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A New Approach to Quantum-Statistical Mechanics

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A new method of calculating the grand partition function of many-body system is developed, adopting extensively the techniques of calculus in quantum field theory. It is shown that the grand partition function, which is a trace of the density matrix expressed in terms of field operators, can be evaluated in a way almost parallel with the evaluation of the vacuum expectation value of the S-matrix in quantum field theory, provided that appropriate modifications in notation and definitions are made. As an example, the method is applied to electron-phonon system. Further, basing on this new formalism, various non-perturbational methods are discussed.

§ 1. Introduction

Stimulated by the studies of cooperative phenomena in quantum statistical system such as ferro- and antiferromagnetism, superconductivity, the λ-transition in liquid helium etc., various methods for the calculation of the partition function of many-body system with interaction have been put forward by many authors. These methods of attack have each its own merit, and in some cases they have been fairly successfully applied to practical problems. For instance, Kubo established an expansion theorem of the density matrix and applied it to ferro- and antiferromagnetism.[1] Schafroth, in his theory of Meissner effect in superconductors, derived a formula in which the density matrix was expressed in powers of the interaction Hamiltonian.[2] Essentially the same formula for the expansion of the density matrix was also obtained by a different method by Chester, who made use of it to discuss the Bose-Einstein condensation of imperfect Bose gas.[3] A quite different way than others to handle the density matrix was invented by Feynman (the method of integral over trajectories), and he applied it to the problem of liquid helium[4]. More recently, Friedman and Butler introduced another technique of manipulating the density matrix and thereby discussed the transition in liquid helium quantitatively.[5]

Generally speaking, however, it seems that major efforts have been made so far to overcome the difficulties encountered in treating the interaction in many-body system, so that there remain unsolved difficulties in taking account of the effect of statistics, especially for Fermion system such as electrons in a superconductor and liquid helium 3, in both of which the role of Fermi statistics seeems to be important. To remedy this point, it may be promising to use the number representation of the second quantization theory for the calculation of the trace of the density matrix. From this view point Ichimura developed a method of expanding the grand partition function in powers of the coupling constant using the number representation.[6] It appears, however, to the present author that his method is unsatisfactory

in the following two points: First it will not be practical in evaluating higher order corrections, because troublesome calculation of an enormous number of terms are needed; Therefore, application of this method will be restricted only to cases in which the effect of higher order perturbations is unimportant. Secondly, while the number representation may be most convenient to take into account the effect of statistics, it has such a defect that it is difficult to treat by this method the problem in configuration space, namely, it is not easy by this method to utilize physical pictures connected with the configuration space. For instance, one cannot utilize the quantity such as the molecular distribution function, which has been useful for the understanding of the cooperative phenomena in classical system.

In this paper we shall present a new approach which seems to be free from the above mentioned shortcomings of the n-representation. We introduce explicitly the quantized field of particles and utilize the various techniques of operator calculus in quantum field theory as far as possible in evaluating the quantum-statistical average of the field quantities. In § 2 and § 3 we give a general formulation of our theory for an example of electron-phonon system. Various results obtained by means of this new method for electron-phonon system are illustrated in § 4. In § 5 non-perturbational treatments are discussed, starting from the formulation given in § 2 and § 3. The last section is devoted to a possible extension of our method to other systems.

§ 2. General formulation

We suppose that the Hamiltonian of a system in question can be divided into two parts

$$H=H_0+H_1, \tag{2·1}$$

each of which is expressed in terms of field quantity as

$$\begin{aligned} H_0&=\int H_0(\boldsymbol{x})\,d^3\boldsymbol{x}, \\ H_1&=\int H_1(\boldsymbol{x})\,d^3\boldsymbol{x}. \end{aligned} \tag{2·2}$$

We shall call $H_0(\boldsymbol{x})$ the Hamiltonian density of free field and $H_1(\boldsymbol{x})$ the density of interaction Hamiltonian. The density matrix of a canonical ensemble $\rho=\exp(-\beta H)$ has to satisfy the Bloch equation

$$-\partial\rho/\partial\beta=(H_0+H_1)\cdot\rho, \qquad \beta=1/kT. \tag{2·3}$$

If we put

$$\exp(-\beta H)=\exp(-\beta H_0)\cdot S(\beta), \tag{2·4}$$

the equation for $S(\beta)$ becomes

$$-\partial S(\beta)/\partial\beta=H_1(\beta)\cdot S(\beta), \tag{2·5}$$

where

$$H_1(t)=\exp(tH_0)\cdot H_1\cdot\exp(-tH_0). \tag{2·6}$$

The solution of (2·5) with initial condition $S(0)=1$ may be written as

$$\begin{aligned} S(\beta) &= \sum_{n=0}^{\infty}(-1)^n \int_0^{\beta} dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} \cdots \int_0^{t_{n-1}} dt_n H_1(t_1) H_1(t_2) \cdots H_1(t_n) \\ &= \sum_{n=0}^{\infty}(-1)^n/n! \int \cdots \int P[H_1(t_1) \cdots H_1(t_n)] dt_1 \cdots dt_n, \end{aligned} \tag{2·7}$$

where P is an ordering operator[7] which re-arranges the operators in the bracket in such an order that the arguments t in them are decreasing in magnitude, that is,

$$\begin{gathered} P[H_1(t_1) \cdots H_1(t_n)] = H_1(t_1') H_1(t_2') \cdots H_1(t_n') \\ t_1' > t_2' > \cdots > t_n'. \end{gathered} \tag{2·8}$$

If we regard

$$\exp(tH_0) \cdot H_1(\boldsymbol{x}) \cdot \exp(-tH_0) = H_1(\boldsymbol{x}, t) \equiv H_1(x) \tag{2·9}$$

as an operator in the four dimensional space with coordinates $x=(\boldsymbol{x}, t)$, then (2·7) can be put into another form

$$S(\beta) = \sum_{n=0}^{\infty}(-1)^n/n! \int \cdots \int P[H_1(x_1) \cdots H_1(x_n)] d^4x_1 \cdots d^4x_n, \tag{2·10}$$

in which $d^4x = d^3\boldsymbol{x}dt$ and the integrations are to be taken over the whole volume with respect to $\boldsymbol{x}_i$ and over the range $(0, \beta)$ with respect to t_i. P is now an operator arranging the operators in the bracket in such an order that the fourth components of coordinates in them are decreasing in magnitude.

The grand partition function of the system is defined by

$$\Xi = Tr[\exp(-\alpha N - \beta H)], \tag{2·11}$$

where N is an operator representing the total number of particles, say, of electrons, and α a selector which is related to the chemical potential per one particle μ through

$$\alpha = -\beta\mu. \tag{2·12}$$

Introducing the following notation

$$\begin{gathered} \Xi_0 = Tr[\exp(-\alpha N - \beta H_0)], \\ \langle \cdots \rangle = Tr[\exp(-\alpha N - \beta H_0) \cdots] / Tr[\exp(-\alpha N - \beta H_0)], \end{gathered} \tag{2·13}$$

we rewrite (2·11) in the following forms:

$$\Xi/\Xi_0 = \langle S(\beta) \rangle \tag{2·14a}$$

$$= 1 + \xi_1 + \xi_2 + \xi_3 + \cdots \tag{2·14b}$$

$$= \exp(C_1 + C_2 + C_3 \cdots), \tag{2·14c}$$

where

$$\xi_n = (-1)^n/n! \int \cdots \int \langle P[H_1(x_1) \cdots H_1(x_n)] \rangle d^4x_1 \cdots d^4x_n. \tag{2·15}$$

The relations between ξ_n's and C_k's are essentially the same as those between the moments and Thiele's semi-invariants in the theory of probability, that is,

$$\begin{aligned}\xi_n&=\sum_{\sum_l l m_l=n} \Pi (C_l)^{m_l}/m_l!\,,\\ C_k&=\sum_{\sum_l l m_l=k} (-1)^{(\Sigma m_l-1)}(\textstyle\sum_l m_l-1)!\quad \Pi(\xi_l)^{m_l}/m_l!\,.\end{aligned}\tag{2·16}$$

Ξ_0 represents the grand partition function of the free system in which the interactions are absent. $\langle\cdots\rangle$ means the quantum-statistical average of a given field quantity denoted by dots referred to the thermal equilibrium realized in the free system.

