20)$$

Then  $G_\varphi^{-1}$  is rewritten as

$$G_\varphi^{-1}(x, x') = \left[ i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 - \langle\varphi(x)\rangle \right] \delta^{(4)}(x-x') - \Sigma_\varphi(x, x'),\quad (3\cdot21)$$

from which we find the relation

$$\Gamma_{\varphi}(\xi, \zeta; x'') = \delta^{(4)}(\xi - \zeta) \delta^{(4)}(\xi - x'') + \frac{\delta \Sigma_{\varphi}(\xi, \zeta)}{\delta \langle \varphi(x'') \rangle}. \quad (3.22)$$

For  $\Delta_{\varphi}$  and  $\langle \varphi \rangle$  we obtain the equations

$$\begin{aligned} \Delta_{\varphi}(x, x') &= U(x - x') - (i\hbar) \text{tr} \iiint d^4x'' d^4\xi' d^4\xi'' d^4\zeta' \Delta_{\varphi}(x, \zeta') \\ &\times \Gamma_{\varphi}(\xi', \xi''; \zeta') G_{\varphi}(\xi'', x'') G_{\varphi}(x'', \xi') U(x'' - x') \end{aligned} \quad (3.23)$$

and

$$\begin{aligned} \langle \varphi(x) \rangle &= \varphi(x) - i\hbar \int d^4x'' U(x - x'') \text{tr} [G_{\varphi}(x'', t''; x'', t'' + 0) \\ &- G(x'', t''; x'', t'' + 0)] \end{aligned} \quad (3.24)$$

from (3.10) and (3.14). Here it may be convenient to introduce the polarization term defined by

$$P_{\varphi}(\zeta', x'') \equiv (i\hbar) \text{tr} \iint d^4\xi' d^4\xi'' \Gamma_{\varphi}(\xi', \xi''; \zeta') G_{\varphi}(\xi'' x'') G_{\varphi}(x'', \xi'), \quad (3.25)$$

so that we can rewrite (3.23) as

$$\Delta_{\varphi}(x, x') = U(x - x') - \iint d^4\zeta' d^4x'' \Delta_{\varphi}(x, \zeta') P_{\varphi}(\zeta', x'') U(x'' - x'). \quad (3.23')$$

Therefore we have formulated a set of six equations in the six unknowns,  $G_{\varphi}$ ,  $\Delta_{\varphi}$ ,  $\Sigma_{\varphi}$ ,  $\Gamma_{\varphi}$ ,  $P_{\varphi}$  and  $\langle \varphi \rangle$ , which are rewritten in matrix form as follows:

$$\left[ \mathbf{p}_0 - \frac{1}{2m} \mathbf{p}^2 - \langle \varphi \rangle - \Sigma_{\varphi} \right] G_{\varphi} = 1, \quad (3.26a)$$

$$\Sigma_{\varphi} = -i\hbar U G + i\hbar \Delta_{\varphi} G_{\varphi} \Gamma_{\varphi}, \quad (3.26b)$$

$$\Delta_{\varphi} = U - \Delta_{\varphi} P_{\varphi} U, \quad (3.26c)$$

$$P_{\varphi} = i\hbar \Gamma_{\varphi} G_{\varphi} G_{\varphi}, \quad (3.26d)$$

$$\Gamma_{\varphi} = 1 + \frac{\delta \Sigma_{\varphi}}{\delta \langle \varphi \rangle}, \quad (3.26e)$$

$$\langle \varphi \rangle = \varphi - i\hbar U (G_{\varphi} - G), \quad (3.26f)$$

where we used the matrix notations, such as  $\langle x | p_0 | x' \rangle \equiv (i\hbar \partial / \partial t) \delta^{(4)}(x - x')$ ,  $\langle x | \mathbf{p} | x' \rangle = (\hbar/i) \nabla \delta^{(4)}(x - x')$ ,  $\langle x | \Sigma_{\varphi} | x' \rangle \equiv \Sigma_{\varphi}(x, x')$ ,  $\langle x | G_{\varphi} | x' \rangle = G_{\varphi}(x, x')$ , and so on.

Here it may be of interest to remark the resemblance of the equation

$$\left[ i\hbar \int d^4x'' U(x - x'') \frac{\delta}{\delta \varphi(x'')} \right] G_{\varphi}(x, x') = \int d^4\zeta \Pi_{\varphi}(x, \zeta) G_{\varphi}(\zeta, x') \quad (3.27)$$

obtained in derivation of (3·26) to the ordinary eigenvalue problem of a differential operator. The ordinary eigenvalue problem is characterized by the equation

$$Ly = \lambda y$$

and a boundary condition imposed on  $y$ , where  $L$  is a differential operator,  $\lambda$  its eigenvalue, and  $y$  its eigenfunction belonging to  $\lambda$ . There,  $\lambda$  and  $y$  depend sensitively on the boundary condition. Corresponding to different boundary conditions, one must find different sets of eigenvalues and eigenfunctions of the same operator  $L$ . Here equate the operator  $i\hbar \int d^4x'' U(x-x'') (\delta/\delta\varphi(x''))$  with  $L$ ,  $\Pi_\varphi$  with  $\lambda$  and  $G_\varphi$  with  $y$ , respectively. Then  $\Pi_\varphi$  may be regarded as an eigenvalue of a functional differential operator. In fact, Eq. (3·27) always has the same form whatever may be the medium, in which the particle moves, and whatever boundary conditions may be imposed on  $G_\varphi$ . However, the equation, after the replacement (3·27), is sensitive to the boundary conditions or the state of the medium. Therefore the replacement (3·27) may be regarded as a sort of eigenvalue equation accompanied with an appropriate boundary condition.

All the needed quantities are obtained from the  $\varphi$ -dependent functions by the limit operation  $\varphi \rightarrow 0$ . Denote every function at the limit  $\varphi = 0$  by the same letter without subscript  $\varphi$ , for example,

$$\Gamma(\xi, \zeta; x'') \equiv \lim_{\varphi \rightarrow 0} \Gamma_\varphi(\xi, \zeta; x'').$$

We then obtain the equation

$$\left[ i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 \right] G(x, x') - \int d^4x'' \Sigma(x, x'') G(x'', x') = \delta^{(4)}(x - x'), \quad (3\cdot28)$$

where

$$\begin{aligned} \Sigma(x, x') &= \bar{V}(x) \delta^{(4)}(x - x') + \Pi(x, x'), \\ \Pi(x, x') &= i\hbar \iint d^4x'' d^4\xi A(x, x') G(x, \xi) \Gamma(\xi, x'; x''). \end{aligned} \quad (3\cdot29)$$

By analogy we shall call  $\Sigma$  the self-energy part. Evidently the function  $\Pi$  includes the term

$$\Pi^{ex}(x, x') \equiv i\hbar U(x - x') G(x, x') \quad (3\cdot30)$$

which is interpreted as the exchange effect between two particles corresponding to the first term  $\bar{V}$  in  $\Sigma$ . This fact will be seen from the comparison of the two terms

$$\begin{aligned} \bar{V}(x)G(x, x') &= -i\hbar \int d^4\xi U(x-\xi)G(\xi, \xi)G(x, x'), \\ \int \Pi^{ex}(x, \xi)G(\xi, x')d^4\xi &= i\hbar \int d^4\xi U(x-\xi)G(x, \xi)G(\xi, x'), \end{aligned} \quad (3.31)$$

in which the latter will be obtained from the first equation by exchange between  $x$  and  $\xi$  in the first arguments of two  $G$ 's in the right member of the first equation. Now we divide  $\Sigma$  into two parts as follows:

$$\Sigma(x, x') = \Sigma^S(x, x') + \Sigma^P(x, x'), \quad (3.32)$$

where

$$\begin{aligned} \Sigma^S(x, x') &\equiv \bar{V}(x)\delta^{(4)}(x-x') + \Pi^{ex}(x, x'), \\ \Sigma^P(x, x') &\equiv \Sigma(x, x') - \Pi^{ex}(x, x'). \end{aligned} \quad (3.33)$$

The meaning or role of the division will later be clarified in the graphical representation and in construction of the effective potential.

Now we can explain the graphical representation.  $G(x, x')$  is graphically represented by drawing a heavy solid line, connecting points  $x$  with  $x'$ , with an arrow toward  $x$  from  $x'$ . According as  $t > t'$  or  $t < t'$ , the line corresponds to a particle line or a hole line in the medium.  $\Delta(x, x')$  is represented by a heavy broken line without an arrow connecting  $x$  and  $x'$ .  $\Gamma(\xi, \zeta; x)$  is the vertex part with an outgoing particle point  $\xi$ , an incoming particle point  $\zeta$  and a force point  $x$ . In the perturbation theories, the unperturbed functions  $G_0$  and  $\Delta_0 = U$  will be represented respectively by a fine solid line and a fine broken line. Now we can draw a graph corresponding to  $\Pi$  in a way suggested by its definition (3.29). Fig. 1 shows the graph of  $\Pi$ . This has the structure similar to the proper self-energy graph of an electron in quantum electrodynamics. The terms of  $\Sigma^S$  are shown in Fig. 2, in which the fine broken line shows the elementary interaction  $U$ . There the above-mentioned exchange is well visualized. The graph of  $P$  is given in Fig. 3.

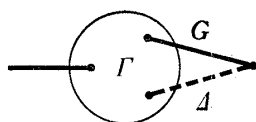


Fig. 1. The graph of  $\Pi$ .

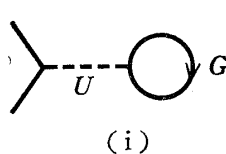


Fig. 2. The graph of  $\Sigma^S$ : (i)  $\bar{V}$  and (ii)  $\Pi^{ex}$ .

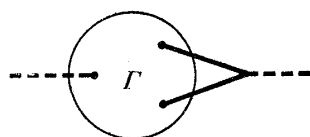
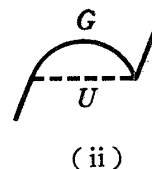


Fig. 3. The graph of  $P$ .

In uniform media all the functions introduced above are independent of the origin of the coordinate system, so that they can be regarded as functions of differences among the space-time variables, that is,

$$\begin{aligned} G(x, x') &= G(x - x'), & \Delta(x, x') &= \Delta(x - x') \\ \Sigma(x, x') &= \Sigma(x - x'), & \Gamma(\xi, \zeta; x'') &= \Gamma(\xi - \zeta; \xi - x'') \end{aligned}$$

and so on.

Therefore it is convenient to write them in the momentum representation or by the Fourier transform. First, for example, consider the Fourier transform\* of  $G(x, x')$  defined by

$$G(p, p') \equiv \iint e^{-i p x} G(x, x') e^{i p' x'} d^4 x d^4 x', \quad (3.34)$$

where  $\hbar p = (\mathbf{P}, P_0)$  is a momentum four-vector and  $p x = (\mathbf{P} \mathbf{x} - p_0 t) / \hbar$ . Because of the uniformity of  $G(p, p')$ , it becomes

$$G(p, p') = (2\pi)^4 G(p) \delta^{(4)}(p - p'), \quad (3.35)$$

where

$$G(p) = \int e^{-i p(x-x')} G(x-x') d^4(x-x'). \quad (3.36)$$

Inversely we have the formula

$$G(x-x') = \frac{1}{(2\pi)^4} \int e^{i p(x-x')} G(p) d^4 p. \quad (3.37)$$

Furthermore one obtains the formulas

$$\begin{aligned} \Delta(x-x') &= \frac{1}{(2\pi)^4} \int e^{i k(x-x')} \Delta(k) d^4 k \\ \Sigma(x-x') &= \frac{1}{(2\pi)^4} \int e^{i p(x-x')} \Sigma(p) d^4 p, \end{aligned} \quad (3.38)$$

by means of the similar procedures. The vertex part is represented by its Fourier transform defined by

$$\begin{aligned} \Gamma(p', p; k) &\equiv \iiint e^{-i p' \xi + i p \zeta - i k x''} \Gamma(\xi - \zeta; \xi - x'') d^4 \xi d^4 \zeta d^4 x'' \\ &= (2\pi)^4 \Gamma(p; k) \delta^{(4)}(p - p' + k), \end{aligned} \quad (3.39)$$

where

$$\Gamma(p; k) \equiv \iiint e^{-i p X} \Gamma(X; Y) e^{i k Y} d^4 X d^4 Y \quad (3.40)$$

\* For all Fourier transforms we shall use the same letters as the functions in the configuration representation. Readers should not confuse them.



which yields

$$\Gamma(\xi - \zeta; \xi - x'') = \frac{1}{(2\pi)^8} \iint e^{i p(\xi - \zeta)} \Gamma(p; k) e^{-i k(\xi - x'')} d^4 p d^4 k. \quad (3.41)$$

The appearance of delta-function in (3.35) or (3.39) is a reflection of the uniformity of the medium. Consequently it must be remembered that the momenta carried by particles are subject to the conservation law in each line or at each vertex.

In the momentum representation Eq. (3.28) becomes

$$\left[ p_0 - \frac{1}{2m} \mathbf{P}^2 - \Sigma(p) \right] G(p) = 1, \quad (3.42)$$

which has the formal solution

$$G(p) = \left[ p_0 - \frac{1}{2m} \mathbf{P}^2 - \Sigma(p) \right]^{-1}. \quad (3.43)$$

The self-energy part  $\Sigma$  has the form

$$\Sigma(p) = \bar{V} + \Pi(p), \quad (3.44)$$

where  $\bar{V}$  is a constant\* as mentioned above and

$$\Pi(p) = \frac{i\hbar}{(2\pi)^4} \int d^4 k \Delta(k) G(p-k) \Gamma(p; k). \quad (3.45)$$

From (3.25) and (3.23') it is easily shown that  $\Delta(k)$  obeys the equation

$$\Delta(k) = U(k) - \Delta(k) P(k) U(k), \quad (3.46)$$

where

$$P(k) = \frac{i\hbar}{(2\pi)^4} \text{tr} \int d^4 p \Gamma(p; k) G(p) G(p-k). \quad (3.47)$$

Eq. (3.46) has the formal solution

$$\Delta(k) = U(k) [1 + P(k) U(k)]^{-1}. \quad (3.48)$$

Thus we could obtain all the functions  $G$ ,  $\Delta$ ,  $\Sigma$ ,  $\Pi$  and  $P$ , if the vertex part  $\Gamma(p; k)$  were given. However  $\Gamma$  cannot be obtained unless we solve the complicated equation containing the functional derivative as follows:

$$\Gamma(p; k) = \delta^{(4)}(p - p' + k) + \lim_{\varphi \rightarrow 0} \frac{\delta}{\delta \langle \varphi(k) \rangle} \Pi_{\varphi}(p', p). \quad (3.49)$$

\* (3.10) yields  $\bar{V} = - (i\hbar) \left( \int U(k) \delta^{(4)}(k) d^4 k \right) \lim_{\varepsilon \rightarrow 0} \frac{1}{(2\pi)^4} \int e^{i p_0 \varepsilon} G(p) d^4 p.$

(For the Fourier transforms of functional derivatives, see Appendix I.) Here the  $\varphi$ -dependent functions have appeared again! Approximate approaches to the Green functions will be discussed in the next section and, for more details, in other articles of the present issue.

### 3.2 Two-particle Green function

In this subsection we shall formulate the equation to be satisfied by the two-particle Green function  $G_{\text{II}}$ . For simplicity, we simply denote the argument variables of  $G_{\text{II}}$  as follows:

$$G_{\text{II}}(1, 2; 1', 2') = (i\hbar)^{-2} \langle T(\psi(1)\psi(2)\psi^*(2')\psi^*(1')) \rangle. \quad (3.50)$$

Differentiating (3.50) with respect to  $t_1$ , we easily obtain the equation

$$i\hbar \frac{\partial}{\partial t_1} G_{\text{II}\varphi}(1, 2; 1', 2') = \delta(1, 1') G_{\varphi}(2, 2') - \delta(1, 2') G_{\varphi}(2, 1') \\ + (i\hbar)^{-2} \langle T \left( i\hbar \frac{\partial \psi(1)}{\partial t_1} \psi(2) \psi^*(2') \psi^*(1') \right) \rangle$$

which, together with (3.5) and (3.6), yields the equation

$$\mathcal{F}_1 G_{\text{II}\varphi}(1, 2; 1', 2') = \delta(1, 1') G_{\varphi}(2, 2') - \delta(1, 2') G_{\varphi}(2, 1'), \quad (3.51)$$

where

$$\mathcal{F}_1 \equiv i\hbar \frac{\partial}{\partial t_1} + \frac{\hbar^2}{2m} \nabla_1^2 - \bar{V}(1) - \langle \varphi(1) \rangle - D(1). \quad (3.52)$$

Here  $D(1)$  is the functional-differential operator written as

$$D(1) \equiv i\hbar \int d(3) \Delta_{\varphi}(1, 3) \frac{\delta}{\delta \langle \varphi(3) \rangle}, \quad (3.53)$$

where we have used the abbreviation  $d(3) = d^4x_3$ . Hence an equation satisfied by  $G_{\text{II}}$  is easily derived from (3.51) and (3.15) in the following form:

$$\mathcal{F}_1 \mathcal{F}_2 G_{\text{II}\varphi}(1, 2; 1', 2') = \delta(1, 1') \delta(2, 2') - \delta(1, 2') \delta(2, 1'). \quad (3.54)$$

However Eq. (3.54) is not what we wanted, because it contains explicitly the functional derivatives.