In order to facilitate the explanation of our further analyses, we consider hereafter as an example the electron-phonon system, whose Hamiltonian is given by[8]

$$H=H_0+H_1,\tag{2·17a}$$

$$H_0=\sum_k \varepsilon_k a_k^* a_k+\tfrac{1}{2}\sum_w \hbar\omega_w(b_w^* b_w+b_w b_w^*),\tag{2·17b}$$

$$\begin{aligned}H_1=&g\sum_{k,w}(\hbar\omega_w/2V)^{1/2}(a_{k+w}^* a_k b_w+a_{k-w}^* a_k b_w^*)\\&+g'/2\sum_w \hbar\omega_w(b_w^* b_w+b_w b_w^*+b_w b_{-w}+b_w^* b_{-w}^*),\end{aligned}\tag{2·17c}$$

where a_k^* and a_k represent, respectively, the creation and annihilation operators of the electron with momentum $\boldsymbol{k}$ and energy ε_k, b_w^* and b_w are the corresponding operators for the phonon with momentum $\boldsymbol{w}$ and energy $\hbar\omega_w$, g and g' are, respectively, a coupling constant and a renormalization constant given by

$$g=(VC^2/NMs^2)^{1/2},\qquad g'=(s_0^2-s^2)/2s^2.\tag{2·18}$$

The meaning of the symbols appearing in (2·18) is as follows: V is the volume of the system, M the mass of an ion, N the total numbers of ions, C the usual interaction constant between electron and lattice, s_0 the sound velocity of free phonons. s_0 is generally different from the real velocity s because there are interactions between electrons and phonons.

Now let us define quantized wave functions of electrons and phonons by

$$\begin{aligned}\psi^*(\boldsymbol{x})&=V^{-1/2}\sum_k a_k^* e^{-i\boldsymbol{k}\cdot\boldsymbol{x}},\\ \psi(\boldsymbol{x})&=V^{-1/2}\sum_k a_k e^{i\boldsymbol{k}\cdot\boldsymbol{x}},\\ \varphi(\boldsymbol{x})&=\sum_k(\hbar ws/2V)^{1/2}(b_w e^{iw\cdot x}+b_w^* e^{-iw\cdot x}).\end{aligned}\tag{2·19}$$

Making use of the commutation relations

$$[a_k,\ a_{k'}^*]_+=\delta_{k,k'},\qquad [b_w,\ b_{w'}^*]_-=\delta_{w,w'},$$

four dimensional fields $\psi^*(x)=\exp(tH_0)\psi^*(\boldsymbol{x})\exp(-tH_0)$ etc. are easily shown to become

$$\psi^*(x)=V^{-1/2}\sum_k a_k^* e^{-i\boldsymbol{k}\cdot\boldsymbol{x}+\varepsilon_k t},$$

$$\psi(x)=V^{-1/2}\sum_k a_k e^{ik\cdot x-\varepsilon_k t}, \tag{2·20}$$

$$\varphi(x)=\sum_w(\hbar ws/2V)^{1/2}(b_w e^{iw\cdot x-\hbar wst}+b_w^* e^{-iw\cdot x+\hbar wst}).$$

Furthermore one can verify by a direct calculation that

$$e^{tH_0}H_1e^{-tH_0}\equiv H_1(t)=g\int\psi^*(x)\psi(x)\varphi(x)d^3x+g'\int\varphi(x)\varphi(x)d^3x,$$

or

$$H_1(x)=g\psi^*(x)\psi(x)\varphi(x)+g'\varphi(x)\varphi(x). \tag{2·21}$$

From (2·14), (2·15) and (2·21), it can be seen that those which we have to know are rules for calculating the averages such as

$$\langle P[\psi^*(x_1)\psi(x_1)\psi^*(x_2)\psi(x_2)\cdots\psi^*(x_n)\psi(x_n)]\rangle$$

and

$$\langle P[\varphi(x_1)\varphi(x_2)\cdots\varphi(x_n)]\rangle. \tag{2·22}$$

We want to emphasize here that a remarkable similarity exists between the evaluation of Ξ/Ξ_0 and that of the vacuum expectation of the so-called S-matrix in quantum field theory. In fact, it will be shown in the next section that all the rules of calculations of the vacum expectation of the field quantities in quantum field theory can be used in the present case with only slight modifications.

§ 3. Computation rules[7)9)10)]

It will be found convenient in later analyses to use in place of the operator P in (2·22) another operator T defined by[9)]

$$T=\delta_P P, \tag{3·1}$$

where δ_P takes 1 or -1 according as the character of the permutation of the electron operators involved is even or odd in going from the written order to the one re-arranged by P. Of course it holds that

$$P[\mathfrak{H}(\psi^*\psi)]=T[\mathfrak{H}(\psi^*\psi)], \tag{3·2}$$

if $\mathfrak{H}(\psi^*\psi)$ is any functional of a product of $\psi^*(x_i)\psi(x_i)$'s as in (2·22). Now let us find the computation rules for $\langle T[\mathfrak{H}(\psi^*\psi)]\rangle$ and $\langle P[\mathfrak{F}(\varphi)]\rangle$, where $\mathfrak{F}(\varphi)$ in any functional of a product of $\varphi(x)$'s. In the first place, we decompose $\psi^*(x)$, $\psi(x)$ and $\varphi(x)$ into two parts respectively according to

$$\begin{aligned}\psi^*(x)&=\psi_+^*(x)+\psi_-^*(x),\\ \psi(x)&=\psi_+(x)+\psi_-(x),\\ \varphi(x)&=\varphi_+(x)+\varphi_-(x).\end{aligned} \tag{3·3}$$

For a given product $X_1X_2\cdots X_n$, where X_i is any one of the components introduced in (3·3), we define an N-product by

$$N[X_1X_2\cdots X_n]=\delta_p X_{1'}X_{2'}\cdots X_{n'}, \tag{3·4}$$

in which the right hand side is a product of the same factors $X_1X_2\cdots X_n$ but ordered in such a manner that all the operators with suffix $-$ stand to the left of all the operators with suffix $+$ and, among the electron operators with the same suffix, all the operators with $*$ stand to the left of those without $*$. δ_p determines the sign of the permutation in the same way as in (3·1).*) For instance,

$$\begin{aligned}
N[\psi^*(x)\psi(x')]&=N[\psi_+^*(x)\psi_+(x')+\psi_+^*(x)\psi_-(x')+\psi_-^*(x)\psi_+(x')+\psi_-^*(x)\psi_-(x')]\\
&=\psi_+^*(x)\psi_+(x')-\psi_-(x')\psi_+^*(x)+\psi_-^*(x)\psi_+(x')+\psi_-^*(x)\psi_-(x'),\\
N[\psi^*(x_1)\psi^*(x_2)\psi(x_3)]&=\psi_-^*(x_1)\psi_-^*(x_2)\psi_-(x_3)+\psi_-^*(x_1)\psi_-^*(x_2)\psi_+(x_3)\\
&\quad-\psi_-^*(x_1)\psi_-(x_3)\psi_+^*(x_2)+\psi_-^*(x_1)\psi_+^*(x_2)\psi_+(x_3)+\psi_-^*(x_2)\psi_-(x_3)\psi_+^*(x_1)\\
&\quad-\psi_-^*(x_2)\psi_+^*(x_1)\psi_+(x_3)+\psi_-(x_3)\psi_+^*(x_1)\psi_+^*(x_2)+\psi_+^*(x_1)\psi_+^*(x_2)\psi_+(x_3),\\
N[\varphi(x_1)\varphi(x_2)]&=\varphi_-(x_1)\varphi_-(x_2)+\varphi_-(x_1)\varphi_+(x_2)+\varphi_-(x_2)\varphi_+(x_1)+\varphi_+(x_1)\varphi_+(x_2),\\
N[\varphi(x_1)\varphi(x_2)\varphi(x_3)]&=\varphi_-(x_1)\varphi_-(x_2)\varphi_-(x_3)+\varphi_-(x_1)\varphi_-(x_2)\varphi_+(x_3)\\
&\quad+\varphi_-(x_1)\varphi_-(x_3)\varphi_+(x_2)+\varphi_-(x_1)\varphi_+(x_2)\varphi_+(x_3)+\varphi_-(x_2)\varphi_-(x_3)\varphi_+(x_1)\\
&\quad+\varphi_-(x_2)\varphi_+(x_1)\varphi_+(x_3)+\varphi_-(x_3)\varphi_+(x_1)\varphi_+(x_2)+\varphi_+(x_1)\varphi_+(x_2)\varphi_+(x_3),
\end{aligned}$$

and so on. Then we can show that an arbitrary T product of electron and phonon field operators is always converted to its corresponding N product through a simple relation. For $T[\psi^*(x)\psi(x')]$, it is easy to verify by a direct calculation that

$$T[\psi^*x)\psi(x')]=\begin{cases} N[\psi^*(x)\psi(x')]+[\psi_+^*(x),\,\psi_-(x')]_+ & t>t'\\ N[\psi^*(x)\psi(x')]+[\psi_+^*(x),\,\psi_-(x')]_+-[\psi^*(x),\,\psi(x')]_+ & t<t'. \end{cases} \tag{3·5}$$

For $P[\varphi(x)\varphi(x')]$, we get

$$P[\varphi(x)\,\varphi(x')]=\begin{cases} N[\varphi(x)\varphi(x')]+[\varphi_+(x),\varphi_-(x')]_- & t>t'\\ N[\varphi(x)\varphi(x')]+[\varphi_+(x'),\,\varphi_-(x)]_- & t<t'. \end{cases} \tag{3·6}$$

Thus if we define two functions $S(x-x')$ and $D(x-x')$ by

$$S(x-x')=\begin{cases} [\psi_+^*(x),\,\psi_-(x')]_+ & t>t'\\ [\psi_+^*(x),\,\psi_-(x')]_+-[\psi^*(x),\,\psi(x')]_+ & t<t' \end{cases} \tag{3·7}$$

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*) Note that there exists a slight difference between our definition of N-product and that used in quantum field theory. This difference arises from the fact that $\psi_+{}^*(x)$ and $\psi_+(x)$ (or $\psi_-{}^*(x)$ and $\psi_-(x)$) do not necessarily anti-commute with each other, and therefore we have to take care of their order in the product.

$$D(x-x')=\begin{cases}[\varphi_+(x),\ \varphi_-(x')]_- & t>t'\\ [\varphi_+(x'),\ \varphi_-(x)]_- & t<t',\end{cases} \tag{3·8}$$

the T-product with two factors is expressed as a sum of the corresponding N-product and S or D function:

$$T[\psi^*(x)\psi(x')]=N[\psi^*(x)\psi(x')]+S(x-x')\ , \tag{3·9}$$

$$P[\varphi(x)\varphi(x')]=N[\varphi(x)\varphi(x')]+D(x-x')\ . \tag{3·9b}$$

Trying similar calculations for the T-products with more factors than two, we are led to a conclusion that any T-product can be expressible as a sum of terms, each of which is composed of an N-product multiplied by S or D functions. More correctly, this statement will be mathematically expressed in the following two lemmas:[10]

Lemma I For any product of $\varphi(x)$'s denoted by $\mathfrak{F}(\varphi)$, it holds that

$$T[\mathfrak{F}(\varphi)]=N[\mathfrak{F}(\varphi')], \tag{3·10}$$

where $\varphi'(x)$ is defined by

$$\varphi'(x)=\varphi(x)+\int d^4x' D(x-x')\,\delta/\delta\varphi(x'). \tag{3·11}$$

$\delta/\delta\varphi(x)$ is an operator characterized by the commutation relation,

$$[\delta/\delta\varphi(x),\ \varphi(x')]_-=\delta(x-x'), \tag{3·12}$$

that is, an operator representing functional differentiation with respect to $\varphi(x)$.

Lemma II For any product of $\psi^*(x)$'s and $\psi(x)$'s, which is denoted by $\mathfrak{H}(\psi^*\psi)$, it holds that

$$T[\mathfrak{H}(\psi^*\psi)]=N[\mathfrak{H}(\psi^{*\prime}\psi')], \tag{3·13}$$

where $\psi^{*\prime}(x)$ and $\psi'(x)$ are defined by

$$\begin{aligned}\psi^{*\prime}(x)&=\psi^*(x)+\int d^4x' S(x-x')\,\delta/\delta\psi(x'),\\ \psi'(x)&=\psi(x)-\int d^4x' S(x'-x)\,\delta/\delta\psi^*(x'),\end{aligned} \tag{3·14}$$

respectively. $\delta/\delta\psi^*(x)$ and $\delta/\delta\psi(x)$ are operators characterized by the following commutation relations:

$$\begin{aligned}&[\delta/\delta\psi(x),\ \psi(x')]_+=[\delta/\delta\psi^*(x),\ \psi^*(x')]_+=\delta(x-x'),\\ &[\delta/\delta\psi(x),\ \psi^*(x')]_+=[\delta/\delta\psi^*(x),\ \psi(x')]_+=0.\end{aligned} \tag{3·15}$$

A proof of these lemmas will be given in appendix. (3·9) are the special cases of (3·10) or (3·13). It should be noted that the above results are valid for an arbitrary choice of the manner of decomposition (3·3). We can, therefore, decompose the field operators in such a way that the resulting computation rules becomes as simple as possible. A possible good choice will be such as to make the averages of N-products $\langle N[\psi^*(x)\psi(x')]\rangle$ and

$\langle N[\varphi(x)\varphi(x')]\rangle$ vanish:

$$\langle N[\psi^*(x)\psi(x')]\rangle=0, \quad \langle N[\varphi(x)\varphi(x')]\rangle=0. \tag{3·16}$$