First we intend to separate the one-particle component from  $G_{\text{II}}$ . For this purpose the equation of  $G$  should be written in the form

$$\iint [G^{-1}(1, 1'') G^{-1}(2, 2'') - W(1, 2; 1'', 2'')] G_{\text{II}}(1'', 2''; 1', 2') d(1'') d(2'') \\ = \delta(1, 1') \delta(2, 2') - \delta(1, 2') \delta(2, 1') \quad (3.55)^*$$

\* To avoid complicated suffices, we shall suppress the subscript  $\varphi$  of  $G$  or  $G_{\text{II}}$ . But Eq. (3.55) holds when  $\varphi$  tends to zero.

or, in the matrix form,

$$[G_1^{-1}G_2^{-1} - W] G_{II} = 1_{12}, \quad (3.55')$$

where  $G^{-1}(1, 1')$  or  $G^{-1}(2, 2')$  is the operator given by (3.17) or (3.21), and  $1_{12}$  stands for the matrix defined by the element  $\langle 12 | 1_{12} | 1'2' \rangle = \delta(1, 1')\delta(1, 2') - \delta(1, 2')\delta(2, 1')$ . The first term in the left member of (3.55) or (3.55') may express the one-particle component of  $G_{II}$ , because the one-particle Green function describes the one-particle propagation in a sense. What we want is the function  $W$  which would represent the sentiales two-particle interactions. The integral form of (3.55) is

$$\begin{aligned} G_{II}(1, 2; 1', 2') &= G(1, 1')G(2, 2') - G(1, 2')G(2, 1') \\ &+ \iiint G(1, 3)G(2, 4)W(3, 4; 3', 4')G_{II}(3', 4'; 1', 2')d(3)d(4)d(3')d(4') \end{aligned} \quad (3.56)$$

or, in the matrix form,

$$G_{II} = G_1G_21_{12} + G_1G_2WG_{II}. \quad (3.56')$$

Applying the operator  $\mathcal{F}_1$  to (3.56), we obtain

$$\begin{aligned} \mathcal{F}_1G_{II}(1, 2; 1', 2') &= \delta(1, 1')G(2, 2') - \delta(1, 2')G(2, 1') \\ &+ \int G(2, 2'') \left[ \iint W(1, 2''; 3', 4')G(3', 4'; 1', 2')d(3')d(4') \right. \\ &- i\hbar \iint \Delta(1, 6)\Gamma(2'', 5'; 6) \left\{ G(1, 1')G(5', 2') - G(1, 2')G(5', 1') \right. \\ &+ \iiint G(1, 3)G(5', 4)W(3, 4; 3', 4') \\ &\quad \left. \times G(3', 4'; 1', 2')d(3)d(4)d(3')d(4') \right\} d(5')d(6) \\ &- i\hbar \iiint G(1, 3)\Delta(1, 6) \frac{\delta}{\delta \langle \varphi(6) \rangle} \left\{ W(3, 2''; 3', 4')G(3', 4'; 1', 2') \right\} \\ &\quad \left. \times d(3)d(6)d(3')d(4') \right] d(2''). \end{aligned}$$

Comparing the last equation with (3.51), the extra term in the right member must vanish, that is to say, we obtain the equation

$$\begin{aligned} &\iint W(1, 2; 3', 4')G_{II}(3', 4'; 1', 2')d(3')d(4') \\ &= i\hbar \iint \Delta(1, 6)\Gamma(2, 5'; 6)G(1, 5'; 1', 2')d(5')d(6) \\ &+ i\hbar \iiint G(1, 3)\Delta(1, 6) \frac{\delta}{\delta \langle \varphi(6) \rangle} [W(3, 2; 3', 4')G(3', 4'; 1', 2')] \\ &\quad \times d(3)d(6)d(3')d(4') \end{aligned} \quad (3.57)$$

or, in the matrix form,

$$WG_{\text{II}} = i\hbar A_{12} \Gamma_2 G_{\text{II}} + i\hbar G_1 A_{12} \frac{\delta}{\delta \langle \varphi_2 \rangle} [WG_{\text{II}}]. \quad (3.57')$$

Denoting the first term in the right member of (3.57) by  $W^{(1)}G_{\text{II}}$ ,  $W^{(1)}$  is written as

$$\begin{aligned} W^{(1)}(1, 2; 3', 4') &\equiv i\hbar \int \int A(1, 6) \Gamma(2, 5'; 6) \langle 1, 5' | 1_{12} | 3', 4' \rangle d(5') d(6) \\ &= i\hbar \int [A(1, 6) \Gamma(2, 4; 6) \delta(1, 3') - A(1, 6) \Gamma(2, 3'; 6) \delta(1, 4')] d(6). \end{aligned} \quad (3.58)$$

This function is graphically represented by a single force-bridge between two particle-lines. See Fig. 4. The two terms in (3.58) express the

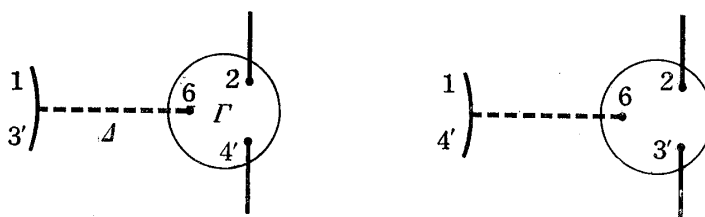


Fig. 4. The graph of  $W^{(1)}$

exchange effect as expected. The last term does not contain any iteration of any graph, but represents more complicated bridges between two particle-lines.

#### §4. Perturbation theory and its foundation

As was seen in last section, we must treat the very complicated equation and then devise a way to obtain the Green function. Most of calculations are usually performed through the perturbation expansion or its modifications. So we shall here explain the formal expansions of the Green function and the related functions into the perturbational series.

If we had the complete knowledge about the wave function belonging to the state of the medium, we could calculate  $\Sigma^s$  and might use it as the starting point of the perturbation theory. However, it is not easy to prepare the correct wave function of the medium, so that we should proceed to the perturbational calculations of  $G$  together with solving the state of the medium. The knowledge about the medium presents the initial and boundary conditions to be imposed upon the Green function  $G$ . From the form of the definition (2.3), it is seen that the perturbation expansion of  $G$  becomes two folds because the state vector  $|m\rangle$  or the density matrix  $\rho$  must be expanded in the perturbation series besides the

Heisenberg operator  $\psi$ . However it may be possible to perform the two expansions by a single procedure such as prepared in quantum field theory. We shall first discuss on it.

Suppose that the total Hamiltonian of the system is divided into two parts, that is,

$$H = H_0 + H_I, \quad (4.1)$$

where  $H_0$  and  $H_I$  are, respectively, the unperturbed and the perturbation Hamiltonian. Further assume that we know the set of eigenvector  $|\phi_m\rangle$  of  $H_0$  obeys the equation

$$H_0 |\phi_m\rangle = E_m^0 |\phi_m\rangle, \quad (4.2)$$

$E_m^0$  being an eigenvalue of  $H_0$  or an unperturbed energy. Corresponding to the division (4.1), it may be useful to express quantities in the interaction representation in which the time evolution operator is defined by

$$U(t, t') = e^{(i/\hbar)H_0 t} e^{-(i/\hbar)H(t-t')} e^{-(i/\hbar)H_0 t'}. \quad (4.3)$$

The  $S$ -matrix can be produced from  $U(t, t')$  by some appropriate limiting procedures<sup>3)</sup>:  $S \equiv U(\infty, -\infty)$ . The  $S$ -matrix is expanded in the perturbation series

$$U(\infty, -\infty) = \sum_{n=0}^{\infty} (i\hbar)^{-n} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} dt_1 \dots dt_n T(H_I(t_1) \dots H_I(t_n)), \quad (4.4)$$

where

$$H_I(t) \equiv \exp\left(\frac{i}{\hbar} H_0 t\right) H_I \exp\left(-\frac{i}{\hbar} H_0 t\right).$$

Now we may write a desired form for the perturbation expansion of  $G$  in the following way:

$$\begin{aligned} G(x, x') &= (i\hbar)^{-1} \langle T(U(\infty, -\infty) \psi_I(x) \psi_I^*(x')) \rangle_0 \\ &= \sum_{n=0}^{\infty} (i\hbar)^{-n-1} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} dt_1 \dots dt_n \langle T(H_I(t_1) \dots H_I(t_n) \psi_I(x) \psi_I^*(x')) \rangle_0, \end{aligned} \quad (4.5)$$

where  $\psi_I$  is the field operator in the interaction representation defined by

$$\psi_I(x) = U^{-1}(t, 0) \psi(x) U(t, 0) \quad (4.6)$$

and  $\langle T(\dots) \rangle_0$  stands for

$$\langle T(\dots) \rangle_0 \equiv \langle \phi_m | T(\dots) | \phi_m \rangle / \langle \phi_m | U(\infty, -\infty) | \phi_m \rangle. \quad (4.7)$$

The Green function in consideration is the one defined by (2.4). (For the definition (2.6), see later discussions.) If the expansion formula

(4.5) is verified, we can use the well-known graphical method as formulated by Feynman<sup>4)</sup> and Dyson<sup>5)</sup> in quantum field theory and by Matsubara<sup>6)</sup> in statistical mechanics. There the expansion could be performed on the basis of the unperturbed Green function

$$G_0(x, x') = (i\hbar)^{-1} \langle \Phi_m | T(\psi_I(x) \psi_I^*(x')) | \Phi_m \rangle. \quad (4.8)$$

Since  $S \equiv U(\infty, -\infty)$  conserves energies, the vector  $S|\Phi_m\rangle$  becomes again an eigenvector of  $H_0$  belonging to  $E_m^0$ . Hence  $S|\Phi_m\rangle$  coincides with  $|\Phi_m\rangle$  except for a numerical factor, if we are concerned with the non-degenerate eigenstate. That is to say, one gets

$$S|\Phi_m\rangle = S_m |\Phi_m\rangle, \quad (4.9)$$

$S_m$  being the numerical factor defined by

$$S_m \equiv \langle \Phi_m | S | \Phi_m \rangle. \quad (4.10)$$

Although Eq. (4.9) is not necessarily valid in degenerate cases, it might be possible to represent the unperturbed state of the medium by a simultaneous eigenstate of  $H_0$  and  $S$ . Eq. (4.5) will be justified only in such cases. Now let us consider the vectors defined by

$$|m^\pm\rangle = U(0, \mp\infty) |\Phi_m\rangle \quad (4.11)$$

for the state of the medium. They are both the eigenvectors of  $H$  belonging to an eigenvalue  $E_m$ , where  $E_m$  may be written in terms of the energy shift as follows:

$$E_m = E_m^0 + \Delta E_m^0. \quad (4.12)$$

The energy shift becomes negligibly small in systems composed of a finite number of particles in an infinitely large volume. For example, this may be understood through a simple scattering of a particle by a fixed potential. However, the energy shift is no longer discarded in some interesting systems which have an infinite number of particles in an infinitely large volume but a finite density. In general, therefore, we have the relation

$$HU(0, -\infty) = U(0, -\infty)(H_0 + \Delta H_0), \quad (4.13)$$

where

$$\Delta H_0 \equiv \sum |\Phi_m\rangle \Delta E_m^0 \langle \Phi_m|. \quad (4.14)$$

This may be evident from (4.12) and (4.11). Now Eqs. (4.9) and (4.11) give us the important relation

$$|m^+\rangle = \frac{1}{S_m^*} U(0, -\infty) S^{-1} |\Phi_m\rangle = \frac{1}{S_m^*} U(0, \infty) |\Phi_m\rangle = \frac{1}{S_m^*} |m^-\rangle. \quad (4.15)$$

Here it is emphasized that Eq. (4.15) is verified only in the media whose unperturbed state can be represented by a simultaneous eigenvector of  $H_0$  and  $S$ . In such cases Eq. (2.4) can be rewritten as

$$G(x, x') = (i\hbar)^{-1} S_m^{-1} \langle m^- | T(\psi(x)\psi^*(x')) | m^+ \rangle. \quad (4.16)$$

Rewriting the expression obtained above, we finally get,

$$G(x, x') = \frac{(i\hbar)^{-1} \langle \Phi_m | T(U(\infty, -\infty)\psi_I(x)\psi_I^*(x')) | \Phi_m \rangle}{\langle \Phi_m | U(\infty, -\infty) | \Phi_m \rangle}. \quad (4.17)$$

Therefore we can perform the perturbation expansion of  $G(x, x')$  by a single procedure produced by expanding  $U(\infty, -\infty)$ , and immediately obtain (4.5). Division by  $S_m = \langle \Phi_m | U(\infty, -\infty) | \Phi_m \rangle$  means that we should omit all graphs that are not connected with  $x$  or  $x'$ . Further it may be worth while to write the following expression of  $G_0$ :

$$G_0(x, t; x', t') = \begin{cases} \frac{1}{i\hbar} \sum_n \chi_n^{(0)}(x) \exp\{- (i/\hbar) E_n^0(t-t')\} \chi_n^{(0)*}(x') & t > t', \\ \frac{-1}{i\hbar} \sum_{\bar{n}} \chi_{\bar{n}}^{(0)*}(x) \exp\{+ (i/\hbar) E_{\bar{n}}^0(t-t')\} \chi_{\bar{n}}^{(0)}(x') & t < t'. \end{cases} \quad (4.18)$$

Here  $\chi_n^{(0)}$  and  $\chi_{\bar{n}}^{(0)}$  are, respectively, the amplitudes of a particle in the  $n$ -th state and of a hole in the  $\bar{n}$ -th state determined by  $H_0$ , which are defined by

$$\begin{aligned} \chi_n^{(0)}(x) &\equiv \langle \Phi_m | \psi(x) | \Phi_{n, m+1} \rangle, \\ \chi_{\bar{n}}^{(0)}(x) &\equiv \langle \Phi_m | \psi^*(x) | \Phi_{\bar{n}, m+1} \rangle, \end{aligned} \quad (4.19)$$

where  $|\Phi_{n, m+1}\rangle$  is the vector representing the  $n$ -th state of the (medium + one particle or hole)-system governed by  $H_0$ .

Next we discuss the Green function defined by (2.6). If any new energy gap or any new bound state is not produced by introducing  $H_I$  into the system governed by  $H_0$ , then we can regard  $\{|m^+\rangle\}$  or  $\{|m^-\rangle\}$  as a complete set and use, for example,  $\{|m^+\rangle\}$  as the vector system over which the summation in the trace of (2.6) is performed. In general cases we have not necessarily the relation (4.15), as pointed out above. However, an appropriate unitary transformation can bring them to a vector set satisfying (4.15). Since the trace is invariant under unitary transformations, we can use the new vector set satisfying (4.15) to perform the summation in the trace. Denoting the new vectors with the same letters, Eq. (2.6) can be rewritten as

$$G(x, x') = (i\hbar)^{-1} \frac{\sum_m \langle m^- | T(\psi(x)\psi^*(x')) e^{-\beta H} | m^+ \rangle S_m^{-1}}{\sum_m \langle m^- | e^{-\beta H} | m^+ \rangle S_m^{-1}}$$

$$= (i\hbar)^{-1} \frac{\sum_m \frac{\langle \Phi_m | U(\infty, 0) T(\psi(x) \psi^*(x')) e^{-\beta H} U(0, -\infty) | \Phi_m \rangle}{\langle \Phi_m | U(\infty, -\infty) | \Phi_m \rangle}}{\sum_m \frac{\langle \Phi_m | U(\infty, 0) e^{-\beta H} U(0, -\infty) | \Phi_m \rangle}{\langle \Phi_m | U(\infty, -\infty) | \Phi_m \rangle}},$$

where (4.15) and (4.11) have been used. Eq. (4.13) yields the relation

$$e^{-\beta H} U(0, -\infty) = U(0, -\infty) e^{-\beta(H_0 + \Delta H_0)},$$

so that one obtains

$$G(x, x') = (i\hbar)^{-1} \frac{\sum_m \frac{e^{-\beta(E_m^0 + \Delta E_m^0)} \langle \Phi_m | T(U(\infty, -\infty) \psi_I(x) \psi_I^*(x')) | \Phi_m \rangle}{\langle \Phi_m | U(\infty, -\infty) | \Phi_m \rangle}}{\sum_m e^{-\beta(E_m^0 + \Delta E_m^0)}}$$

or

$$= (i\hbar)^{-1} \frac{\text{Tr}\{e^{-\beta(H_0 + \Delta H_0)} T(U(\infty, -\infty) \psi_I(x) \psi_I^*(x'))\}_{\text{Connected}}}{\text{Tr}\{e^{-\beta(H_0 + \Delta H_0)}\}}, \quad (4.20)$$

where  $\text{Tr}(\dots)_{\text{connected}}$  is defined by the right members themselves in (4.20). If considered by (4.20), the perturbation expansion of this Green function contains twofold procedures for  $U(\infty, -\infty)$  and  $\Delta H_0$ . The fact that the perturbation series of  $G$  cannot be obtained by a single procedure makes the problems very complicated. If only  $U(\infty, -\infty)$  is expanded, we will reach similar expansion formula or similar graphs with understanding that we should use the function

$$G_0(x, x') = (i\hbar)^{-1} \frac{\text{Tr}\{e^{-\beta(H_0 + \Delta H_0)} T(\psi_I(x) \psi_I^*(x'))\}}{\text{Tr}\{e^{-\beta(H_0 + \Delta H_0)}\}} \quad (4.21)$$

as the zeroth-order Green function.  $G_0$  defined by (4.21) obeys the same equation to be satisfied by (4.8), but it must be subject to another boundary condition different from the one imposed on (4.8). In spite of the easy form of equation, therefore, the explicit form of  $G_0$  can not be obtained unless we can solve the energy spectrum of the total Hamiltonian. Nevertheless one might devise a way to calculate  $G$ . If  $\Delta H_0$  can be calculated by some types of approximation methods, for example, the perturbation method or the variational method, we have only to substitute it into (4.21). We prefer such a method to the formal expansion of the factor  $\exp(-\beta H)$ , because some parts of all contributions of  $\Delta H_0$  to  $G$  may be summed up by the exponential function. Finally we remark the simplest two cases; (i)  $\Delta E_m^0$  is a constant for all states, and (ii)  $\Delta E_m^0 = \lambda E_m^0$ ,  $\lambda$  being independent of  $m$ . In the first case we can directly drop out the term  $H$  from (4.20) and (4.21), so the expansion of  $G$  contains only a



single procedure caused by  $U(\infty, -\infty)$ . In the second case, if we know  $\lambda$ , we have only to modify  $\beta$  or another parameter in  $H_0$  and to drop out  $\Delta H_0$  from (4.20) and (4.21).

In the following of this section, we assume the full knowledge about  $G_0(x, x')$  and formulate the formal expansion of the Green function and the related functions. This will be explained on the basis developed in the previous section, without resorting to the direct use of (4.5) or (4.21). First we suppose that  $H_0$  has the form

$$H_0 \equiv \int \psi^*(x) \left( -\frac{\hbar^2}{2m} \nabla^2 \right) \psi(x) d^3x + \iint \psi^*(x) \Xi(x, x') \psi(x') d^4x' d^3x, \quad (4.22)$$

where  $\Xi(x, x')$  is, in general, the non-local potential appropriately chosen. In this case the one-particle function  $G$  obeys the equation

$$\left[ i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 \right] G_0(x, x') - \int d^4x'' \Xi(x, x'') G_0(x'', x') = \delta^{(4)}(x - x'). \quad (4.23)$$

If we use  $G_0$  as the starting point of perturbation theory, it is convenient to rewrite the equation of  $G$  in the following integral equation

$$G(x, x') = G_0(x, x') + \iint d^4x'' d^4x''' G_0(x, x'') \times [\Sigma(x'', x''') - \Xi(x'', x''')] G(x''', x') \quad (4.24)$$

or symbolically,

$$G = G_0 + G_0 [\Sigma - \Xi] G. \quad (4.25)$$

The convergence or accuracy of the perturbation series essentially relies on the choice of  $\Xi$ . If in passing of the particle in consideration the medium is almost always in its ground state, we may consider the static approximation to be good and choose  $\Xi$  as

$$\Xi = \Sigma^s [G_0]. \quad (4.26)$$

This may be regarded as simple application of the Hartree-Fock method to our problem. For this choice we should solve the equation (in the symbolical matrix form)

$$\left[ p_0 - \frac{1}{2m} p^2 + \Sigma^s [G_0] \right] G_0 = 1, \quad (4.27)$$

which may be treated by the successive iteration. Besides (4.26), we have other possibilities of choosing  $\Xi$ , for example, those suggested by

Brueckner's method. Detailed discussions will be given elsewhere in this issue.

The perturbation series of  $G$  is obtained by successive iteration, where the perturbation series of  $\Sigma$  is required. To get the series of  $\Sigma$ , we should prepare the series of  $\Delta$ ,  $P$  and  $\Gamma$ . The perturbation series of  $\Delta$  is immediately obtained as follows:

$$\begin{aligned} \Delta(x, x') = & U(x-x') - (i\hbar) \iint d^4x'' d^4\zeta' U(x'-x'') \text{tr}[G_0(x'', \zeta') G_0(\zeta', x'')] \\ & \times U(x-\zeta') + \dots, \end{aligned} \tag{4.28}$$

where we have used the lowest-order term of  $P$  in the series

$$P(\zeta', x'') = i\hbar \text{tr}[G_0(x'', \zeta') G_0(\zeta', x'')] + \dots \tag{4.29}$$

Similarly we get

$$\Gamma(\xi, \zeta; x'') = \delta^{(4)}(\xi-\zeta) \delta^{(4)}(\xi-x'') + i\hbar U(\xi-\zeta) G_0(\xi, x'') G_0(x'', \zeta) + \dots \tag{4.30}$$

The graphs corresponding to the perturbation series of  $\Delta$  are shown in Fig. 5 and the graph of  $\Gamma$  in Fig. 6. The series produced by iteration of

Fig. 5. Graphical representation of the series of  $\Delta$ .

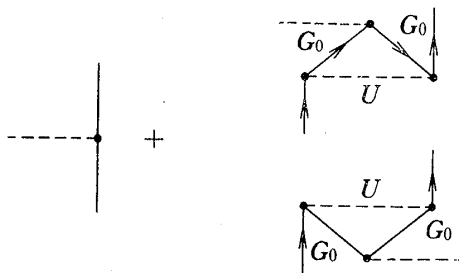
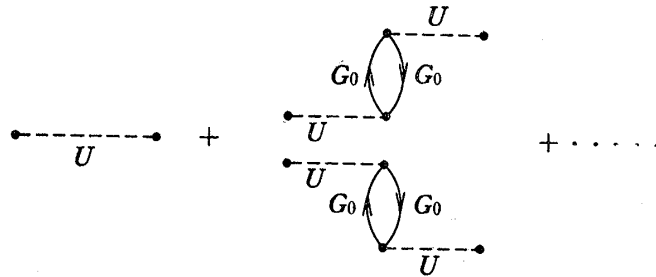
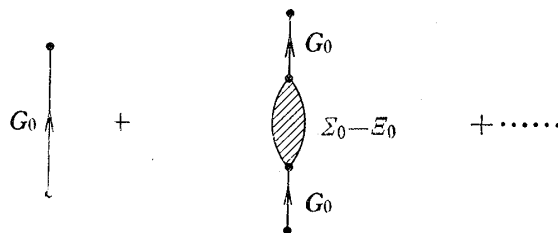


Fig. 6. Graphical representation of the series of  $\Gamma$ .

Fig. 7. Graphical representation of the series of  $G$ .



(4.24) or (4.25) is graphically represented as in Fig. 7, but the concrete form of  $(\Sigma - \mathcal{E})$  depends on the choice of  $\mathcal{E}$ . The graphs of  $\Sigma^S$  can simply be drawn by substituting the graphs of  $G$  into the heavy solid line in Fig. 2. In the graphs all the fine lines correspond to the unperturbed function. Next we write the perturbation series for

$$\begin{aligned} \Sigma^F(x, x') = & - (i\hbar)^2 \iint d^4x'' d^4\zeta' U(x' - x'') G_0(x'', \zeta') G_0(\zeta', x'') \\ & \times U(x - \zeta') G_0(x, x') \\ & + (i\hbar)^2 \iint d^4x'' d^4\xi U(x - x'') G_0(x, \xi) U(\xi - x') G_0(\xi, x'') G_0(x'', x') \\ & + \dots, \end{aligned} \tag{4.31}$$

which is graphically represented in Fig. 8. In particular, the first two terms are interpreted as the exchange-pair between two excited particles or holes. See Fig. 9. As understood from Fig. 8 or Fig. 9, the function  $\Sigma^F$  describes all the reactions to the one-particle (or hole) motions from

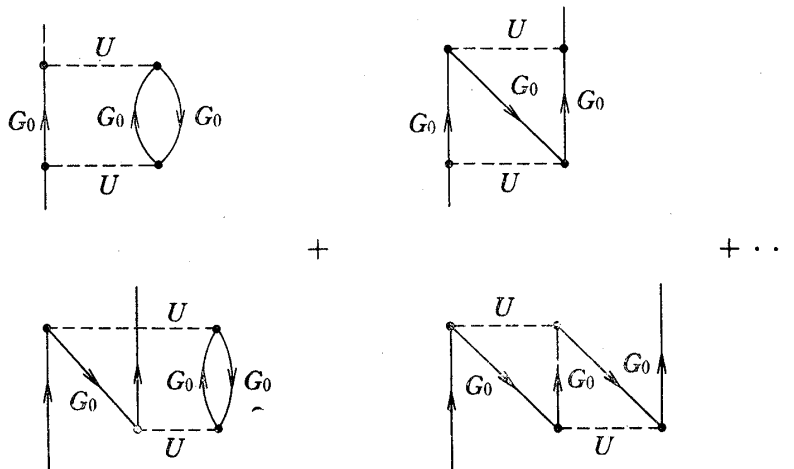


Fig. 8. Graphical representation of the series of  $\Sigma^F$ .

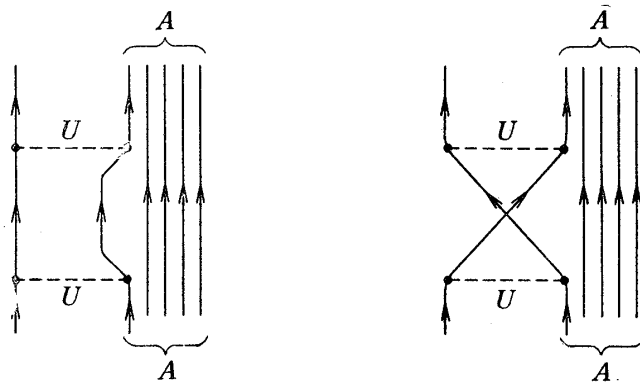


Fig. 9. Interpretation of the first two terms of (4.12).

virtual or provisional excitations of the medium caused by passing of a particle or hole.

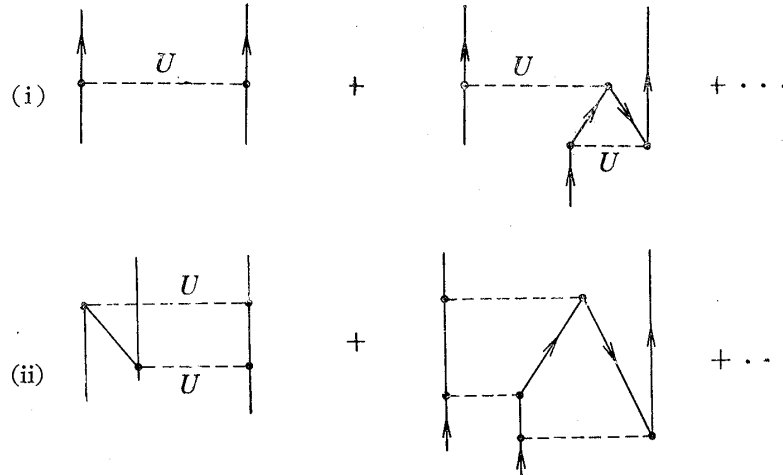


Fig. 10. Graphical representation of the series of  $W$ :  
(i) Graphs of  $W^{(1)}$  and (ii) Graphs of  $W - W^{(1)}$ .

Finally we write the series of the interaction function  $W$  operating on the two-particle Green function in the graphical representation. See Fig. 10.

### §5. Spectral representation and its application

We shall now consider the spectral representation of the Green function in this section. This approach has extensively been developed by Landau,<sup>8)</sup> Galitskii-Migdal<sup>9)</sup> and Martin-Schwinger.<sup>7)</sup> Since we are interested in the problems in uniform media and in the absence of external field, the function depends only on the difference of two coordinates,  $\mathbf{x} = \mathbf{x}_1 - \mathbf{x}_2$ ,  $t = t_1 - t_2$ . The problems in the presence of external field will be considered later in the section.<sup>7), 9), 10)</sup>

The space-time dependence of the matrix element of operator  $\psi(\mathbf{x})$  is given by

$$\psi_{nm}(\mathbf{x}, t) = \psi_{nm}^{(0)} \exp\{i(\mathbf{k}_{nm}\mathbf{x} - \omega_{nm}t)\} \quad (5.1)$$

in the representation making the total Hamiltonian diagonal, where

$$\hbar\mathbf{k}_{nm} = \mathbf{P}_n - \mathbf{P}_m, \quad \hbar\omega_{nm} = E_{nm} = E_n - E_m$$

and  $n$  and  $m$  refer to the states in consideration.  $E_n(E_m)$ ,  $\mathbf{P}_n(\mathbf{P}_m)$  and  $N_n(N_m)$  are the total energy, momentum and total number of particles of state  $n(m)$ , respectively. By means of these matrix elements, the one particle Green function defined by (2.3) or (2.6) can be expressed as

$$\begin{aligned}
G(\mathbf{x}, t) &= (i\hbar)^{-1} \sum_{n,m} \exp\{-\beta(E_n - \mu N_n - \mathcal{Q})\} \\
&\quad \times |\psi_{nm}^{(0)}|^2 \exp\{i(\mathbf{k}_{nm}\mathbf{x} - \omega_{nm}t)\} \quad \text{for } t > 0 \\
&= \pm (i\hbar)^{-1} \sum_{n,m} \exp\{-\beta(E_m - \mu N_m - \mathcal{Q})\} \\
&\quad \times |\psi_{nm}^{(0)}|^2 \exp\{i(\mathbf{k}_{nm}\mathbf{x} - \omega_{nm}t)\} \quad \text{for } t < 0, \quad (5.2)
\end{aligned}$$

or

$$\begin{aligned}
&= \pm (i\hbar)^{-1} \sum_{n,m} |\psi_{nm}^{(0)}|^2 \exp\{-\beta(E_n - \mu N_n - \mathcal{Q})\} \\
&\quad \times \exp\{\beta(E_{nm} + \mu)\} \exp\{i(\mathbf{k}_{nm}\mathbf{x} - \omega_{nm}t)\} \quad \text{for } t < 0,
\end{aligned}$$

where  $\mathcal{Q}$  is Gibbs potential of the system. The last formula is derived from the fact

$$\begin{aligned}
\psi_{nm} &\neq 0 && \text{when } N_m = N_n + 1 \\
&= 0 && \text{otherwise.}
\end{aligned}$$

The plus or minus sign in (5.2) corresponds to the bosons or fermions, respectively. In the absence of interaction among particles (5.2) turns out to be

$$\begin{aligned}
G_0(\mathbf{x}, t) &= (i\hbar)^{-1} \int d\mathbf{k} \langle 1 - n_{\mathbf{k}} \rangle \exp\{i(\mathbf{k}\mathbf{x} - \omega t)\} \quad t > 0 \\
&= (i\hbar)^{-1} \int d\mathbf{k} \langle n_{\mathbf{k}} \rangle \exp\{i(\mathbf{k}\mathbf{x} - \omega t)\} \quad t < 0. \quad (5.3)
\end{aligned}$$

where  $\langle n_{\mathbf{k}} \rangle = \langle a_{\mathbf{k}}^* a_{\mathbf{k}} \rangle$  denotes the expectation value of number operator. The momentum representation of the Green function defined by

$$G(\mathbf{k}, t) = \int G(\mathbf{x}, t) \exp(-i\mathbf{k}\mathbf{x}) d^3x$$

can be obtained from (5.3) in the form

$$\begin{aligned}
G_0(\mathbf{k}, t) &= (i\hbar)^{-1} (2\pi)^{-3} \langle 1 - n_{\mathbf{k}} \rangle \exp(-i\omega t) \quad t > 0 \\
&= \pm (i\hbar)^{-1} (2\pi)^{-3} \langle n_{\mathbf{k}} \rangle \exp(-i\omega t) \quad t < 0. \quad (5.4)
\end{aligned}$$

The Fourier transform of the Green function defined by (3.34) is

$$\begin{aligned}
G(\mathbf{k}, \varepsilon) &= -(2\pi)^3 \left\{ \pm \sum_{n,m} |\psi_{nm}^{(0)}|^2 \exp\{-\beta(E_m - \mu N_m - \mathcal{Q})\} \frac{1}{\varepsilon - E_{nm} - i\delta} \right. \\
&\quad \left. + \sum_{n,m} |\psi_{nm}^{(0)}|^2 \exp\{-\beta(E_n - \mu N_n - \mathcal{Q})\} \frac{1}{\varepsilon - E_{nm} + i\delta} \right\} \delta^{(3)}(\mathbf{k}_{nm} - \mathbf{k}), \quad (5.5)
\end{aligned}$$

where  $\delta$  denotes a positive infinitesimal quantity. In the limiting case of large system with a given density or in the limit of continuous quantum

number, we can write (5.5) in the following form

$$G(\mathbf{k}, \varepsilon) = \int_0^\infty dE \left\{ \frac{A(\mathbf{k}, E)}{\varepsilon - E - i\delta} + \frac{B(\mathbf{k}, E)}{\varepsilon - E + i\delta} \right\}, \quad (5.6)$$

where  $A(\mathbf{k}, E)$  and  $B(\mathbf{k}, E)$  are defined as limiting functions in such a way

$$\begin{aligned} A(\mathbf{k}, E)dE &= \lim(\mp)(2\pi)^3 \sum_{n,m} |\psi_{nm}^{(0)}|^2 \exp\{-\beta(E_n - \mu N_n - \Omega)\} \\ &\quad \times \delta^{(3)}(\mathbf{k}_{nm} - \mathbf{k}) \quad E < E_{nm} < E + dE \\ B(\mathbf{k}, E)dE &= \lim(-)(2\pi)^3 \sum_{n,m} |\psi_{nm}^{(0)}|^2 \exp\{-\beta(E_n - \mu N_n - \Omega)\} \\ &\quad \times \delta^{(3)}(\mathbf{k}_{nm} - \mathbf{k}) \quad E < E_{nm} < E + dE. \end{aligned} \quad (5.7)$$

This expression (5.6) is essentially same as Lehmann's expansion in the quantum field theory.