This choice yields for $S(x-x')$ and $D(x-x')$ the results of the form:

$$S(x-x')=\begin{cases} V^{-1}\sum_{k} f_k e^{-ik\cdot(x-x')+\varepsilon_k(t-t')} & t>t', \\ V^{-1}\sum_{k}(f_k-1)e^{-ik\cdot(x-x')+\varepsilon_k(t-t')} & t<t', \end{cases} \tag{3·17a}$$

$$D(x-x')=\sum_{w}(\hbar ws/2V)\left[(N_w+1)e^{iw\cdot(x-x')-\hbar ws|t-t'|}\right.$$
$$\left.+N_w e^{-iw\cdot(x-x')+\hbar ws|t-t'|}\right], \tag{3·17b}$$

where f_k and N_w represent the average numbers of free electrons with momentum $\boldsymbol{k}$ and of free phonons with momentum $\boldsymbol{w}$ in thermal equilibrium at temperature T, namely

$$f_k=\langle a_k^* a_k\rangle=(e^{\alpha+\beta\varepsilon_k}+1)^{-1}$$
$$N_w=\langle b_w^* b_w\rangle=(e^{\beta\hbar ws}-1)^{-1}. \tag{3·18}$$

(3·17) are readily proved with the help of (3·9), (3·16) and (3·20). Although the averages of N-products of higher order do not necessarily vanish, it happens that they are such small quantities that their contributions to the grand partition function can be ignored in the limit of $N\to\infty$, $V\to\infty$ (keeping N/V as a constant). To see this fact, we shall consider $\langle T[\psi^*(x)\psi(x)\psi^*(x')\psi(x')]\rangle$ as an example. According to the lemma II, we get

$$\begin{aligned}\langle T[\psi^*(x)\psi(x)\psi^*(x')\psi(x')]\rangle &= \langle N[\psi^{*\prime}(x)\psi'(x)\psi^{*\prime}(x')\psi'(x')]\rangle \\ &= \langle N[\psi^*(x)\psi(x)\psi^*(x')\psi(x')]\rangle - S(x-x')\langle N[\psi^*(x')\psi(x)]\rangle \\ &\quad - S(x'-x)\langle N[\psi^*(x)\psi(x')]\rangle + S(x-x)\langle N[\psi^*(x')\psi(x')]\rangle \\ &\quad + S(x'-x')\langle N[\psi^*(x)\psi(x)]\rangle - S(x-x')S(x'-x) + S(x-x)S(x'-x') \\ &= \langle N[\psi^*(x)\psi(x)\psi^*(x')\psi(x')]\rangle - S(x-x')S(x'-x) \\ &\quad + S(x-x)S(x'-x'),\end{aligned} \tag{3·19}$$

in which the condition $\langle N[\psi^*(x)\psi(x')]\rangle=0$ has been used. On the other hand, if one compute the left-hand side of (3·19) directly, it will follow that

$$\langle T[\psi^*(x)\psi(x)\psi^*(x')\psi(x')]\rangle$$
$$=\begin{cases} V^{-2}\sum_{k}\sum_{l}\sum_{m}\sum_{n}\langle a_k^* a_l a_m^* a_n\rangle e^{-i[(k-l)x+(m-n)x']+(\varepsilon_k-\varepsilon_l)t+(\varepsilon_m-\varepsilon_n)t'} & t>t', \\ V^{-2}\sum_{k}\sum_{l}\sum_{m}\sum_{n}\langle a_k^* a_l a_m^* a_n\rangle e^{-i[(k-l)x'+(m-n)x]+(\varepsilon_k-\varepsilon_l)t'+(\varepsilon_m-\varepsilon_n)t} & t<t'. \end{cases} \tag{3·20}$$

The average $\langle a_k^* a_l a_m^* a_n\rangle$ vanishes for all values of $(\boldsymbol{k}\,\boldsymbol{l}\,\boldsymbol{m}\,\boldsymbol{n})$ except for the follwing three cases:

a) $\boldsymbol{k=l\neq m=n}$,

b) $\boldsymbol{k=n\neq l=m}$,

c) $\boldsymbol{k=l=m=n}$.

Referring to the definition of $S(x-x')$ given by (3·17a), one can easily see that case a) gives us the term $S(x-x)S(x'-x')$ in the right hand side of (3·10), and the case b) the term $S(x-x')S(x'-x)$, so that

$$\langle N[\psi^*(x)\psi(x)\psi^*(x')\psi(x')]\rangle = V^{-2}\sum_k \langle a_k^* a_k a_k^* a_k\rangle, \tag{3·21}$$

which is, however, smaller than the other two terms by a factor $1/V$, owing to the contraction of the summation over momenta from double to single. The same reasoning prevails for all the averages of N-products, and the average of an N-product with $2n$ factors is generally shown to be a quantity of the order of $(1/V^{n-1})$ if the c-number terms composed of $S(x-x')$ and $D(x-x')$ alone are regarded as the quantities of the order of unity. Thus, on disregarding all the averages of N-products, we are led to a simple computation rule for $\langle T[H_1(x_1)\cdots H_1(x_n)]\rangle$, that is;

(1) substitute for every field operator $\psi^*(x)$, $\psi(x)$ and $\varphi(x)$ the quantities $\psi^{*\prime}(x)$, $\psi'(x)$ and $\varphi'(x)$ defined by (3·14) and (3·15) respectively,

(2) perform the operations indicated by $\delta/\delta\psi^*(x)$, $\delta/\delta\psi(x)$ and $\delta/\delta\varphi(x)$ with the help of the commutation relations (3·12) and (3·15),

(3) retain only such terms that do not contain N-product as a factor.

We can reformulate these results by noting that equs. (3·11) and (3·14) can be respectively in the form

$$\begin{aligned} e^{\Delta}\varphi(x)e^{-\Delta} &= \varphi'(x), \\ e^{\Sigma}\psi^*(x)e^{-\Sigma} &= \psi^{*\prime}(x), \\ e^{\Sigma}\psi(x)e^{-\Sigma} &= \psi'(x), \end{aligned} \tag{3·22}$$

where

$$\begin{aligned} \Delta &= \tfrac{1}{2}\iint dxdy\, D(x-y)\,\delta/\delta\varphi(x)\,\delta/\delta\varphi(y), \\ \Sigma &= \iint dxdy\, S(x-y)\,\delta/\delta\psi(y)\,\delta/\delta\psi^*(x), \end{aligned} \tag{3·23}$$

as can be readily proved by a direct calculation. Let $\mathfrak{G}(\psi^*, \psi, \varphi)$ be any functional of the field operators $\psi^*(x)$, $\psi(x)$ and $\varphi(x)$. then

$$\langle T[\mathfrak{G}(\psi^*, \psi, \varphi)]\rangle = \langle N[e^{\Delta}e^{\Sigma}\mathfrak{G}(\psi^*, \psi, \varphi)e^{-\Delta}e^{-\Sigma}]\rangle. \tag{3·24}$$

In this formalism the grand partition function given by (2·14) can be put into a compact form :

$$\begin{aligned} \Xi/\Xi_0 &= \langle T[\exp -\int H_1(x)dx]\rangle = \langle T[\mathfrak{S}]\rangle \\ &= \langle N[e^{\Delta}e^{\Sigma}\mathfrak{S}e^{-\Delta}e^{-\Sigma}]\rangle \end{aligned}$$

or

$$\Xi/\Xi_0=\langle N[e^{A}e^{\Sigma}\mathfrak{S}]\rangle, \tag{3·25}$$

because we can disregard the factor $e^{-A}e^{-\Sigma}$ since there is nothing for it to operate on. Serial expansion of exponential function in powers of $\int H_1(x)dx$ leads us to the formula (2·14b).