With aid of the well-known formula

$$\frac{1}{i} \int_0^\infty e^{\pm i\alpha x} dx = i\pi\delta(\alpha) \pm P\left(\frac{1}{\alpha}\right)$$

and from (5.2), (5.5) is expressed in the form as

$$\begin{aligned} G(\mathbf{k}, \varepsilon) &= (2\pi)^3 \sum_{n,m} |\psi_{nm}^{(0)}|^2 \exp\{-\beta(E_n - \mu N_n - \Omega)\} \delta^{(3)}(\mathbf{k}_{nm} - \mathbf{k}) \\ &\quad \times \left[ P\left(\frac{1}{E_{nm} - \varepsilon}\right) (1 \pm e^{\beta(E_{nm} + \mu)}) + \pi i \delta(E_{nm} - \varepsilon) (1 \pm e^{\beta(E_{nm} + \mu)}) \right]. \end{aligned} \quad (5.8)$$

Using the expression (5.8), we can obtain the relations connecting the real part of the Green function  $G'$  with its imaginary part  $G''$ . In case of the Bose field the relation is

$$G'(\mathbf{k}, \varepsilon) = \frac{1}{\pi} P \int_{-\infty}^\infty \tanh \frac{\beta(z + \mu)}{2} \frac{G''(\mathbf{k}, \varepsilon)}{z - \varepsilon} dz, \quad (5.9)$$

and in case of the Fermi field we obtain

$$G'(\mathbf{k}, \varepsilon) = \frac{1}{\pi} P \int_{-\infty}^\infty \coth \frac{\beta(z + \mu)}{2} \frac{G''(\mathbf{k}, \varepsilon)}{z - \varepsilon} dz. \quad (5.9')$$

As a useful application of the spectral representation of the two particle Green function we consider the current caused by external field, which is expressed by a vector potential  $A(\mathbf{x}, t)$ . In this case the following terms must be added to the total Hamiltonian

$$H_I = -\frac{1}{c} \int A(\mathbf{x}, t) \mathbf{j}^{(0)}(\mathbf{x}, t) d^3\mathbf{x} - \frac{1}{2c} \int A(\mathbf{x}, t) \mathbf{j}^{(1)}(\mathbf{x}, t) d^3\mathbf{x},$$

where

$$\mathbf{j}^{(0)}(\mathbf{x}, t) = \frac{e}{2m} \left[ -\frac{\hbar}{i} \nabla \psi^*(\mathbf{x}, t) \psi(\mathbf{x}, t) + \psi^*(\mathbf{x}, t) \frac{\hbar}{i} \nabla \psi(\mathbf{x}, t) \right]$$

and

$$\mathbf{j}^{(1)}(\mathbf{x}, t) = \frac{e^2}{mc} \psi^*(\mathbf{x}, t) \psi(\mathbf{x}, t) \mathbf{A}(\mathbf{x}, t). \quad (5.10)$$

Taking into account the contributions up to the first order terms in  $\mathbf{A}$ , we have

$$\mathbf{j}^{(0)}(\mathbf{x}, t) = \mathbf{j}_0(\mathbf{x}, t) - \frac{1}{ic\hbar} \int_0^t dt' \int d^3x' [\mathbf{j}_0(\mathbf{x}, t), \mathbf{j}_0(\mathbf{x}', t')] \mathbf{A}(\mathbf{x}', t') \quad t > t', \quad (5.11)$$

where  $\mathbf{j}_0(\mathbf{x}, t)$  is the current density operator in the absence of external field. Using the two particle Green function defined by (3.50), we obtain the following relation:

$$\begin{aligned} \langle \mathbf{j}_0(\mathbf{x}, t) \mathbf{j}_0(\mathbf{x}', t') \rangle &= \left( \frac{e\hbar}{2mi} \right)^2 \lim_{\substack{\mathbf{x}_1 \rightarrow \mathbf{x}_2 = \mathbf{x} \\ \mathbf{x}'_1 \rightarrow \mathbf{x}'_2 = \mathbf{x}'}} \lim_{\substack{t_1 \rightarrow t_2 = t \\ t'_1 \rightarrow t'_2 = t'}} (\nabla_1 - \nabla_2) (\nabla'_1 - \nabla'_2) \\ &\times \langle \psi^*(\mathbf{x}_1 t_1) \psi(\mathbf{x}_2 t_2) \psi^*(\mathbf{x}'_1 t'_1) \psi(\mathbf{x}'_2 t'_2) \rangle \\ &= \left( \frac{e\hbar^2}{2m} \right)^2 \lim_{\substack{\mathbf{x}_1 \rightarrow \mathbf{x}_2 = \mathbf{x} \\ \mathbf{x}'_1 \rightarrow \mathbf{x}'_2 = \mathbf{x}'}} \lim_{\substack{t_1 \rightarrow t_2 = t \\ t'_1 \rightarrow t'_2 = t'}} (\nabla_1 - \nabla_2) (\nabla'_1 - \nabla'_2) G_{\text{II}}(\mathbf{x}_2 t_2, \mathbf{x}'_2 t'_2; \mathbf{x}_1 t_1, \mathbf{x}'_1 t'_1). \end{aligned} \quad (5.12)$$

Therefore, the current can be expressed in terms of the two particle Green function

$$\begin{aligned} \langle \mathbf{j}(\mathbf{x}, t) \rangle &= \frac{e^2}{mc} \langle \psi^*(\mathbf{x}, t) \psi(\mathbf{x}, t) \rangle \mathbf{A}(\mathbf{x}, t) \\ &+ \frac{1}{ic\hbar} \left( \frac{e\hbar^2}{2m} \right)^2 \int_0^t dt' \int d^3x' \lim (\nabla_1 - \nabla_2) (\nabla'_1 - \nabla'_2) \\ &\times G_{\text{II}}(\mathbf{x}_2 t_2, \mathbf{x}'_2 t'_2; \mathbf{x}_1 t_1, \mathbf{x}'_1 t'_1) \mathbf{A}(\mathbf{x}, t) + \text{c.c.} \end{aligned} \quad (5.13)$$

Thus the two particle Green function gives us sufficient information for calculating the current density to the first order term of  $\mathbf{A}(\mathbf{x}, t)$ .<sup>12)</sup>

The Fourier transform of (5.12) can be expressed as follows.

$$\begin{aligned} F_{in}(\mathbf{k}\omega; \mathbf{k}'\omega') &= -\frac{1}{(2\pi)^8} \iint (\mathbf{k} + 2\mathbf{k}_1)_i (\mathbf{k}' + 2\mathbf{k}'_2)_n \\ &\times G_{\text{II}}(\mathbf{k} + \mathbf{k}_1, \omega + \omega_1, \mathbf{k}' + \mathbf{k}'_1, \omega' + \omega'_1; \mathbf{k}_1, \omega_1, \mathbf{k}'_1, \omega'_1) d\mathbf{k}_1 d\mathbf{k}'_1 d\omega_1 d\omega'_1, \end{aligned} \quad (5.14)$$

where

$$G_{\text{II}}(\mathbf{x}_1 t_1, \mathbf{x}_2 t_2; \mathbf{x}'_1 t'_1, \mathbf{x}'_2 t'_2)$$

$$= \frac{1}{(2\pi)^{16}} \iiint \exp\{i(\mathbf{k}_1\mathbf{x}_1 + \mathbf{k}_2\mathbf{x}_2 - \mathbf{k}'_1\mathbf{x}'_1 - \mathbf{k}'_2\mathbf{x}'_2) - i(\omega_1 t_1 + \omega_2 t_2 - \omega'_1 t'_1 - \omega'_2 t'_2)\} \\ \times G_{\Pi}(\mathbf{k}_1\omega_1, \mathbf{k}_2\omega_2; \mathbf{k}'_1\omega'_1, \mathbf{k}'_2\omega'_2) d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}'_1 d\mathbf{k}'_2 d\omega_1 d\omega_2 d\omega'_1 d\omega'_2 \quad (5.15)$$

and

$$F_{ln}(\mathbf{x}, t; \mathbf{x}', t') = \frac{1}{(2\pi)^3} \int \exp\{i(\mathbf{k}\mathbf{x} - \mathbf{k}'\mathbf{x}') - i(\omega t - \omega' t')\} \\ \times F_{ln}(\mathbf{k}\omega; \mathbf{k}'\omega') d\mathbf{k} d\mathbf{k}' d\omega d\omega'. \quad (5.16)$$

Hereafter we shall use the correlation function  $F(\mathbf{x}, t; \mathbf{x}', t')$  instead of the two-particle Green function. The second term of (5.11) is also expressed in terms of correlation functions of the currents as,

$$-\frac{1}{i\hbar} \int_0^t dt' \int d^3\mathbf{x}' \langle \mathbf{j}_0(\mathbf{x}', t') \mathbf{j}_0(\mathbf{x}, t + i\beta\hbar) - \mathbf{j}_0(\mathbf{x}, t) \mathbf{j}_0(\mathbf{x}', t + i\beta\hbar) \rangle \\ \times \mathbf{A}(\mathbf{x}, t). \quad (5.17)$$

Introducing the symmetrized product

$$S_{kl}(\mathbf{x}, t; \mathbf{x}', t') = \langle \{ \mathbf{j}_k(\mathbf{x}, t), \mathbf{j}_l(\mathbf{x}', t') \} \rangle \\ = \langle \mathbf{j}_k(\mathbf{x}, t) \mathbf{j}_l(\mathbf{x}', t') + \mathbf{j}_l(\mathbf{x}', t') \mathbf{j}_k(\mathbf{x}, t) \rangle \\ = F_{kl}(\mathbf{x}, t; \mathbf{x}', t') + F_{lk}(\mathbf{x}', t'; \mathbf{x}, t)$$

and its Fourier transform defined by

$$S_{kl}(\mathbf{x}, \mathbf{x}', \omega) = \int S_{kl}(\mathbf{x}, \mathbf{x}'; t - t') e^{i\omega(t-t')} d(t-t'), \quad (5.18)$$

the expectation value of the commutator of  $\mathbf{j}_k(\mathbf{x}, t)$  and  $\mathbf{j}_l(\mathbf{x}', t')$  is written in the following form:

$$\langle [\mathbf{j}_k(\mathbf{x}, t), \mathbf{j}_l(\mathbf{x}', t')] \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \tanh \frac{\beta\hbar\omega}{2} S_{kl}(\mathbf{x}, \mathbf{x}'; \omega), \quad (5.19)$$

where the invariant property of trace for cyclic permutation of operators has been used.

Restricting the problem under the consideration to a uniform medium, we can define the momentum representation of  $S_{kl}(\mathbf{x}, \mathbf{x}'; \omega)$  by

$$S_{kl}(\mathbf{k}, \omega) = \int d^3(\mathbf{x} - \mathbf{x}') e^{-i\mathbf{k}(\mathbf{x} - \mathbf{x}')} S_{kl}(\mathbf{x} - \mathbf{x}'; \omega). \quad (5.20)$$

Since the tensor elements  $S_{kl}(\mathbf{k}, \omega)$  are expressed by

$$S_{kl}(\mathbf{k}, \omega) = \delta_{kl} S_1(\mathbf{k}^2, \omega^2) + (\mathbf{k}_k \mathbf{k}_l - k^2 \delta_{kl}) S_2(\mathbf{k}^2, \omega^2), \quad (5.21)$$

Eq. (5.14) can be written in terms of (5.21),



$$\begin{aligned} \langle [\mathbf{j}_k(\mathbf{x}, t), \mathbf{j}_i(\mathbf{k}', t')] \rangle &= \frac{1}{(2\pi)^4} \left[ \delta_{ki} \frac{\partial}{\partial t'} \int_{-\infty}^{\infty} d\omega \int d^3\mathbf{k} e^{-i\omega(t-t') + i\mathbf{k}(\mathbf{x}-\mathbf{x}')} S_1(\mathbf{k}^2, \omega^2) \right. \\ &\quad \left. \times \frac{1}{i\omega} \tanh \frac{\beta\hbar\omega}{2} + (\nabla'_i \nabla'_i - \delta_{ki} \nabla_i^2) \int_{-\infty}^{\infty} d\omega \int d^3\mathbf{k} e^{-i\omega(t-t') + i\mathbf{k}(\mathbf{x}-\mathbf{x}')} S_2(\mathbf{k}^2, \omega^2) \tanh \frac{\beta\hbar\omega}{2} \right]. \end{aligned} \quad (5.22)$$

In our problem the electric field  $\mathbf{E}(\mathbf{x}, t)$  and magnetic field  $\mathbf{H}(\mathbf{x}, t)$  are determined (from the vector potential  $\mathbf{A}(\mathbf{x}, t)$ ) by the formulas

$$\mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{A}}{\partial t}, \quad \nabla \times \mathbf{H} = (\nabla \nabla - \nabla^2) \mathbf{A}.$$

We thereby obtain, after a little manipulation, the following form

$$\begin{aligned} \langle \mathbf{J}(\mathbf{x}, t) \rangle &= \int d^3\mathbf{x}' \int_0^t dt' \left\{ \sigma(\mathbf{x}-\mathbf{x}', t-t') \mathbf{E}(\mathbf{x}', t') \right. \\ &\quad \left. + c \frac{\partial}{\partial t} r(\mathbf{x}-\mathbf{x}', t-t') \nabla \times \mathbf{H} \right\}, \end{aligned} \quad (5.23)^*$$

where

$$\begin{aligned} \sigma(\mathbf{x}-\mathbf{x}', t-t') &= \frac{1}{(2\pi)^4 \hbar} \int_{-\infty}^{\infty} d\omega \int d^3\mathbf{k} e^{-i\omega(t-t') + i\mathbf{k}(\mathbf{x}-\mathbf{x}')} S_1(\mathbf{k}^2, \omega^2) \frac{\tanh(\beta\hbar\omega/2)}{\omega} \\ r(\mathbf{x}-\mathbf{x}', t-t') &= \frac{1}{(2\pi)^4 \hbar c^2} \int_{-\infty}^{\infty} d\omega \int d^3\mathbf{k} e^{-i\omega(t-t') + i\mathbf{k}(\mathbf{x}-\mathbf{x}')} S_2(\mathbf{k}^2, \omega^2) \frac{\tanh(\beta\hbar\omega/2)}{\omega}. \end{aligned}$$

From these relations we can calculate electric conductivity, polarizability and magnetic susceptibility by the Fourier transform. The real part and the imaginary part of the Fourier transform of  $\sigma$  or  $r$  satisfy the well-known Kramers-Kronig's dispersion relation.

## §6. Connection with reaction matrix

The advantage and powerfulness of the Green function lie in the fact that one can formulate complicated problems without resorting to the concrete knowledge of the system in consideration or the nature of interactions intervening. Therefore, the structure or the formal aspect of the theory will be clarified, and the perspective to advance the theory into new stages will be given through the study of the Green function. Such

\* In derivation of (5.23) we get the non gauge-invariant extra term directly proportional to the vector potential itself which has the factor  $\left( \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{\tanh\left(\frac{1}{2}\beta\hbar\omega\right)}{\omega} S_1(\mathbf{k}^2\omega^2) - \frac{ne^2}{m} \right)$ , in its integrand,  $n$  being the particle density per unit volume. However, this term should vanish by virtue of the conservation law of charge, so that we obtain the sum rule  $\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{1}{\omega} \tanh\left(\frac{1}{2}\beta\hbar\omega\right) S_1(\mathbf{k}^2\omega^2) = \frac{ne^2}{m}$  for the spectral distribution function  $S_1(\mathbf{k}^2\omega^2)$ .

usefulness, however, is also its inconvenience at the same time. Being able to discuss formal aspects of the system, we are in rather difficult situation to calculate physically interesting quantities in practice. We have to admit some approximation to the Green function. For such a purpose it may be convenient to use another method which, however, is closely connected with the Green function. The method of the reaction matrix seems to serve our purpose. Actually it is known that the direct approximation to the Green function leads to the usual Brueckner reaction matrix for the ground-state energy and generalizations thereof. Brueckner and his collaborators<sup>13)</sup> extensively developed nuclear many-body problems based upon the reaction matrix. Goldstone,<sup>14)</sup> Thouless<sup>15)</sup> examined in greater detail Brueckner's theory, and enriched the contents of the theory. An approach similar to this problem has also been used by Klein<sup>16)</sup> and Prange.

With the aid of the appropriately defined reaction matrix they elucidated the Brueckner's theory for infinite nuclear matter. In this section we shall briefly review the use of the reaction matrix based upon the works by above mentioned people.

Now looking back §3 we have derived single-particle and two-particle Green function there.

$$\begin{aligned} \left[ i\hbar \frac{\partial}{\partial t_1} + \frac{\hbar^2}{2m} \nabla^2 \right] G(1, 1') - i\hbar \int d^3(1'') U(1-1'') G_{\text{II}}(1'', 1; 1'', 1') \\ = \delta^{(4)}(1-1') \end{aligned} \quad (6.1)$$

and

$$\begin{aligned} G_{\text{II}}(1, 2; 1', 2') = G(1, 1')G(2, 2') - G(1, 2')G(2, 1') \\ + \int G(1, 3)G(2, 4) W(3, 4; 3', 4') G_{\text{II}}(3', 4'; 1', 2') d(3)d(4)d(3')d(4') \end{aligned} \quad (6.2)$$

or symbolically,

$$G_{\text{II}} = G_1 G_2 1_{12} + G_1 G_2 W G_{\text{II}}. \quad (6.2')$$

Here relevant definitions or notions are the same as the ones used in §3.

Actually  $W$  is considered to be functional of the propagator  $G$ , and  $G$  in turn depends on  $W$ . So the solution to such coupled equations as (6.1) and (6.2) is extremely difficult and seems to be impossible to obtain in practice.

The following two approximations, however, may enable us to step further, to neglect the dependence of propagator on  $W$ , or to ignore the dependence of the interaction operator on  $G$ .

Now we shall introduce the function defined by

$$\begin{aligned} \mathcal{K}(1, 2; 1', 2') &= U(1-2)\delta^{(3)}(1-1')\delta^{(3)}(2-2')\delta_t(1-2) \\ &+ \int U(1-1'')\mathfrak{G}_{\text{II}}(1'', 2''; 1', 2')U(2-2'')d(1'')d(2''), \end{aligned} \quad (6.3)$$

where  $\mathfrak{G}$  satisfies the equation formally same as (6.1) in which all time integrations are construed to extend only over the past, i. e.,

$$\begin{aligned} \mathfrak{G}(1, 1') &= G^{(0)}(1, 1') + i\hbar \int d^3(1'')d^3\mathbf{y}'' \int_{-\infty}^0 dt'' G^{(0)}(1, 1'') \\ &\times U(1''-y'')\mathfrak{G}_{\text{II}}(\mathbf{y}''t'', 1''; \mathbf{y}''t'', 1'). \end{aligned} \quad (6.4)$$

Correspondingly,

$$\begin{aligned} \mathfrak{G}_{\text{II}}(1, 2; 1', 2') &= \mathfrak{G}(1, 1')\mathfrak{G}(2, 2') - \mathfrak{G}(1, 2')\mathfrak{G}(2, 1') \\ &+ \int d^{(3)}(3) \int d^{(3)}(4) \int d^{(3)}(3') \int d^{(3)}(4') \int d_t(3)d_t(4)d_t(3')d_t(4') \\ &\times \mathfrak{G}(1, 3)\mathfrak{G}(2, 4)w(3, 4; 3', 4')\mathfrak{G}_{\text{II}}(3', 4'; 1', 2'). \end{aligned} \quad (6.5)$$

These are the model single-particle and two-particle propagators defined by Klein and Prange, respectively, which are essentially the same as Thouless'  $R$  and  $L$ . It can easily be seen from (6.2) and (6.3) that  $\mathcal{K}$  satisfies the integral equation

$$\begin{aligned} \mathcal{K}(1, 2; 1', 2') &= U(1-2)\delta^{(3)}(1-1')\delta^{(3)}(2-2')\delta_t(1-2) \\ &+ \int_{t'}^t d_t(t'') \int_{t'}^{t''} d_t(2'') \int d^{(3)}(1'') \int d^{(3)}(2'') U(1-2)\delta(1-2) \\ &\times \mathfrak{G}(1, 1'')\mathfrak{G}(2, 2'')\mathcal{K}(1'', 2''; 1', 2') \quad t \geq t' \\ &= 0 \quad t < t'. \end{aligned} \quad (6.6)$$

This is then the reaction matrix which forms the basis of Brueckner's work.

Let us define the Fourier transforms by

$$\begin{aligned} \mathcal{K}_{mnpq} &= \int d^3x_1 d^3x_2 d^3x'_1 d^3x'_2 \exp(imx_1 + inx_2) \mathcal{K}(x_1x_2; x'_1x'_2) \\ &\times \exp(-ipx'_1 - iqx'_2), \\ \mathcal{K}(t) &= \frac{1}{2\pi} \int dE e^{-iEt} \mathcal{K}(E), \\ \mathfrak{G}_p &= \int e^{-ip(x-x')} \mathfrak{G}(x, x') d^{(3)}(x-x'). \end{aligned} \quad (6.7)$$

Then (6.6) can be written in the Fourier transform as

$$\mathcal{K}_{mnpq}(E) = U_{mnpq} + \sum_{k,l} U_{mnkl} \mathcal{R}_{kl} \mathcal{K}_{klpq} \quad (6.8)$$

where summation should be restricted to the states above the Fermi sea.  $\mathcal{R}_{kl}^+(E)$  is the convolution of the two single-particle propagators defined by

$$\mathcal{R}_{kl}^+(E) = \frac{i}{2\pi} \int_{-\infty}^{\infty} dE_1 \mathfrak{G}_k^+(E_1) \mathfrak{G}_l^+(E - E_1). \quad (6.9)$$

Here a (+) subscript denotes relevant quantities for particle which are analytic in the upper half-plane.

Now performing the Fourier transform and separating the Green function into two parts, one obtains the equations

$$\mathfrak{G}_k^+(E) = G_k^{(0)+}(E) \left[ 1 + \frac{1}{2\pi i} \int dE_1 \sum_{l < k_F} \mathcal{K}_{klkl}(E + E_1) \mathfrak{G}_l^-(E_1) \mathfrak{G}_k^+(E) \right], \quad (6.10)$$

$$\begin{aligned} \mathfrak{G}_k^-(E) = G_k^{(0)-}(E) & \left[ 1 - \frac{1}{(2\pi i)^2} \int_{-\infty}^{\infty} dE_1 dE_2 \right. \\ & \left. \times \frac{\sum_{l < k_F} \mathcal{K}_{klkl}(E_1) \mathfrak{G}_k^-(E_2) \mathfrak{G}_l^-(E_1 - E_2)}{E - E_2 - i\delta} \right], \end{aligned} \quad (6.11)$$

where  $G_k^{(0)\pm}(E)$  is the unperturbed propagator for particle (hole).  $\mathfrak{G}^-$  represents the corresponding hole Green function which are analytic in the lower half-plane, and has such a simple solution as

$$\mathfrak{G}_k^-(E) = -\frac{1}{E - \varepsilon_k^- - i\delta}, \quad (6.12)$$

where

$$\varepsilon_k^- = \frac{\hbar^2 k^2}{2m} + \sum_{l < k_F} [\mathcal{K}_{klkl}(\varepsilon_k^- + \varepsilon_l^-) - \mathcal{K}_{klkl}(\varepsilon_k^- + \varepsilon_l^-)]. \quad (6.13)$$

With the aid of analytic properties of  $\mathfrak{G}_k^+(E)$  it turns out to be

$$\begin{aligned} \mathfrak{G}_k^+(E) &= - \left[ E - \frac{\hbar^2 k^2}{2m} + \frac{1}{2\pi i} \int dE_1 \sum_l \mathcal{K}_{klkl}(E + E_1) \mathfrak{G}_l^-(E_1) + i\delta \right]^{-1} \\ & \quad \text{for } l > k_F \\ &= 0 \quad \text{for } l < k_F. \end{aligned} \quad (6.14)$$

If we make an approximation usually done in which we replace the denominator of (6.14) by its real part,  $\mathcal{K}_{klkl}(E + \varepsilon_l^-)$  can be replaced by  $\text{Re} \mathcal{K}_{klkl}(\varepsilon_k^+ + \varepsilon_l^-)$ .  $\varepsilon_k^+$  satisfies

$$\varepsilon_k^+ = \frac{\hbar^2 k^2}{2m} + \sum_{l < k_F} \text{Re} [\mathcal{K}_{klkl}(\varepsilon_k^+ + \varepsilon_l^-) - \mathcal{K}_{klkl}(\varepsilon_k^+ + \varepsilon_l^-)] \quad k > k_F. \quad (6.15)$$

Correspondingly (6.8) can be written in this approximation as follows,

$$\mathcal{K}_{mnpq}(E) = U_{mnpq} + \sum_{kl > k_F} U_{mnkl} \frac{1}{E - \epsilon_k^+ - \epsilon_l^- + i\delta} \mathcal{K}_{klpq}(E). \quad (6 \cdot 16)$$

This is the reaction matrix neglecting “off-the-energy-shell” propagation. (6·15) and (6·16) are the equations to obtain interaction energy of a pair of particles. The energy is determined through the solution of the reaction matrix  $\mathcal{K}$ . On the other hand  $\mathcal{K}$  depends on the energy in the intermediate states which must also be determined by the reaction matrix. The system of these equations has such a complicated structure of the infinite ladder of equations, that we do not enter here into the detailed discussion of the solution. Brueckner et al. succeeded to reduce the ladder to a single equation without approximation by introducing a parameter with an infinite range in the denominator of the integral equation for the reaction matrices. Readers may refer to the original paper on these discussions.

Finally we record the total energy of the ground state obtained in our approximation:

$$\begin{aligned} E(A) &= \frac{3}{5} Ak_F^2 + \frac{1}{2} \int d(1)d^{(3)}(2)d(1')d^{(3)}(2') \int_{-\infty}^0 d_t(2') \\ &\quad \times \mathcal{K}(12, 1'2') [\mathfrak{G}(1', 1)\mathfrak{G}(2', 2) - \mathfrak{G}(1', 2)\mathfrak{G}(2', 1)] \\ &= \frac{3}{5} Ak_F^2 + \frac{1}{2} \sum_{mn} [\mathcal{K}_{mnmn}(\epsilon_m^- + \epsilon_n^-) - \mathcal{K}_{mnmn}(\epsilon_m^- + \epsilon_n^-)]. \end{aligned}$$

## §7. Amplitudes and their equations

In many-particle systems we can often observe the systematic one- or two-particle motions. There the surrounding particles behave as if they were a sort of medium for the systematic motions of one or two particle in consideration. Such a motion may be described by the one- or two-particle amplitude. In the present section we shall define them in a reasonable way and study the equations satisfied by them. In particular, the one-particle amplitude will be explained in detail through investigation of the problems of the nuclear optical model and of the Hydrogen-like motion of an electron in insulator.

### 7.1 Definitions of amplitudes and effective potential

First we consider the one-particle amplitude. Suppose that the system is in a state represented by a vector  $|E, \alpha\rangle$ , where  $E$  is the energy of the system and  $\alpha$  other quantum numbers. Now we know that the vector  $\psi^*(x)|m\rangle$  asymptotically approaches to the vector representing the state in which a particle is found at a point  $x$  in the medium whose state is

$|m\rangle$ . Therefore it may be inferred that the one-particle amplitude defined by

$$\chi(\mathbf{x}) \equiv \langle m | \psi(\mathbf{x}) | E, \alpha \rangle \quad (7.1)$$

describes, in an asymptotical sense, the systematic one-particle motions in the many-particle system. Here it is noted that  $\psi$  is the field operator in the Heisenberg representation. When a systematic one-particle motion is observed, the state vector  $|E, \alpha\rangle$  may be written down as follows:

$$|E^+, \alpha\rangle = \lim_{t_0 \rightarrow \infty} \frac{1}{t_0} \int_{-\infty}^{t_1} dt \int d^3\mathbf{x} \psi^*(\mathbf{x}, t) |m\rangle \varphi_0(\mathbf{x}) e^{-(i/\hbar)Et + (t_1 - t/t_0)}, \quad (7.2a)$$

or

$$|E^-, \alpha\rangle = \lim_{t_0 \rightarrow \infty} \frac{1}{t_0} \int_{t_1}^{\infty} dt \int d^3\mathbf{x} \psi^*(\mathbf{x}, t) |m\rangle \varphi_0(\mathbf{x}) e^{-(i/\hbar)Et + (t - t_1/t_0)}. \quad (7.2b)$$

Here  $|E^+, \alpha\rangle$  and  $|E^-, \alpha\rangle$  correspond, respectively, to an initial state and a final state of the medium in  $|m\rangle$  and a particle in  $\varphi(\mathbf{x})$ . From the definition it is quite easy to show the equation

$$(E - H) |E^\pm, \alpha\rangle = 0, \quad (7.3)$$

where the energy of the state  $|m\rangle$  is put zero. From (7.3) one gets the equation

$$i\hbar \frac{d}{dt_1} |E^\pm, \alpha\rangle = (E - H) |E^\pm, \alpha\rangle = 0. \quad (7.4)$$

In other words, the state  $|E^\pm, \alpha\rangle$  is an eigenvector of the total Hamiltonian belonging to an eigenvalue  $E$  and is independent of  $t_1$ . Hence the time-interval  $(t_1, -\infty)$  is chosen in a remote past, while  $(\infty, t_1)$  in a remote future. To show (7.3), we have only to apply  $H$  to the right member of (7.2) to commute  $H$  with  $\psi^*$  and to perform integration by parts. Next we can show that  $|E^+, \alpha\rangle$  and  $|E^-, \alpha\rangle$  are subject to the outgoing-wave and the ingoing-wave boundary conditions, respectively. This will be seen in the following: The expression (7.2) can be rewritten as

$$|E^\pm, \alpha\rangle = \lim_{t_0 \rightarrow \infty} \frac{\pm (\hbar/t_0)}{i(H - E_p) \pm (\hbar/t_0)} |\varphi_0\rangle,$$

or

$$= |\varphi_0\rangle + \lim_{t_0 \rightarrow \infty} \frac{1}{(E - H_0) \pm i(\hbar/t_0)} H_1 |E^\pm, \alpha\rangle, \quad (7.5)$$

where we have used the equation

$$\psi(\mathbf{x}, t) = \exp\{(i/\hbar)Ht\} \psi(\mathbf{x}) \exp\{-(i/\hbar)Ht\}$$

and the abbreviation

$$|\varphi_0\rangle \equiv \int d^3x \psi^*(\mathbf{x}) |m\rangle \varphi_0(\mathbf{x}).$$

The form (7.5) shows explicitly the boundary conditions. Thus we can write the amplitude  $\chi$  as

$$\begin{aligned} \chi(\mathbf{x}, t) &= \lim_{t_0 \rightarrow \infty} \frac{1}{t_0} \int_{-\infty}^{t_1} dt' \int d^3x' \langle m | \psi(\mathbf{x}, t) \psi^*(\mathbf{x}', t') | m \rangle \varphi_0(\mathbf{x}') e^{-(i/\hbar)Et' + (t' - t_1/t_0)} \\ &= \lim_{t_0 \rightarrow \infty} \frac{i\hbar}{t_0} \int_{-\infty}^{t_1} dt' \int d^3x' G(\mathbf{x}, t; \mathbf{x}', t') \varphi_0(\mathbf{x}') e^{-(i/\hbar)Et' + (t' - t_1/t_0)}, \end{aligned} \quad (7.6)$$

where the definition (2.4) has been used.

The time in  $\chi(\mathbf{x}, t)$  does not take a value in the time-interval  $(t_1, -\infty)$ , because the time-interval was chosen in a remote past. Consequently the amplitude should obey the equation

$$\left( i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 \right) \chi(\mathbf{x}) - \int d^4x' \Sigma(\mathbf{x}, \mathbf{x}') \chi(\mathbf{x}') = 0, \quad (7.7)$$

where we have used the equation (3.28) of the Green function.

All the above formulas and equations can describe the one-hole propagations in the medium, if we replace  $\psi^*$  by  $\psi$  and reverse the order in time.

Next we shall derive the effective potential for the one-particle motions in the medium. From the definition it is easily shown that the amplitude  $\chi(\mathbf{x})$  oscillates harmonically in time, namely,

$$\chi(\mathbf{x}, t) = \chi(\mathbf{x}, 0) e^{-(i/\hbar)Et}. \quad (7.8)$$

Hence we can rewrite the last term of the left member of (7.7) as follows:

$$\int d^4x' \Sigma(\mathbf{x}, \mathbf{x}') \chi(\mathbf{x}') = \int d^3x' \langle \mathbf{x} | \mathcal{V}_E | \mathbf{x}' \rangle \chi(\mathbf{x}', t), \quad (7.9)$$

where

$$\langle \mathbf{x} | \mathcal{V}_E | \mathbf{x}' \rangle \equiv \int dt' \Sigma(\mathbf{x}, t; \mathbf{x}', t') e^{(i/\hbar)E(t-t')}. \quad (7.10)$$

In derivation of (7.9), we have assumed that the medium is uniform in time, or in other words,  $\Sigma(\mathbf{x}, \mathbf{x}')$  is a function of  $(t-t')$  with respect to time variable. The function  $\langle \mathbf{x} | \mathcal{V}_E | \mathbf{x}' \rangle$  is nothing but the effective potential for the one-particle motion in question. As is seen from (7.10), the effective potential is, in general, non-local and dependent of energy  $E$ . Only when the wave-length of the incident particle is much longer than the characteristic length for non-locality (in other words, the correlation

length), we can treat as the local potential

$$\mathcal{V}_E(\mathbf{x}) \equiv \int d^3\mathbf{x}_0 \left\langle \mathbf{x} - \frac{1}{2}\mathbf{x}_0 \left| \mathcal{V}_E \right| \mathbf{x} + \frac{1}{2}\mathbf{x}_0 \right\rangle. \quad (7.11)$$

First we discuss the properties of  $\mathcal{V}_E^S$ , corresponding to  $\Sigma^S$  defined by (3.33), which is regarded as the contribution of the medium in the fixed state. From (3.33) and (7.10) we immediately get the formula

$$\langle \mathbf{x} | \mathcal{V}_E^S | \mathbf{x}' \rangle = \bar{V}(\mathbf{x}) \delta(\mathbf{x} - \mathbf{x}') + i\hbar G(\mathbf{x}, 0; \mathbf{x}', 0) V(\mathbf{x} - \mathbf{x}'). \quad (7.12)$$

Therefore the static part  $\mathcal{V}_E^S$  never depends on the energy  $E$ . Furthermore, it is easy to prove the hermitian property of  $\mathcal{V}_E^S$ , that is,

$$\langle \mathbf{x} | \mathcal{V}_E^S | \mathbf{x}' \rangle = \{ \langle \mathbf{x}' | \mathcal{V}_E^S | \mathbf{x} \rangle \}^*. \quad (7.13)$$

The hermitian property of  $\mathcal{V}_E^S$  tells us the facts that  $\mathcal{V}_E^S$  is never responsible for probability dissipation of the one-particle amplitude in consideration, in other words, for the real excitations of the medium. Such properties of  $\mathcal{V}_E^S$  show that  $\mathcal{V}_E^S$  is worthy to be called the *static* part of the effective potential.