In actual calculations dealing with eq. (3·25), it is more convenient to employ the so-called Feynman graphs. Each term in the expansion of the right hand side of (3·25) can be analyzed into various Feynman graphs according to the following rules: On carrying out the rearrangments of operators and retaining only the terms which do not contain N-product, for every factor $D(x-x')$ a dotted (phonon) line is drawn connecting the points x and x'; for every factor $S(x-x')$ a directed (electron) line is drawn from x to x'. Thus each term in the expansion of the right hand side of (3·25) is composed of a number of Feynman graphs, to each of which a product function of $S(x-x')$ and $D(x-x')$ corresponds. The final result we want is obtained by integrating with respect to all the coordinates involved in each Feynman graphs and by summing up all the terms contributed from possible Feynman graphs.

§ 4. Illustrations

Having established the computation rules, we will apply them to the calculations of ξ_n and C_n with small n for the electron-phonon system. What we are going to calculate is

$$\begin{aligned}\xi_n&=(-1)^n/n!\int\cdots\int\langle T[H_1(x_1)\cdots H_1(x_n)]\rangle dx_1\cdots dx_n,\\ H_1(x)&=g\psi^*(x)\psi(x)\varphi(x)+g'\varphi(x)\varphi(x).\end{aligned} \tag{4·1}$$

In analyzing ξ_n into Feynman graphs, the following view points are useful: We think that to each $\psi^*(x)$ corresponds an electron line starting from the point x, to each $\psi(x)$ corresponds an electron line entering into the point x, and to each $\varphi(x)$ coreesponds a phonon line joining at the point x. Thus $H_1(x)$ represents a point x, at which either three lines, two electron lines and a phonon line, join with strength g, or two phonon lines are connected with strength g'. We can, therefore, carry out the analysis of ξ_n by drawing all the graphs in which n vertices are connected with each other, either by two electron lines outgoing and incoming and a phonon line, or by two phonon lines. We need not consider the term in ξ_n which contain the factors $\varphi(x)$'s of odd numbers. Furthermore, many graphs may be left out of consideration on account of the rule that an electron line is forbidden to join a point to itself. This additional rule comes out from the fact that since a constant factor $S(0)$ corresponds to such an electron line that joins a point to itself, the integration with respect to the coordinate of this vertix is to be reduced to the form $\int D(x)dx$, which evidently vanishes in virtue of (3·17b). In Fig. 1 various Feynman graphs appearing in the lower order terms of ξ_n's are shown. A comparison of the results from Feynman graph analysis with that of a straightfoward application of the computation rules reveals that

the sign of each graph is determined as + or − according to whether the number of closed electron line loops involved in the Feynman graph is odd or even.

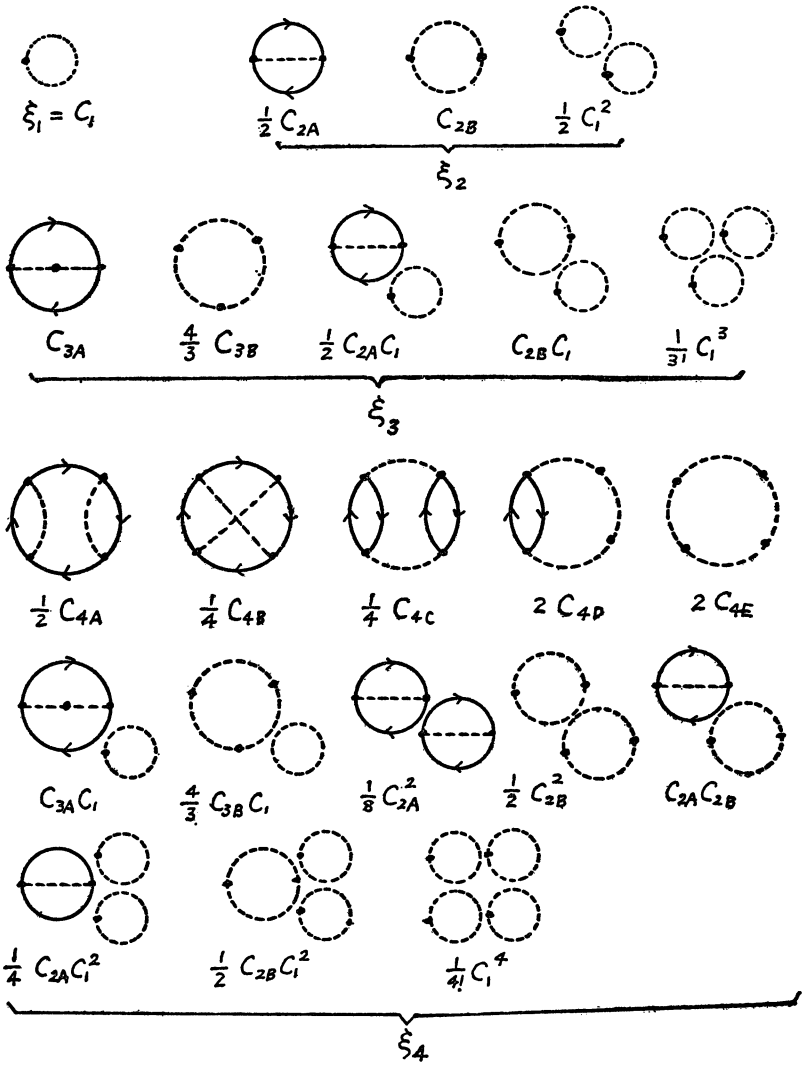

Fig. 1. Various Feynman graphs appearing in ξ_1, ξ_2, ξ_3 and ξ_4.

Referring to the relations between $\hat{\varsigma}_n$ and C_k given by (2·16), we can see from Fig. 1 that C_k is exclusively constructed of connected Feynman graphs with k vertices. This sesult is of some importance, because the free energy of the system is given by

$$\begin{aligned} F &= -N\mu - kT \log \Xi \\ &= -N\mu - kT \log \Xi_0 - kT(C_1 + C_2 + C_3 \cdots), \end{aligned} \tag{4·2}$$

which is to be proportional to the whole volume of the system V. For every connected Feynman graphs, the result of the integrations with respect to all the involved coordinates but one turns out to be independent of a remaining coordinate, and the integration with respect to the last coordinate simply gives a factor βV, so that the above requirement that (4·2) is to be proportional to V is always fulfilled if every C_k consist of connected Feynman graphs alone. It should be noted that this proportionality $F \propto V$ is not justified when the averages of N-products disregarded above are take into consideration.

The integrations with respect to the coordinates can be quite easily performed, at least for small n. We shall show below only two lowest order terms in Fig. 1 ·

$$C_1 = \int D(0)\,dx = \beta V \sum_w \hbar w s (N_w + 1/2),$$

$$C_{2A} = \iint S(x-x')S(x'-x)D(x-x')\,dx\,dx' \qquad (4\cdot3)$$

$$= \left[-\sum_k \sum_w \frac{w f_k (1-f_{k+w})}{\varepsilon_{k+w} - \varepsilon_k + \hbar w s} + \sum_k \sum_w \frac{w N (f_{k+w} - f_k)}{\varepsilon_{k+w} - \varepsilon_k + \hbar w s} \right] \beta V,$$

which are in agreement with those obtained by other authors.[8]

The merits of the present method are, apart from the simplicity of its computation rules, that it enables us to get a deep insight into the structures of the higher order perturbations through the Feynman graphs, and hence to go beyond the usual perturbational calculation. For instance, we can carry out a partial summation of serial terms up to infinite order, by adding certain special Feynman graphs. Thus the so-called renormalization procedures developed in quantum field theory will become available to various degrees. An