The non-hermitian property of the effective potential originates in the fluctuation part  $\Sigma^F$  defined by (3.33). Denote the contribution of  $\Sigma^F$  to the effective potential by  $\mathcal{V}_E^F$ . The fluctuation part  $\mathcal{V}_E^F$  is, in general, decomposed into the hermitian part  $\mathcal{V}_E^{Fr}$  and the anti-hermitian part  $\mathcal{V}_E^{Fi}$ , that is,

$$\mathcal{V}_E^F \equiv \mathcal{V}_E^{Fr} - i\mathcal{V}_E^{Fi}. \quad (7.14)$$

Both the matrices  $\mathcal{V}_E^{Fr}$  and  $\mathcal{V}_E^{Fi}$  are hermitian. In order to illustrate the concrete form of  $\mathcal{V}_E^F$ , we shall calculate the function  $\langle \mathbf{x} | \mathcal{V}_E^F | \mathbf{x}' \rangle$  to the lowest order in the perturbation theory formulated in §4. Substituting (3.33) into the definition of  $\mathcal{V}_E^F$  and using the explicit formulas (4.18) and (4.31), we obtain, after some calculations, the contribution of the first two terms of (4.31) to the effective potential as follows:

$$\begin{aligned} \langle \mathbf{x} | \mathcal{V}_E^F | \mathbf{x}' \rangle &= (i\hbar)^{-1} \sum_{l\bar{m}\bar{n}} \int_{-\infty}^t dt' \exp\{(i/\hbar)(E - E_l^0 - E_{\bar{m}}^0 - E_{\bar{n}}^0)(t - t')\} \\ &\quad \times F_{l\bar{m}\bar{n}}(\mathbf{x}) F_{l\bar{m}\bar{n}}^*(\mathbf{x}') \\ &\quad - (i\hbar)^{-1} \sum_{l\bar{m}\bar{n}} \int_t^{\infty} dt' \exp\{(i/\hbar)(E + E_l^0 + E_{\bar{m}}^0 + E_{\bar{n}}^0)(t - t')\} \\ &\quad \times F_{l\bar{m}\bar{n}}^*(\mathbf{x}) F_{l\bar{m}\bar{n}}(\mathbf{x}'), \end{aligned} \quad (7.15)$$

where we have used the abbreviation



$$\begin{aligned}
 F_{l\bar{m}n}(\mathbf{x}) &\equiv \int d^3\mathbf{x}'' V(\mathbf{x}-\mathbf{x}'') \chi_m^{(0)}(\mathbf{x}'') \chi_{l'n}^{(0)}(\mathbf{x}, \mathbf{x}''), \\
 F_{\bar{l}m\bar{n}}(\mathbf{x}) &\equiv \int d^3\mathbf{x}'' V(\mathbf{x}-\mathbf{x}'') \chi_m^{(0)}(\mathbf{x}'') \chi_{l'n}^{(0)}(\mathbf{x}, \mathbf{x}'').
 \end{aligned}
 \tag{7.16}$$

Here  $\chi_{l'n}^{(0)}$  and  $\chi_{\bar{l}\bar{n}}^{(0)}$  are, respectively, defined by

$$\begin{aligned}
 \chi_{l'n}^{(0)}(\mathbf{x}, \mathbf{x}'') &\equiv \frac{1}{\sqrt{2}} \{ \chi_l^{(0)}(\mathbf{x}) \chi_n^{(0)}(\mathbf{x}'') - \chi_n^{(0)}(\mathbf{x}) \chi_l^{(0)}(\mathbf{x}'') \}, \\
 \chi_{\bar{l}\bar{n}}^{(0)}(\mathbf{x}, \mathbf{x}'') &\equiv \frac{1}{\sqrt{2}} \{ \chi_{\bar{l}}^{(0)}(\mathbf{x}) \chi_{\bar{n}}^{(0)}(\mathbf{x}'') - \chi_{\bar{n}}^{(0)}(\mathbf{x}) \chi_{\bar{l}}^{(0)}(\mathbf{x}'') \}.
 \end{aligned}
 \tag{7.17}$$

The functions  $F_{l\bar{m}n}$  and  $F_{\bar{l}m\bar{n}}$  have the properties

$$F_{l\bar{m}n} = -F_{\bar{n}m\bar{l}}, \quad F_{\bar{l}m\bar{n}} = -F_{\bar{n}m\bar{l}}
 \tag{7.18}$$

due to the anti-symmetric properties of  $\chi_{l'n}^{(0)}$  and  $\chi_{\bar{l}\bar{n}}^{(0)}$ . To evaluate the time integrals in (7.15), we can use

$$\begin{aligned}
 (i\hbar)^{-1} \int_{-\infty}^t dt' \exp\left[\frac{i}{\hbar} a(t-t')\right] &= -i\pi\delta(a) + \text{P} \frac{1}{a}, \\
 -(i\hbar)^{-1} \int_t^{\infty} dt' \exp\left[\frac{i}{\hbar} a(t-t')\right] &= i\pi\delta(a) + \text{P} \frac{1}{a}.
 \end{aligned}
 \tag{7.19}$$

Hence we can immediately write down  $\mathcal{V}_E^{Fr}$  and  $\mathcal{V}_E^{Fi}$  as follows:

$$\begin{aligned}
 \langle \mathbf{x} | \mathcal{V}_E^{Fr} | \mathbf{x}' \rangle &= \text{P} \sum_{l\bar{m}n} \frac{F_{l\bar{m}n}(\mathbf{x}) F_{l\bar{m}n}^*(\mathbf{x}')}{E - E_l^0 - E_m^0 - E_n^0} \\
 &\quad + \text{P} \sum_{\bar{l}m\bar{n}} \frac{F_{\bar{l}m\bar{n}}^*(\mathbf{x}) F_{\bar{l}m\bar{n}}(\mathbf{x}')}{E + E_{\bar{l}}^0 + E_m^0 + E_{\bar{n}}^0},
 \end{aligned}
 \tag{7.20}$$

$$\begin{aligned}
 \langle \mathbf{x} | \mathcal{V}_E^{Fi} | \mathbf{x}' \rangle &= \pi \sum_{l\bar{m}n} \delta(E - E_l^0 - E_m^0 - E_n^0) F_{l\bar{m}n}(\mathbf{x}) F_{l\bar{m}n}^*(\mathbf{x}') \\
 &\quad - \pi \sum_{\bar{l}m\bar{n}} \delta(E + E_{\bar{l}}^0 + E_m^0 + E_{\bar{n}}^0) F_{\bar{l}m\bar{n}}^*(\mathbf{x}) F_{\bar{l}m\bar{n}}(\mathbf{x}').
 \end{aligned}
 \tag{7.21}$$

It is easy to prove the hermiticity of  $\mathcal{V}_E^{Fr}$  and  $\mathcal{V}_E^{Fi}$ . The last term in the right member of (7.21) vanishes in the cases of particle propagation, because it is impossible to realize the energy relation  $E + E_{\bar{l}}^0 + E_m^0 + E_{\bar{n}}^0 = 0$ , corresponding to spontaneous excitations of the medium. Inversely, the first term vanishes for hole propagation, since the energy relation  $E - E_l^0 - E_m^0 - E_n^0 = 0$  is never realized. For the moment we shall discuss the particle propagation.

From (7.20) and (7.21) we can calculate the expectation value of  $\mathcal{V}_E^F$  for the amplitude  $\chi$  as follows:

$$\begin{aligned}
(\chi, \mathcal{V}_E^{Fr} \chi) &\equiv \iint \chi^*(\mathbf{x}) \langle \mathbf{x} | \mathcal{V}_E^{Fr} | \mathbf{x}' \rangle \chi(\mathbf{x}') d^3x d^3x' \\
&= P \sum_{l\bar{m}n} \frac{|\langle \chi | V | l\bar{m}n \rangle|^2}{E - E_l^0 - E_m^0 - E_n^0} + P \sum_{l\bar{m}\bar{n}} \frac{|\langle m | V | \chi l\bar{m}\bar{n} \rangle|^2}{E + E_l^0 + E_m^0 + E_n^0}, \quad (7.22)
\end{aligned}$$

$$(\chi, \mathcal{V}_E^{Fi} \chi) \equiv \iint \chi^*(\mathbf{x}) \langle \mathbf{x} | \mathcal{V}_E^{Fi} | \mathbf{x}' \rangle \chi(\mathbf{x}') d^3x d^3x' \equiv \frac{\hbar}{2} w_E, \quad (7.23)$$

where

$$w_E \equiv \frac{2\pi}{\hbar} \sum_{l\bar{m}n} \delta(E - E_l^0 - E_m^0 - E_n^0) |\langle \chi | V | l\bar{m}n \rangle|^2. \quad (7.24)$$

Here we have used the abbreviations

$$\begin{aligned}
\langle \chi | V | l\bar{m}n \rangle &\equiv \int \chi^*(\mathbf{x}) F_{l\bar{m}n}(\mathbf{x}) d^3x, \\
\langle m | V | \chi l\bar{m}\bar{n} \rangle &\equiv \int \chi(\mathbf{x}) F_{l\bar{m}\bar{n}}(\mathbf{x}) d^3x. \quad (7.25)
\end{aligned}$$

Thus we know that  $\mathcal{V}_E^{Fi}$  has a positive expectation value, and that  $w_E$  is nothing but the time rate of the transition probability for exciting the medium or for decay of its excited state. This is the situation just expected, because the anti-hermitian part  $\mathcal{V}_E^{Fi}$ , responsible for the probability dissipation of the one-particle amplitude, is one of the contribution of the fluctuation part  $\Sigma^F$  represented by Fig. 8 to the effective potential. There it is noted that the probability dissipation of the one-particle amplitude is caused by the pair-excitations of the medium. For hole propagation we have the negative expectation value of  $\mathcal{V}_E^{Fi}$ . It is reasonable, however, because hole propagation can be regarded as the time-reversed process of particle propagation. The expression (7.22) for the expectation value of  $\mathcal{V}_E^{Fr}$  has a strong resemblance to the self-energy of a particle or to the level shift in quantum field theory. In fact, the hermitian part  $\mathcal{V}_E^{Fr}$  is responsible for modification of effective mass or for the shifts of the resonance level. Therefore the fluctuation part  $\mathcal{V}_E^F$  represents reactions of virtual or provisional excitations of the medium to the one-particle motion in consideration.

Finally we explain the equation satisfied by the two-particle amplitude defined by

$$\chi_{II}(x_1, x_2) \equiv \langle m | T(\psi(x_1)\psi(x_2)) | E, \alpha \rangle \quad (7.26)$$

which may be interpreted in an asymptotic sense such as given for the one-particle amplitude. When a sort of systematic two-particle motion can be observed, the vector  $|E, \alpha\rangle$  may be written down as follows:

$$|E^+, \alpha\rangle \equiv \lim_{t_0 \rightarrow \infty} \frac{1}{t_0^2} \int_{-\infty}^{t_1} dt'_1 \int_{-\infty}^{t_1} dt'_2 \int d\mathbf{x}'_1 d\mathbf{x}'_2 \psi^*(\mathbf{x}'_1, t'_1) \psi^*(\mathbf{x}'_2, t'_2) |m\rangle \varphi_0(\mathbf{x}'_1, \mathbf{x}'_2)$$

$$\times \exp\left\{\left(-\frac{i}{\hbar}\right)E_1 t'_1 + \frac{t'_1 - t_1}{t_0}\right\} \cdot \exp\left\{\left(-\frac{i}{\hbar}\right)E_2 t'_2 + \frac{t'_2 - t_1}{t_0}\right\}, \quad (7.27)$$

where  $E = E_1 + E_2$  is given.  $|E^-, \alpha\rangle$  is expressed in an analogous way. It is also easy to prove that  $|E^+, \alpha\rangle$  is an eigenvector of  $H$  belonging to an eigenvalue  $E$  and is independent of  $t$ . From (7.26) and (7.27) it follows that

$$\begin{aligned} \chi_{\text{II}}(1, 2) &= \lim_{t_0 \rightarrow \infty} \frac{(i\hbar)^2}{t_0^2} \int_{-\infty}^{t_1} dt'_1 \int_{-\infty}^{t'_1} dt'_2 \int d^3 x'_1 d^3 x'_2 G(\mathbf{x}_1 t_1, \mathbf{x}_2 t_2; \mathbf{x}'_1 t'_1, \mathbf{x}'_2 t'_2) \\ &\times \varphi_0(\mathbf{x}'_1, \mathbf{x}'_2) \exp\left\{-\frac{i}{\hbar} E_1 t'_1 + \frac{t'_1 - t_1}{t_0}\right\} \cdot \exp\left\{-\frac{i}{\hbar} E_2 t'_2 + \frac{t'_2 - t_1}{t_0}\right\}. \end{aligned} \quad (7.28)$$

Thus, since the interval  $(t_1, -\infty)$  is chosen in a remote past, the amplitude  $\chi(\mathbf{x}_1, \mathbf{x}_2)$  should obey the equation

$$\iint [G^{-1}(1, 1')G^{-1}(2, 2') - W(1, 1'; 2, 2')] \chi_{\text{II}}(1', 2') d(1') d(2') = 0 \quad (7.29)$$

or symbolically

$$G_1^{-1} G_2^{-1} \chi_{\text{II}} - W \chi_{\text{II}} = 0. \quad (7.30)$$

Using the one-particle Green functions, one can easily rewrite Eq. (7.28) in the integral equation

$$\begin{aligned} \chi_{\text{II}}(1, 2) &= \chi_{\text{II}}^{(0)}(1, 2) + \iiint G(1, 1') G(2, 2') W(1', 2'; 3, 4) \chi_{\text{II}}(3, 4) \\ &\times d(1') d(2') d(3) d(4), \end{aligned} \quad (7.31)$$

where the inhomogeneous term  $\chi_{\text{II}}^{(0)}(1, 2)$  is defined by

$$\chi_{\text{II}}^{(0)}(1, 2) = \chi_1(1) \chi_2(2) - \chi_1(2) \chi_2(1) \quad (7.32)$$

for some scattering problems,  $\chi_1$  and  $\chi_2$  being the one-particle amplitude, and corresponding to propagations of the incident two particles without interactions. Eq. (7.32) can be replaced by

$$\begin{aligned} \chi_{\text{II}}^{(0)}(1, 2) &= \lim_{t_0 \rightarrow \infty} \frac{(i\hbar)^2}{t_0^2} \iint_{-\infty}^{t_1} dt'_1 dt'_2 \iint d^3 x'_1 d^3 x'_2 [G_0(1; \mathbf{x}'_1, t'_1) G_0(2; \mathbf{x}'_2, t'_2) \\ &- G_0(1; \mathbf{x}'_2, t'_2) G_0(2; \mathbf{x}'_1, t'_1)] \varphi_0(\mathbf{x}'_1, \mathbf{x}'_2) \\ &\times \exp\left\{-\frac{i}{\hbar} E_1 t'_1 + \frac{t'_1 - t_1}{t_0}\right\} \cdot \exp\left\{-\frac{i}{\hbar} E_2 t'_2 + \frac{t'_2 - t_1}{t_0}\right\} \end{aligned} \quad (7.33)$$

with  $E = E_1 + E_2$ . When we are concerned with a bound state in which  $E < 0$ , the integral with respect to time in (7.33) would vanish because

the function  $[G_0(1; \mathbf{x}'_1, t'_1)G(2; \mathbf{x}'_2, t_2) - \dots]$  contains only positive frequencies. Therefore the amplitude for a bound state satisfies the integral equation\*

$$\chi_{\text{II}}(1, 2) = \iiint G(1, 1')G(2, 2')W(1', 2'; 3, 4)\chi_{\text{II}}(3, 4)d(1')d(2')d(3)d(4). \quad (7.34)$$

The equations of the types, such as (7.29), (7.31) and (7.34), were first introduced by Nambu<sup>17)</sup> for a special case and developed by Kita,<sup>18)</sup> Bethe and Salpeter,<sup>19)</sup> Gell-Mann and Low,<sup>20)</sup> and Schwinger<sup>21)</sup> for some general cases in quantum field theory. In particular, Eq. (7.34) is often called the "Bethe-Salpeter" equation.

## 7.2 Nuclear optical model

As is well known, the giant resonances in nuclear reactions are observed in the cross sections for the elastic scattering of neutrons at low energies by large nuclei, if averaged at each energy point over some spread. They can also be expected in observations using incident beams with some energy spread. Following Weisskopf et al., the giant resonances can be well reproduced by a one-particle Schroedinger equation with a complex potential for an incident neutron. Such a complex potential is called the *optical potential*, whose imaginary part is responsible for the probability dissipation of the one-particle amplitude due to occurrence of other inelastic collisions. Thus the optical model may be accepted by the notion of an irreversible process, in which one observes a sort of one-particle motions as an average or coarse-grained motion of the many-particle system in consideration. The above-mentioned average comes from the energy spread of incident beams. Hayakawa et al.<sup>21)</sup> considered the beam to be a short wave packet with time-length  $t_0$  corresponding to the above energy spread  $E_p \simeq (\hbar/t_0)$ . However, it may hardly be acceptable to consider the short wave packet as the one produced in actual instruments. One may rather prefer considering the actual beam like a mixed beam to regarding it as a single and short wave packet. The mixed beam consists of a random mixture of a number of long wave packets, in which each wave packet has a sharply determined energy but its center of energy distributes over the range  $\Delta E_p$ . In both cases we may expect the same aspect of irreversible processes as suggested from discussions given by Van Hove<sup>22)</sup> and Toda.<sup>23)</sup> At any rate, it becomes necessary for derivation of the coarse-grained one-particle motion to discard or to average the fine interactions within a short time-interval at each time. To discard the short interval is equivalent to ignoring the high frequency parts. Therefore

\* Note that Gell-Mann and Low devised the so-called "L-operation" for the purpose of omission of the inhomogeneous term. Our derivation of (7.34) never necessitates such an ambiguous manipulation.

deviations from the coarse-grained motion come to be of random fluctuations on such a time scale. For the usage of a single wave packet, however, one may pay close attention to the randomness. If the wave packet has a long time-length enough to discriminate the average spacing of fine-structure levels of the whole system, we could observe a new type of systematic motions of the system, for example, the compound nucleus. In order that we can observe the coarse-grained one-particle motions, or in other words, the optical model in nuclear reactions, the packet should be so designed as to have a length much shorter than the time corresponding to the average spacing of the fine-structure levels. Otherwise, we would observe the many-particle motions themselves, as the systematic ones.

Here we shall briefly explain the nuclear optical model, in particular, the derivation of the optical potential from the fundamental many-particle equation. For simplicity, we suppose that the beam is a single wave packet with time-length  $t_0$  and energy spread  $\Delta E_p \simeq (\hbar/t_0)$  around its center  $E_p$ . For a mixed beam, the discussions given below will not be essentially modified; see Van Hove<sup>22)</sup> and Toda,<sup>23)</sup> and Namiki.<sup>24)</sup> The scattering state caused by such an incident wave packet is written as

$$|E_p^+\rangle = \sum_{E, \alpha} a(E, \alpha) |E^+, \alpha\rangle, \quad (7.35)$$

where  $a(E, \alpha)$  is a smooth function having non-zero values only in the range  $\Delta E_p$  around its center  $E_p$ . The state  $|E_p^+\rangle$  can also be represented by

$$|E_p^+\rangle = \frac{1}{t_0} \int_{-\infty}^{t_1} dt' \int d^3x' \psi^*(x', t') |A\rangle \varphi_p(x') e^{-(i/\hbar)E_p t' + (t' - t_1/t_0)}, \quad (7.36)$$

where  $\varphi(x)$  is a function corresponding to the initial wave packet. Here  $|A\rangle$  stands for the vector representing the ground state of the target nucleus. If  $|A\rangle$  is an eigenvector of the total momentum operator, the system is uniform and then we cannot observe the optical (or effective) potential located at a point with a nuclear size. Consequently we should prepare the vector  $|A\rangle$ , by which the localized center-of-mass of the target nucleus is represented. In the same way as (7.2), one can easily prove that

$$\begin{aligned} (E_p - H) |E_p^+\rangle &= O(\Delta E_p), \\ i\hbar \frac{d}{dt_1} |E_p^+\rangle &= (E - H) |E_p^+\rangle = O(\Delta E_p), \\ |E_p^+\rangle &= \frac{(\hbar/t_0)}{i(H - E_p) + (\hbar/t_0)} |\varphi_p\rangle + O(\Delta E_p), \end{aligned} \quad (7.37)$$

as expected. Thus  $|E_p^+\rangle$  is regarded as an approximate eigenvector of  $H$  belonging to an eigenvalue  $E_p$ , so that the amplitude

$$\chi_p(\mathbf{x}, t) \equiv \langle A | \psi(\mathbf{x}, t) | E_p^+ \rangle \quad (7.38)$$

oscillates in a nearly harmonic way during the packet passes. Consequently the amplitude  $\chi_p$  obeys the one-particle Schroedinger equation

$$\left[ i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 \right] \chi_p(\mathbf{x}, t) - \int d^3\mathbf{x}' \langle \mathbf{x} | \mathcal{V}_p | \mathbf{x}' \rangle \chi_p(\mathbf{x}', t) = 0, \quad (7.39)$$

where  $\mathcal{V}_p$  is nothing but the so-called "optical potential" and defined by

$$\mathcal{V}_p \equiv \sum_E w(E) \mathcal{V}_E,$$

or

$$\equiv \int dt' e^{(i/\hbar)E_p(t-t') - (t-t')/t_0} \Sigma(\mathbf{x}, t; \mathbf{x}', t'), \quad (7.40)$$

$w_E$  being a smooth function\* with non-zero values only in the range  $\Delta E$  around its center  $E_p$ . Here  $\mathcal{V}_E$  is the effective potential defined in the previous subsection. The static part of  $\mathcal{V}_p$  is exactly equal to that of  $\mathcal{V}_E$ . To obtain the explicit formula for the fluctuation part of  $\mathcal{V}_p$ , we have only to replace the delta-function and the principal part of the expressions such as (7.20) and (7.21) of  $\mathcal{V}_E$  with the smooth functions corresponding to them as follows:

$$\begin{aligned} \delta(a) &\rightarrow \frac{1}{\pi} \frac{(\hbar/t_0)}{a^2 + (\hbar/t_0)^2}, \\ \text{P} \frac{1}{a} &\rightarrow \frac{a}{a^2 + (\hbar/t_0)^2}. \end{aligned} \quad (7.41)$$

The deviations of one-particle amplitude from the average become random on a rough time scale, if the systematic motion of the system is of the one-particle motion. It will be proved that such random deviations are subject to the fluctuation-dissipation theorem, if the system is excited in quasi-equilibrium. For details, see Namiki's paper.<sup>24)</sup>

### 7.3 One electron in insulators and semi-conductors

The many-particle approach developed in this article has various fields of its application not only to nuclear many-body problem but also to problems in solid state physics. We shall give here another typical example of our formalism in solid state physics. Consider a motion of one electron in insulators and semi-conductors. This problem has long been familiar but difficult subject. When we want to take into account the effect of all other electrons properly, we are inevitably forced to treat with many-body

\*  $w(E)$  must be so normalized that  $\sum_E w(E) = 1$ .

problems. That is, electrically and magnetically susceptible media should be described from the many-particle point of view. Then the situation is just analogous to that encountered in the nuclear many-body problem, where one incident nucleon plus target nucleus was successfully described in terms of the nuclear optical potential as discussed in great detail in the previous section.

Klein<sup>25)</sup> has already developed the discussion on this subject along the line mentioned above. His guiding image was the analogy between the system, impurity plus electron imbedded in the crystal, and the hydrogen atom, proton plus electron imbedded in the vacuum. Being originated in the nuclear reaction because of the close connection with previous argument, our idea is essentially the same as that of Klein's.

Considering the case of a perfect insulator which contains  $N$  electrons, with a single extra electron (or hole) and a small external charge  $q$  imbedded in it, Kohn<sup>26)</sup> has shown that the  $(N \pm 1)$ -particle Schrodinger equation could be reduced—for the low lying states—to a single particle equation of the form

$$\left[ -\frac{\hbar^2}{2m^*} \nabla^2 \mp \frac{eq}{\kappa^* r} \right] \chi(r) = E\chi(r). \quad (7.42)$$

Here  $m^*$  is the effective mass of an electron in the conduction band, and  $\kappa^*$  the effective dielectric constant of the medium. This equation was derived on the basis of the single-particle model. Kohn<sup>27)</sup>, further in his succeeding paper, was able to show that  $\kappa^* = \kappa$  indeed, where  $\kappa$  is the conventionally defined static dielectric constant of the solid. Our purpose is to provide a foundation to such an approach as the reduction to the single-particle equation.

Let  $E_0$  and  $E(N+1, k, \alpha)$  be energy of the ground state of the insulator and perfect insulator plus one electron, respectively. Here  $k$  denotes the momentum of an electron in the crystal and  $\alpha$  represents other relevant quantum numbers. Then

$$E(N+1, k, 0) - E_0 = \epsilon(k) \quad (7.43)$$

$$\simeq \epsilon_0 + \epsilon_1 k^2 \quad \text{for small } k,$$

where

$$\epsilon_0 = E(N+1, 0, 0) - E_0 \quad \text{the binding energy of the extra electron}$$

and

$$\epsilon_1 = m/m^*, \quad \text{the ratio of actual to effective electron mass.}$$

We are interested in the lowest band, states characterized by (7.43). In our insulator, they are distinguished from all other states  $E(N+1, k, \alpha)$  by the condition

$$E(N+1, k, \alpha) - E_0 \geq \epsilon_0 + \Delta E \quad \alpha \neq 0, \quad (7.44)$$

where  $\Delta E$  plays the role of energy gap against excitation of an "electron" in the system of  $N+1$  electrons. Because of relations of the above type, we can safely introduce a distinction between single-particle and collective states. As explained in great detail at the beginning of this section, it is very useful to introduce a suitable amplitude or one-particle wave function, which makes possible to describe many of the properties of the single particle states.

Analogous to (7.38) we shall introduce the function defined by

$$\chi_k(\mathbf{x}, t) \equiv \langle 0 | \psi(\mathbf{x}, t) | E(N+1, k, 0) \rangle, \quad (7.45)^*$$

where  $|E(N+1, k, 0)\rangle$  and  $|0\rangle$  stand for a wave packet of  $N+1$  particle eigenstates of the "one-particle" variety and the ground state of the perfect crystal, respectively.  $\chi_k(\mathbf{x}, t)$  may be interpreted as the amplitude for finding the ground state of the perfect crystal, if we remove an "electron" at the point  $(\mathbf{x}, t)$  from the state  $|E(N+1; k, 0)\rangle$ .

One can prove that  $\chi_k(\mathbf{x}, t)$  should satisfy the one-particle Schroedinger equation

$$\left[ i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 \right] \chi_k(\mathbf{x}, t) - \int d^3\mathbf{x}' dt' \Sigma(\mathbf{x}, t; \mathbf{x}', t') \chi_k(\mathbf{x}', t') = 0. \quad (7.46)$$

Taking into account the harmonically oscillating behavior of  $\chi_k(\mathbf{x}, t)$ , in time, we can rewrite the last term of (7.46) in the following way,

$$\int d^3\mathbf{x}' dt' \Sigma(\mathbf{x}, t; \mathbf{x}', t') = \int d\mathbf{x}' \langle \mathbf{x} | \mathcal{V}_k | \mathbf{x}' \rangle \chi_k(\mathbf{x}', t) \quad (7.47)$$

where

$$\langle \mathbf{x} | \mathcal{V}_k | \mathbf{x}' \rangle \equiv \int dt' \Sigma(\mathbf{x}, t; \mathbf{x}', t') e^{(i/\hbar)\epsilon(k)(t-t')}. \quad (7.48)$$

Then (7.46) turns out to be

\* If our system is described by the Hamiltonian

$$H_0 = \frac{\hbar^2}{2m} \int d^3\mathbf{x} \nabla \psi^*(\mathbf{x}) \nabla \psi(\mathbf{x}) + \frac{e^2}{2} \int d^3\mathbf{x} d^3\mathbf{x}' \psi^*(\mathbf{x}) \psi^*(\mathbf{x}') \\ \times \frac{1}{|\mathbf{x} - \mathbf{x}'|} \psi(\mathbf{x}) \psi(\mathbf{x}') + e \int d^3\mathbf{x} d^3\mathbf{x}' \psi^*(\mathbf{x}) \psi(\mathbf{x}) \frac{1}{|\mathbf{x} - \mathbf{x}'|} \rho_L(\mathbf{x}'),$$

where  $\rho_L(\mathbf{x})$  represents a fixed lattice charge density,

$$H_0 \Psi(N, k, \alpha) = E_0(N, k, \alpha) \Psi(N, k, \alpha),$$

here  $N$  and  $k$  being the number of electrons and the crystal momentum, respectively.  $\{\Psi(N, k, \alpha)\}$  forms the complete set of eigenstates.



$$\left[ i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 \right] \chi_k(\mathbf{x}, t) - \int d^3\mathbf{x}' \langle \mathbf{x} | \mathcal{V}_k | \mathbf{x}' \rangle \chi_k(\mathbf{x}', t) = 0. \quad (7.49)$$

This form of the equation permits us to interpret the function  $\langle \mathbf{x} | \mathcal{V}_k | \mathbf{x}' \rangle$  as the effective potential for the one-particle motion. Thus the  $(N \pm 1)$ -particle Schroedinger equation could be reduced to a single-particle equation. It should be, however, emphasized that, contrary to the nuclear optical potential, the effective potential  $\langle \mathbf{x} | \mathcal{V}_k | \mathbf{x}' \rangle$  defined here has not anti-hermitian part because all the real excitations are discarded for the medium particles. With the aid of the renormalization technique like those in quantum field theory, one may prove that the above equation is reducible to (7.42) with interpretation of the effective mass and the dielectric constant. For details, see Klein's original paper.<sup>25)</sup>

### Appendix I

#### Functional differentiation

As a quantity taking a complex number depending on the functional form of a function (say  $\varphi(x)$ ), we can consider a *functional* which is usually denoted by  $F[\varphi]$ . For example, the typical forms may be conceived by an integral containing  $\varphi$  in its integrand, the value of  $\varphi$  at a fixed point, and so on. If the functional is continuous in some sense for variations of its argument function, we can define the *functional differentiation* of the functional with respect to its argument function. A natural way to define the functional derivative, denoted by  $\delta F[\varphi] / \delta \varphi(x)$ , is the following:

$$\int \frac{\delta F[\varphi]}{\delta \varphi(x)} f(x) dx = \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} \{ F[\varphi + \varepsilon f] - F[\varphi] \}, \quad (A.1)$$

where  $f(x)$  is an arbitrary but smooth and integrable function. From the definition it is quite easy to see that the functional differentiation has the properties satisfied by the differential operation, namely, that

$$\begin{aligned} \frac{\delta}{\delta \varphi(x)} a &= 0, \\ \frac{\delta}{\delta \varphi(x)} \{ aF[\varphi] + bG[\varphi] \} &= a \frac{\delta F[\varphi]}{\delta \varphi(x)} + b \frac{\delta G[\varphi]}{\delta \varphi(x)}, \\ \frac{\delta}{\delta \varphi(x)} F[\varphi] G[\varphi] &= \frac{\delta F[\varphi]}{\delta \varphi(x)} G[\varphi] + F[\varphi] \frac{\delta G[\varphi]}{\delta \varphi(x)}, \end{aligned} \quad (A.2)$$

where  $F$  and  $G$  are functionals of  $\varphi$ , and  $a$  and  $b$  arbitrary functions independent of  $\varphi$ .

Now consider some simple examples. For the functional  $F[\varphi]$

$= \int u(x)\varphi(x)dx$ , the above definition integral becomes

$$\begin{aligned} \int \frac{\delta F[\varphi]}{\delta \varphi(x)} f(x) dx &= \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} \left\{ \int u(x) \{ \varphi(x) + \varepsilon f(x) \} dx - \int u(x) \varphi(x) dx \right\} \\ &= \int u(x) f(x) dx. \end{aligned}$$

Since the relation holds for an arbitrary  $f$ , one gets

$$\frac{\delta}{\delta \varphi(x)} \int u(x') \varphi(x') dx' = u(x). \quad (\text{A}\cdot\text{3})$$

For the functional  $F[\varphi] \equiv \varphi(a)$ , we have

$$\int \frac{\delta F[\varphi]}{\delta \varphi(x)} f(x) dx = \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} [\varphi(a) + \varepsilon f(a) - \varphi(a)] = f(a),$$

which yields the well-known formula

$$\frac{\delta}{\delta \varphi(x)} \varphi(a) = \delta(x-a). \quad (\text{A}\cdot\text{4})$$

The above examples illustrate the linear functionals of  $\varphi$ , so that their derivatives are no longer dependent of  $\varphi$ . However, we will often encounter with the functionals non-linearly depending on  $\varphi$ . For them we can define the higher-order derivatives in a way analogous to ordinary derivatives. The second-order derivative is defined by

$$\begin{aligned} &\int \frac{\delta^2 F[\varphi]}{\delta \varphi(x) \delta \varphi(x')} f(x) g(x') dx dx' \\ &= \lim_{\substack{\varepsilon \rightarrow 0 \\ \varepsilon' \rightarrow 0}} \frac{1}{\varepsilon \varepsilon'} \{ F[\varphi + \varepsilon f + \varepsilon' g] - F[\varphi + \varepsilon f] - F[\varphi + \varepsilon' g] + F[\varphi] \}. \end{aligned} \quad (\text{A}\cdot\text{5})$$

For  $F[\varphi] \equiv \{\varphi(a)\}^2$  the definition immediately gives us

$$\frac{\delta^2}{\delta \varphi(x) \delta \varphi(x')} \{\varphi(a)\}^2 = 2\delta(x-a)\delta(x'-a).$$

It is true to define the  $n$ -th order derivative of a functional by the form analogous to the ordinary one. Therefore we may make use of the Taylor type of series as written in §1.