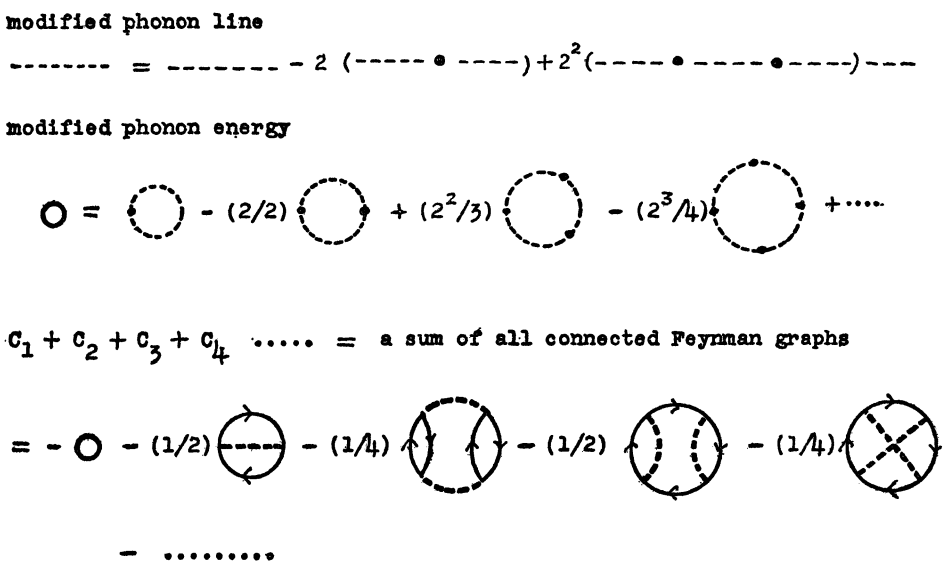

Fig. 2. Elimination of the term $g'\varphi(x)\varphi(x)$ in $H_1(x)$. This is effected by employing a re-defined phonon line in place of ------

example: It is immediately suggested by inspecting Fig. 1 that the effect of the second term in (4·1) can be eliminated by re-defining the phonon line and the phonon energy as illustrated in Fig. 2.

This means in the mathematical formula that $D(x-x')$ is to be replaced by

$$D^*(x-x') = D(x-x') - 2g'\int D(x-x_1)E(x_1-x')\,dx_1 + (2g')^2\iint D(x-x_1)D(x_1-x_2)D(x_2-x')\,dx_1dx_2\cdots \tag{4·4}$$

The evaluation of $D^*(x-x')$ is not difficult (see appendix *B*), the result being conveniently expressed in terms of the Fourier component as

$$D^*(\boldsymbol{k}, t) = 1/g'\int_1^\infty \xi^{-\alpha} D(\xi\boldsymbol{k}, t)\,d\xi, \tag{4·5}$$

where

$$D(\boldsymbol{k}, t) = \int D(\boldsymbol{x}, t)\, e^{i\boldsymbol{k}\cdot\boldsymbol{x}} d^3\boldsymbol{x}, \tag{4·6}$$

and

$$\alpha = (1+3g')/g'. \tag{4·6}$$

(4·5) and (4·7) show that for small g' $D^*(x-x')$ is nearly equal to $D(x-x')$, whereas for large g' it becomes proportional to $1/g'$. This reduction in magnitude of $D^*(x-x')$, in turn, acts to prevent the sound velocity from suffering large alteration due to electron-phonon interaction. Such a situation remedies a certain difficulty occurred in a perturbational treatment of sound velocity re-normalization.[11] But we shall leave this problem for another occasion.

§ 5. Non-perturbational treatment

The treatment described in the preceding sections is essentially an expansion of the grand partition function in powers of the coupling constant, so that, for the case of strong coupling it will not be useful as it stands. It is, however, possible to put forward a method which is free from the serial expansion procedure.[10]

We consider a set of functions defined by

$$\begin{aligned} G_1(x\,;x') &= \langle T[\psi^*(x)\psi(x')\mathfrak{S}]\rangle/\langle T[\mathfrak{S}]\rangle, \\ G_2(xy\,;x'y') &= \langle T[\psi^*(x)\psi^*(y)\psi(y')\psi(x')\mathfrak{S}]\rangle/\langle T[\mathfrak{S}]\rangle, \\ G_3(xyz\,;x'y'z') &= \langle T[\psi^*(x)\psi^*(y)\psi^*(z)\psi(z')\psi(y')\psi(x')\mathfrak{S}]\rangle/\langle T[\mathfrak{S}]\rangle, \end{aligned} \tag{5·1}$$

and so on, where

$$\mathfrak{S} = \exp\Big[-\int H_1(x)\,dx\Big], \qquad H_1(x) = g\psi^*(x)\psi(x)\varphi(x). \tag{5·2}$$

(For the sake of simplicity, we shall omit the term $g'\varphi(x)\varphi(x)$ for a while.) Following the terminology used in quantum field theory, we shall call them the Green function of one-electron, of two-electrons and so on. As is evident from the definitions, however, they correspond to the coordinate representation of the reduced density matrices in the grand canonical ensemble, and play a role similar to the molecular distribution function in classical statistical mechanics. For phonon we define in a similar way

$$\Delta_1(xx') = \langle T[\varphi(x)\varphi(x')\mathfrak{S}]\rangle / \langle T[\mathfrak{S}]\rangle, \quad \text{etc.} \tag{5·3}$$

Now, we will show that these Green functions satisfy a set of coupled integral equations. To do this we apply the equation (3·24) to (5·1) and (5·3). Then, for instance, we obtain

$$G_1(xx') = \langle N[e^{\Delta}e^{\Sigma}\psi^*(x)\psi(x')\mathfrak{S}]\rangle / \langle T[\mathfrak{S}]\rangle. \tag{5·4}$$

Here let us commute e^{Σ} through $\psi^*(x)$. Referring to the relations

$$\begin{aligned} e^{\Sigma}\psi^*(x) &= \psi^*(x)\,e^{\Sigma} + \int dy\, S(x-y)\,\delta/\delta\psi(y)\,e^{\Sigma}, \\ e^{\Sigma}\psi(x) &= \psi(x)\,e^{\Sigma} - \int dy\, S(y-x)\,\delta/\delta\psi^*(y)\,e^{\Sigma}, \end{aligned} \tag{5·5}$$

we see that the result is

$$G_1(xx') = \langle N[e^{\Delta}\int dy\, S(x-y)\,\delta/\delta\psi(y)\,e^{\Sigma}\psi(x')\mathfrak{S}]\rangle / \langle T[\mathfrak{S}]\rangle. \tag{5·6}$$

The term which contains the factor $\psi^*(x)$ standig to the left of e^{Σ} is omitted, because we are ignoring the average of N-product. Since the operator $\delta/\delta\psi(y)$ commutes with Σ, we can perform the indicated differentiation in (5·6) by noting that

$$\begin{aligned} &[\delta/\delta\psi(y),\ \psi(x')]_+ = \delta(y-x'), \\ &\delta/\delta\psi(y)\,\mathfrak{S} = g\psi^*(y)\varphi(y)\mathfrak{S}, \end{aligned} \tag{5·7}$$

and we obtain

$$G_1(xx') = S(x-x') + g\int S(x-y)\,dy \langle N[e^{\Delta}e^{\Sigma}\psi^*(y)\psi(x')\varphi(y)\mathfrak{S}]\rangle / \langle T[\mathfrak{S}]\rangle. \tag{5·8}$$