Finally we remark on the Fourier transformation of functionals and functional derivatives. First we write the Fourier transformation of the argument function, namely

$$\tilde{\varphi}(k) \equiv \tilde{\varphi}_-(-k) = \int e^{-ikx} \varphi(x) dx,$$

$$\varphi(x) = \frac{1}{2\pi} \int e^{ikx} \tilde{\varphi}(k) dk. \quad (\text{A}\cdot 6)$$

The Fourier transform  $\tilde{F}$  of a functional  $F$  may be defined by

$$\tilde{F}[\tilde{\varphi}] \equiv F[\varphi]. \quad (\text{A}\cdot 7)$$

For example, the Fourier transforms of  $F_1[\varphi] \equiv \int u(x)\varphi(x)dx$  and  $F_2[\varphi] \equiv \varphi(a)$  are given from the integrals

$$\begin{aligned} \tilde{F}_1[\tilde{\varphi}] &\equiv \frac{1}{2\pi} \int u(x) \left( \int e^{-ikx} \tilde{\varphi}(-k) dk \right) dx, \\ \tilde{F}_2[\tilde{\varphi}] &\equiv \frac{1}{2\pi} \int e^{-ika} \tilde{\varphi}(-k) dk, \end{aligned}$$

which yields  $\tilde{F}_1 = (1/2\pi)\tilde{u}(k)$  and  $\tilde{F}_2 = (1/2\pi)e^{-ika}$  as expected. Now we can define the Fourier transform of the functional derivative by

$$\int \frac{\delta \tilde{F}[\tilde{\varphi}]}{\delta \tilde{\varphi}(-k)} \tilde{\varphi}(-k) dk = \int \frac{\delta F[\varphi]}{\delta \varphi(x)} \varphi(x) dx, \quad (\text{A}\cdot 8)$$

which can be derived from (A.1) and (A.7). (A.7) and (A.6) yield the formulas

$$\begin{aligned} \frac{\delta \tilde{F}[\tilde{\varphi}]}{\delta \tilde{\varphi}(k)} &= \int e^{-ikx} \frac{\delta F[\varphi]}{\delta \varphi(x)} dx, \\ \frac{\delta F[\varphi]}{\delta \varphi(x)} &= \frac{1}{2\pi} \int e^{ikx} \frac{\delta \tilde{F}[\tilde{\varphi}]}{\delta \tilde{\varphi}(k)} dk. \end{aligned} \quad (\text{A}\cdot 9)$$

## Appendix II

### *Schwinger's dynamical principle*

Schwinger<sup>2)</sup> formulated the most fundamental principle of quantum mechanics in a variational form. His dynamical principle says that, if one takes small variations of initial and final conditions and the Lagrangian function, then the corresponding variation of the transition probability amplitude should obey the variational equation

$$\delta \langle F | I \rangle = \frac{i}{\hbar} \langle F | \delta \int L d^4x | I \rangle, \quad (\text{A}\cdot 10)$$

where  $L$  is the Lagrangian density of the system. This dynamical principle unifies all the fundamental equations and relations in quantum mechanics, that is, the Schrodinger equation, the Heisenberg equation, the commutation

relations, the conservation laws, and so on. In practice the principle is useful for calculating the functional derivatives of amplitudes or matrix elements with respect to external sources or fields.

The Schwinger's principle may easily be accepted if one considers it from Feynman's point of view using the path integral. Feynman presented the amplitude in the form of the so-called path integral:

$$\langle F|I\rangle = \sum_{\text{path}} \exp\left(\frac{i}{\hbar} \int L d^4x\right),$$

where summation is over all possible forms of functions describing the field. From this expression we have

$$\delta \langle F|I\rangle = \sum_{\text{path}} \frac{i}{\hbar} \delta \int L d^4x \exp\left(\frac{i}{\hbar} \int L d^4x\right),$$

whose right member is nothing but the right member of (A·10) because of the correspondence rule between the path-integral formalism and the usual operator formalism.

Now let us calculate the functional derivatives of the amplitudes and the matrix elements with respect to the external sources,  $J(x)$  and  $\eta(x)$ , introduced in §2. For a small variation  $\varepsilon f(x)$  in the source function of bosons ( $\varepsilon$  being a small number), we have the variation of the action function

$$\delta \int L d^4x = - \int \phi(x) \varepsilon f(x) d^4x.$$

Then the Schwinger's principle becomes

$$\delta \langle F|I\rangle = \frac{1}{i\hbar} \int \langle F|\phi(x)|I\rangle \varepsilon f(x) d^4x.$$

On the other hand, the right member can be written as

$$\delta \langle F|I\rangle = \langle F|I\rangle_{J+\varepsilon f} - \langle F|I\rangle_J = \int \frac{\delta \langle F|I\rangle}{\delta J(x)} \varepsilon f(x) d^4x.$$

Thus we immediately obtain the formula

$$\frac{\delta}{\delta J(x)} \langle F|I\rangle = \frac{1}{i\hbar} \langle F|\phi(x)|I\rangle. \quad (\text{A}\cdot 11)$$

Similarly one gets

$$\begin{aligned} \frac{\delta}{\delta \eta(x)} \langle F|I\rangle &= \frac{1}{i\hbar} \langle F|\psi^*(x)|I\rangle, \\ \frac{\delta}{\delta \eta^*(x)} \langle F|I\rangle &= \frac{1}{i\hbar} \langle F|\psi(x)|I\rangle, \end{aligned} \quad (\text{A}\cdot 12)$$

for the spinor field. Next we differentiate the matrix element  $\langle F|Q(x)|I\rangle$  of an operator  $Q(x)$  with respect to  $J(x')$  and  $\eta(x')$ . For  $t > t'$  the derivative is written as

$$\begin{aligned} \frac{\delta}{\delta J(x')} \langle F|Q(x)|I\rangle &= \sum_m \langle F|Q(x)|mt_1\rangle \frac{\delta \langle mt_1|I\rangle}{\delta J(x')} \\ &= \frac{1}{i\hbar} \langle F|Q(x)\phi(x')|I\rangle, \end{aligned}$$

where  $t_1$  is a time taken between  $t$  and  $t'$ , while one has

$$\begin{aligned} \frac{\delta}{\delta J(x')} \langle F|Q(x)|I\rangle &= \frac{1}{i\hbar} \sum_m \frac{\delta \langle F|mt_1\rangle}{\delta J(x')} \langle mt_1|Q(x)|I\rangle \\ &= \frac{1}{i\hbar} \langle F|\phi(x')Q(x)|I\rangle \end{aligned}$$

for  $t < t'$ . For spinor field we must pay attention on the anti-commutativity of the spinor sources with the other spinors. The variation of the matrix element must be written as

$$\delta \langle F|Q(x)|I\rangle = \frac{1}{i\hbar} \langle F|Q(x) \int \psi^*(x') \delta\eta(x') d^4x' |I\rangle$$

or

$$= \frac{1}{i\hbar} \langle F| \int \psi^*(x') \delta\eta(x') d^4x' Q(x) |I\rangle,$$

according as the non-zero point of  $\delta\eta(x')$  is earlier or later than  $t$ . The right member for  $t' > t$  becomes

$$\pm \frac{1}{i\hbar} \int \langle F|\psi^*(x')Q(x)|I\rangle \delta\eta(x') d^4x',$$

where the sign  $\pm$  is caused from exchange between  $Q(x)$  and  $\delta\eta(x')$ . Thus we can obtain

$$\begin{aligned} \frac{\delta}{\delta J(x')} \langle F|Q(x)|I\rangle &= \frac{1}{i\hbar} \langle F|T(Q(x)\phi(x'))|I\rangle, \\ \frac{\delta}{\delta \eta(x')} \langle F|Q(x)|I\rangle &= \frac{1}{i\hbar} \langle F|T(Q(x)\psi^*(x'))|I\rangle, \\ \frac{\delta}{\delta \eta^*(x')} \langle F|Q(x)|I\rangle &= \frac{1}{i\hbar} \langle F|T(Q(x)\psi(x'))|I\rangle, \quad (\text{A}\cdot 13) \end{aligned}$$

where  $T$  stands for the well-known time-ordering symbol. From (A·12) and (A·13) it is easy to derive the formulas

$$\frac{\delta}{\delta J(x')} \langle Q(x) \rangle = \frac{1}{i\hbar} \{ \langle T(Q(x)\phi(x')) \rangle - \langle Q(x) \rangle \langle \phi(x') \rangle \},$$

$$\begin{aligned}\frac{\delta}{\delta\eta(x')} \langle Q(x) \rangle &= \frac{1}{i\hbar} \{ \langle T(Q(x)\psi^*(x')) \rangle - \langle Q(x) \rangle \langle \psi^*(x') \rangle \}, \\ \frac{\delta}{\delta\eta^*(x')} \langle Q(x) \rangle &= \frac{1}{i\hbar} \{ \langle T(Q(x)\psi(x')) \rangle - \langle Q(x) \rangle \langle \psi(x') \rangle \},\end{aligned}\tag{A.14}$$

where the symbols  $\langle \dots \rangle$  are defined by (1.11a') or (1.11b').

In §3 the real scalar external field  $\varphi(x)$  is introduced by adding  $-\psi^*(x)\psi(x)\varphi(x)$  to the Lagrangian density. The functional derivative with respect to  $\varphi(x)$  is similarly derived from the Schwinger's principle, namely, one gets

$$\begin{aligned}\frac{\delta}{\delta\varphi(x')} \langle Q(x) \rangle &= \frac{1}{i\hbar} \{ \langle T(Q(x)\psi^*(x')\psi(x')) \rangle \\ &\quad - \langle Q(x) \rangle \langle \psi^*(x')\psi(x') \rangle \}.\end{aligned}\tag{A.15}$$

### Appendix III

#### *Polaron problem*

To illustrate the Green function method, we shall deal with another example, the polaron problem, in which an electron moves in a polar crystal. The system is governed by the Hamiltonian

$$\begin{aligned}H &= \int \psi^*(x) \left[ -\frac{\hbar^2}{2m} \nabla^2 \right] \psi(x) d^3x + \frac{1}{2} r \int \{ [\dot{\mathbf{P}}(x)]^2 + \omega^2 [\mathbf{P}(x)]^2 \} d^3x \\ &\quad + e \int \mathbf{P}(x) \cdot \nabla \int \frac{\delta(t-t')}{|\mathbf{x}-\mathbf{x}'|} \psi^*(x') \psi(x') d^4x' d^3x,\end{aligned}\tag{A.16}$$

where  $\psi$  is the electron field and  $\mathbf{P}$  the polarization field in the crystal. The constant  $r$  is given by

$$r = \frac{\omega^2}{4\pi} \left( \frac{1}{\epsilon_\infty} - \frac{1}{\epsilon} \right),$$

$\epsilon$  being the dielectric constant and  $\epsilon_\infty$  the optical one. The commutation relations are formulated as

$$\begin{aligned}[\dot{P}_i(\mathbf{x}, t), P_m(\mathbf{x}', t)] &= -\frac{i\hbar}{r} \delta_{im} \delta(\mathbf{x} - \mathbf{x}') \\ [P_l(\mathbf{x}, t), P_m(\mathbf{x}', t)] &= 0,\end{aligned}\tag{A.17}$$

for the polarization field, besides usual ones for the electron field. As is easily seen, the polarization field can be described by the scalar phonon field  $\phi$  defined by

$$\mathbf{P} = \frac{1}{4\pi} \nabla \phi, \quad \text{or} \quad \phi(\mathbf{x}, t) = - \int \frac{\nabla' \cdot \mathbf{P}(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} d^3x'. \quad (\text{A}\cdot 18)$$

In terms of  $\phi$  we write the Hamiltonian as

$$H = \int \psi^*(\mathbf{x}) \left[ -\frac{\hbar^2}{2m} \nabla^2 + e\phi(\mathbf{x}) \right] \psi(\mathbf{x}) d^3x \\ + \frac{r}{2(4\pi)^2} \int [(\nabla \dot{\phi}(\mathbf{x}))^2 + \omega^2 (\nabla \phi(\mathbf{x}))^2] d^3x \quad (\text{A}\cdot 19)$$

and the commutation relations as

$$[\dot{\phi}(\mathbf{x}, t), \phi(\mathbf{x}', t)] = -\frac{4\pi}{r} (i\hbar) \frac{1}{|\mathbf{x} - \mathbf{x}'|}, \\ [\phi(\mathbf{x}, t), \phi(\mathbf{x}', t)] = 0. \quad (\text{A}\cdot 20)$$

It must be noted that the commutator between  $\dot{\phi}$  and  $\phi$  is not proportional to  $\delta(\mathbf{x} - \mathbf{x}')$  but to  $|\mathbf{x} - \mathbf{x}'|^{-1}$ . The fact shows that, in contrast with cases of  $\delta(\mathbf{x} - \mathbf{x}')$ , the components of  $\phi$  with high momenta are reduced by the factor  $|\mathbf{k}|^{-2}$ , and that the theory does not contain any divergence.

For the sake of mathematical convenience, let us artificially introduce the external source of the phonon field by adding

$$\int \phi(\mathbf{x}) J(\mathbf{x}) d^3x \quad (\text{A}\cdot 21)$$

to the Hamiltonian. In the same way as in Appendix II, we can derive the formula

$$i\hbar \frac{\delta}{\delta J(\mathbf{x})} \langle Q \rangle = \langle T(Q\phi(\mathbf{x})) \rangle - \langle Q \rangle \langle \phi(\mathbf{x}) \rangle \quad (\text{A}\cdot 22)$$

for the expectation value of an operator  $Q$ . Now we consider the Green functions

$$G(\mathbf{x}, \mathbf{x}') = (i\hbar)^{-1} \langle T(\psi(\mathbf{x})\psi^*(\mathbf{x}')) \rangle \\ K(\mathbf{x}, \mathbf{x}') = \frac{\delta \langle \phi(\mathbf{x}) \rangle}{\delta J(\mathbf{x}')} = (i\hbar)^{-1} \{ \langle T(\phi(\mathbf{x})\phi(\mathbf{x}')) \rangle \\ - \langle \phi(\mathbf{x}) \rangle \langle \phi(\mathbf{x}') \rangle \}, \quad (\text{A}\cdot 23)$$

for the electron and the phonon fields, respectively. At the limit  $J=0$ , the term  $\langle \phi(\mathbf{x}) \rangle$  must vanish. In the presence of  $J$  the field equations become

$$\left( i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 - e\phi(\mathbf{x}) \right) \psi(\mathbf{x}) = 0,$$

$$\left(\frac{\partial^2}{\partial t^2} + \omega^2\right)\phi(x) = -\frac{4\pi}{r} \int U(x-x') [J(x') + e\psi^*(x')\psi(x')] d^4x', \quad (\text{A}\cdot\text{24})$$

where  $U(x-x') \equiv |x-x'|^{-1}\delta(t-t')$ . The second equation is rewritten as

$$\left(\frac{\partial^2}{\partial t^2} + \omega^2\right)\nabla^2\phi(x) = \frac{(4\pi)^2}{r} [J(x) + e\psi^*(x)\psi(x)], \quad (\text{A}\cdot\text{25})$$

because of the formula  $\nabla^2 U(x-x') = -(4\pi)\delta^{(4)}(x-x')$ . From (A·23) and (A·24) or (A·25), it follows that

$$\begin{aligned} \left(i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\nabla^2\right)G(x, x') - e(i\hbar)^{-1}\langle T(\phi(x)\psi(x)\psi^*(x')) \rangle &= \delta^{(4)}(x-x'), \\ \left(\frac{\partial^2}{\partial t^2} + \omega^2\right)\nabla^2 K(x, x') - \frac{(4\pi)^2}{r} e \frac{\delta}{\delta J(x')} \langle \psi^*(x)\psi(x) \rangle &= \frac{(4\pi)^2}{r} \delta(x-x'). \end{aligned}$$

By virtue of (A·22), we immediately obtain

$$\begin{aligned} e\langle T(\phi(x)\psi(x)\psi^*(x')) \rangle &= e \frac{\delta}{\delta J(x)} \langle T(\psi(x)\psi^*(x')) \rangle \\ &+ e(i\hbar)^{-1} \langle \phi(x) \rangle \langle T(\psi(x)\psi^*(x')) \rangle \\ &= \int \Sigma(x, \zeta) G(\zeta, x') d^4\zeta + e \langle \phi(x) \rangle G(x, x') \\ e \frac{\delta}{\delta J(x')} \langle \psi^*(x)\psi(x) \rangle &= - \int \Pi(x, x'') K(x'', x') d^4x'', \end{aligned}$$

where

$$\begin{aligned} \Sigma(x, \zeta) &\equiv i\hbar e^2 \iint G(x, \xi) K(x'', x) \Gamma(\xi, \zeta; x'') d^4\xi d^4x'', \\ \Pi(x, x'') &\equiv i\hbar e^2 \iint G(x, \xi) \Gamma(\xi, \zeta; x'') G(\zeta, x) d^4\xi d^4\zeta, \end{aligned} \quad (\text{A}\cdot\text{26})$$

being defined by

$$\Gamma(\xi, \zeta; x'') \equiv - \frac{\delta G^{-1}(\xi, \zeta)}{e \delta \langle \phi(x'') \rangle}. \quad (\text{A}\cdot\text{27})$$

Therefore the equations of  $G$  and  $K$  are symbolically written in the form

$$\begin{aligned} \left[ i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\nabla^2 - e\langle \phi \rangle - \Sigma \right] G &= 1, \\ \left[ \left( \frac{\partial^2}{\partial t^2} + \omega^2 \right) \nabla^2 + \frac{(4\pi)^2}{r} \Pi \right] K &= \frac{(4\pi)^2}{r} \cdot 1, \end{aligned} \quad (\text{A}\cdot\text{28})$$

where

$$\Sigma = i\hbar e^2 G K \Gamma,$$



$$\begin{aligned} \Pi &= i\hbar e^2 G \Gamma G, \\ \Gamma &= 1 + \frac{\delta \Sigma}{\delta \langle \phi \rangle}. \end{aligned} \quad (\text{A}\cdot\text{29})$$

Hence we have five equations among the five unknowns,  $G$ ,  $K$ ,  $\Pi$ ,  $\Sigma$  and  $\Gamma$ .

At the limit  $J=0$  (or  $\langle \phi \rangle=0$ ), the “self-energy” part  $\Sigma$  gives us the effective mass of a polaron.

**Note added in proof:** The authors have recently found A. Klein’s and M. Yasuno’s unpublished works. Klein derived the Hugenholtz-Van Hove theorem on single-particle energies and the Landau theory of Fermi liquids by means of extensive use of the Green function method. Yasuno formulated, in the framework of the Green function method, the single-particle energies and the effective potentials for the single-particle motion in the nuclear matter. There Yasuno presented an interesting method in which the hierarchy of the equations of Green functions is stopped at the two-particle Green function and then the three-particle Green function is replaced by a sum of appropriate products of the one- and two-particle Green functions. In particular, his discussions are given for the relations between the single-particle behaviors and the Brueckner’s reaction matrix, and the plasma-type excitation terms. Concerning discussions in § 3, readers may find the more-refined form of the theory in Yasuno’s paper which will be published in near future in *Progress of Theoretical Physics*.

### References

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