Let us further commute e^{Δ} through $\psi^*(y)$, $\psi(x')$ and $\varphi(y)$, referring to the relations

$$e^{\Delta}\varphi(y) = \varphi(y)\,e^{\Delta} + \int dz\, D(y-z)\,\delta/\delta\varphi(z)\,e^{\Delta} \tag{5·9}$$

and

$$\delta/\delta\varphi(z)\,\mathfrak{S} = -g\psi^*(z)\psi(z)\mathfrak{S}. \tag{5·10}$$

The result is

$$G_1(xx') = S(x-x') - g^2\int\int dy\,dz\, S(z-y)\,D(y-z)\,\langle T[\psi^*(y)\psi(x')\psi^*(z)\psi(z)\mathfrak{S}]\rangle / \langle T[\mathfrak{S}]\rangle$$

$$=S(x-x')-g^2\iint S(x-y)D(y-z)G_2(yz;x'z)\,dy\,dz, \tag{5·11}$$

where the use of the definition for $G_2(xy;x'y')$ has been made. Thus $G_1(xx')$ is shown to be coupled with $G_2(xy;x'y')$ through an equation (5·11). Repeating the same procedures, we can easily prove that G_k is directly connected with G_{k-1} and G_{k+1} through an integral equation similar to (5·11). For example

$$G_2(xy;x'y')=S(x-x')G_1(yy')-S(x-y')G_1(yx')$$
$$-g^2\int S(x-x_1)D(x_1-y_1)G_3(yx_1y_1;y'x'y_1)\,dx_1dy_1. \tag{5·12}$$

These coupled equations connecting the Green functions of varicus order bear a resemblance to the integral equations satisfied by the molecular distribution functions of various orders, discovered by Born-Green[12] and Kirdwood[13] in classical statistical mechanics. Although it is a very difficult task to solve these equations, one might be able to find an approximation of breaking off the infinite chain of equations into a closed system of few equations.

It is, however, more convenient to handle an equation containing one electron Green function alone, if such an equation exists. In fact, we can derive such an equation by making use of a trick of introducing an auxiliary external field.[14] We define $\mathfrak{S}$ in place of (5·2) by

$$\mathfrak{S}=\exp[-\int\{g\psi^*(x)\psi(x)\varphi(x)+\psi^*(x)\phi(x)\psi(x)\}\,dx], \tag{5·13}$$

where $\phi(x)$ is a c-number field which is to be made vanish in the final result. Then following the same procedures as in deriving (5·11), we get

$$G_1(xx')=S(x-x')-\int dy\,S(x-y)\langle T[\psi(x')\delta/\delta\psi(y)\mathfrak{S}]\rangle/\langle T[\mathfrak{S}]\rangle.$$

Now in view of (5·13) it immediately follows that

$$\delta/\delta\psi(y)\mathfrak{S}=\{g\psi^*(y)\varphi(y)+\phi(y)\psi^*(y)\}\mathfrak{S},$$

and hence

$$G_1(xx')=S(x-x')+\int S(x-y)\phi(y)G_1(yx')\,dy$$
$$+g\int dy\,S(x-y)\langle N[e^{\Delta}e^{\Sigma}\psi^*(y)\psi(x')\varphi(y)\mathfrak{S}]\rangle/\langle T[\mathfrak{S}]\rangle$$
$$=S(x-x')+\int S(x-y)\phi(y)G_1(yx')\,dy$$
$$-g^2\iint S(x-y)D(y-\xi)G_2(y\xi;x'\xi)\,dy\,d\xi. \tag{5·14}$$

The last expression in (5·14) has been attained by commuting e^{Δ} with $\varphi(y)$ and carrying out the differentiation. In order to express G_2 in terms of G_1, we have to regard $G_1(xx')$

as a functional of the auxiliary field $\phi(x)$. Then we can proceed as follows:

$$\begin{aligned} G_2(x\xi\,;y\xi) &= \langle T[\psi^*(x)\psi^*(\xi)\psi(\xi)\psi(y)\mathfrak{S}]\rangle/\langle T[\mathfrak{S}]\rangle \\ &= -\langle T[\psi^*(x)\psi(y)\delta/\delta\phi(\xi)\mathfrak{S}]\rangle/\langle T[\mathfrak{S}]\rangle \\ &= -\delta/\delta\phi(\xi)\langle T[\psi^*(x)\psi(y)\mathfrak{S}]\rangle/\langle T[\mathfrak{S}]\rangle. \end{aligned} \tag{5·15}$$

Inserting (5·15) into (5·14) and carrying out a slight manipulation, we arrive at

$$\begin{aligned} G(xx') = S(xx') &+ \int S(x-y)\phi(y)G(y,x')dy \\ &+ g^2\iint S(x-y)D(y-\xi)\delta/\delta\phi(\xi)G(yx')d\xi dy. \end{aligned} \tag{5·16}$$

On the other hand, $S(x-x')$ satisfies the following differential equation:

$$\left[\frac{\partial}{\partial t}+\frac{\hbar^2}{2m}\Delta\right]S(\boldsymbol{x},t)=\delta(\boldsymbol{x})\delta(t)=\delta(x), \tag{5·17}$$

which can be easily proved by a direct operation of $(\partial/\partial t+\hbar^2/2m\cdot\Delta)$ on $S(x)$ defined by (3·17a). Operating $(\partial/\partial t+\hbar^2/2m\cdot\Delta)$ on (5·16) from left, and making use of (5·17), (5·16) is converted to

$$\begin{aligned} \left\{\frac{\partial}{\partial t}+\frac{\hbar^2}{2m}\Delta\right\}G(xx') &= \delta(x-x')+\phi(x)G(xx') \\ &+ g^2\int D(x-\xi)\delta/\delta\phi(\xi)G(xx')d\xi\,. \end{aligned} \tag{5·18}$$

A similar equation for one-nucleon Green function in meson field was solved by Edwards and Peierls by introducing a special technique of Fourier transformation in functional space.[15] A similar method may be available in the present case.

Another and more tractable method to deal with the grand partition function will be the generalized Hartree approximation. Recently Kinoshita and Nambu have developed a theory of Hartree field for a system composed of a number of particles and a intermediary Bose field.[16] A similar method will be also applicable to the present case, and will be especially useful for the investigation of the cooperative phenomena such as superconductivity.

We shall take again the electron-phonon system as an example. According to the general theory described in § 2 and § 3, the grand partition function is given by

$$\Xi/\Xi_0=\langle T[\exp\{-\int H_1(x)dx\}]\rangle, \tag{5·19}$$

which is valid for an arbitrary choice of H_0 and H_1. We assume, therefore, that the free Hamiltonian has, instead of (2·17b), the following form

$$\bar{H}=\sum_k E_k a_k^* a_k+\sum_w W_w(b_w^* b_w+\tfrac{1}{2}) \tag{5·20}$$

and the interaction Hamiltonian is chosen so as to make it hold that

$$\int \bar{H}_1(x)\,dx=\int e^{t\bar{H}_0}H_1 e^{-t\bar{H}_0}dt=\tfrac{1}{2}\iint T[\psi^*(x)\phi(x-x')\psi(x')]dxdx'$$
$$+\tfrac{1}{4}\iint P[\varphi(x)\chi(x-x')\varphi(x')]dxdx'+g\int\psi^*(x)\psi(x)\varphi(x)\,dx, \qquad (5\cdot21)$$

where $\phi(x-x')$ represents a sort of Hartee field for electron, E_k the energy of electron moving in this Hartree field, $\chi(x-x')$ and W_w are the corresponding quantities for phonon. $\psi^*(x)$, $\psi(x)$ and $\varphi(x)$ are respectively defined by

$$\begin{aligned}\psi^*(x)&=V^{-1/2}\sum_k a_k^* e^{-ik\cdot x+E_k t},\\ \psi(x)&=V^{-1/2}\sum_k a_k\, e^{ik\cdot x-E_k t},\\ \varphi(x)&=\sum_w (W_w/2V)^{1/2}(b_w^* e^{-iw\cdot x+W_w t}+b_w e^{iw\cdot x-W_w t})\end{aligned} \qquad (5\cdot22)$$

in place of (2·20). With the aid of (5·22), each term in the right hand side of (5·21) can be written down as a function of a_k^*, a_k, b_w^* and b_w, the results being

$$\begin{aligned}&\tfrac{1}{2}\iint T[\psi^*(x)\phi(x-x')\psi(x')]dxdx'\\ &\quad=\int dt\, e^{t\bar{H}_0}[\tfrac{1}{2}\sum_k \phi(k,\,-E_k)\,(a_k^* a_k-a_k a_k^*)]e^{-t\bar{H}_0},\\ &\tfrac{1}{4}\int P[\varphi(x)\chi(x-x')\varphi(x')]dxdx'\\ &\quad=\tfrac{1}{2}\int dt\, e^{t\bar{H}_0}[\sum_w W_w\chi(w,\,-W_w)\,(b_w^* b_w+b_w b_w^*+b_w b_{-w}+b_w^* b_{-w}^*)]e^{-t\bar{H}_0},\\ &g\int\psi^*(x)\psi(x)\varphi(x)\,dx\\ &\quad=\int dt\, e^{t\bar{H}_0}[g\sum_k\sum_w (W_w/2V)^{1/2}(a_{k-w}^* a_k b_w^*+a_{k+w}^* a_k b_w)]e^{-t\bar{H}_0},\end{aligned} \qquad (5\cdot23)$$

where $\phi(k, E)$ and $\chi(w, W)$ are, respectively, the Fourier-Laplace transform of $\phi(x)$ and $\chi(x)$ defined by

$$\begin{aligned}\phi(k,E)&=\iint\phi(x,\,t)\,e^{ik\cdot x-Et}d^3x\,dt,\\ \chi(w,\,W)&=\iint\chi(x,\,t)\,e^{ik\cdot x-Wt}d^3x\,dt.\end{aligned} \qquad (5\cdot24)$$

Combining (5·23) with (5·20) we see that

$$\bar{H}_1=g\sum_k\sum_w (W_w/2V)^{1/2}(a_{k-w}^* a_k b_w^*+a_{k+w}^* a_k b_w)+\sum_k\phi(k,\,-E_k)\,a_k^* a_k-\tfrac{1}{2}\sum_k\phi(k,\,-E_k)$$
$$+\tfrac{1}{2}\sum_w W_w\chi(w,\,-W_w)\,(b_w^* b_w+b_w b_w^*+b_w^* b_{-w}+b_w^* b_{-w}^*).$$

Since the sum of $\bar{H}_0$ and $\bar{H}_1$ has to be taken equal to the original total Hamiltonian given

by (2·17), apart from a constant,

$$\bar{H}_0+\bar{H}_1=H+C,$$

it follows by comparing (5·25) with (2·17) that

$$\varepsilon_k=E_k+\phi(k,\ -E_k), \tag{5·26a}$$

$$\hbar ws=W_w, \tag{5·26b}$$

$$g'=\chi(w,\ -W_w), \tag{5·26c}$$

$$C=-\tfrac{1}{2}\sum\phi(k,\ -E_k). \tag{5·26d}$$

Eqs. (5·26) provide physical meanings for the Hartree field $\phi(x)$ and $\chi(x)$, that is, the Fourier-Laplace component of $\phi(x)$ equals the difference between the enenery of a free electron and that of an electron moving in the Hartree field, and the Fourier-Laplace component of $\chi(x)$ gives what we called renormalization constant in § 2. In order to determine $\phi(x)$ and $\chi(x)$ self-consistently, we shall apply the theory of Green function described in the beginning of this section. Define the Green function $G(xx')$ and $\Delta(xx')$ by

$$\begin{aligned} G(xx')&=\langle T[\psi^*(x)\psi(x')\mathfrak{S}]\rangle/\langle T[\mathfrak{S}]\rangle,\\ \Delta(xx')&=\langle T[\varphi(x)\varphi(x')\mathfrak{S}]\rangle/\langle T[\mathfrak{S}]\rangle \end{aligned} \tag{5·27}$$

with

$$\begin{aligned} \mathfrak{S}=\exp\Big[-\{g\int\psi^*(x)\psi(x)\varphi(x)dx+\tfrac{1}{2}\iint\psi^*(x)\phi(x-x')\psi(x')dxdx'\\ +\tfrac{1}{4}\iint\varphi(x)\chi(x-x')\varphi(x')dxdx'\}\Big]. \end{aligned} \tag{5·28}$$

If we content ourselves with the expressions up to the second order in the coupling constant g, the coupled equations for $G(x-x')$ and $\Delta(x-x')$, which are derived through the procedures described above, can be easily solved by an iteration procedure. We shall give here only the results;

$$\begin{aligned} G(xx')=S(x-x')+\tfrac{1}{2}\iint S(z-y)\phi(x-y)S(z-x')dydz\\ +g^2\iint S(x-y)D(y-z)S(y-z)S(z-x')dydz, \end{aligned} \tag{5·29}$$

$$\begin{aligned} \Delta(xx')=D(x-x')-\tfrac{1}{2}\iint D(x-y)\chi(y-z)D(z-x')dydz\\ +g^2\iint D(x-y)D(x'-z)S(y-z)S(z-y)dydz. \end{aligned} \tag{5·30}$$

In this approximation, it will be natural to determine $\phi(x)$ and $\chi(x)$ in such a way that

$$G(xx')=S(x-x'),\quad \Delta(xx')=D(x-x'), \tag{5·31}$$

because the equations (5·21) state that electrons and phonons behave in the respective

Hartree field as if they are independent of each other. This statement is in accord with the basic assumption in Hartree approximation. From (5·29), (5·30) and (5·31) $\phi(x)$ and $\chi(x)$ are determined as

$$\phi(z-y)=-2g^2D(y-z)S(y-z), \tag{5·32}$$

$$\chi(y-z)=-2g^2S(y-z)S(z-y). \tag{5·33}$$

Here we shall briefly discuss the results derived from the equations (5·32) and (5·33), leaving the details to a later publicatoin.

Performing the Fourier-Lapace transformations of (5·32) and (5·33) with the help of (3·17), we readily get

$$\phi(\boldsymbol{k}, -E_k)=\frac{g^2}{V}\sum_{w}\hbar ws\left[\frac{(N_w+1)(1-f_{k-w})}{E_{k-w}-F_k+\hbar ws}+\frac{N_w(1-f_{k+w})}{E_{k+w}-E_k-\hbar ws}\right], \tag{5·34}$$

$$\chi(\boldsymbol{w}, -W_k)=\frac{2g^2}{V}\sum_{k}\frac{f_k(1-f_{k-w})}{E_{k-w}-E_k+W_w}. \tag{5·35}$$

Referring to (5·26), the equation (5·35) gives the change in the sound velocity of phonon caused by the electron-phonon interaction, if the dispersion of sound velocity is ignored. The result obtained here is nearly the same as that calculated by Fröhlich. (5·34) combined with (5·26a), on the other hand, give an equation to determine E_k. On neglecting N_w at very low temperatures, it becomes

$$E_k=\varepsilon_k-\frac{g^2}{V}\sum_{w}\hbar ws\frac{(1-f_{k-w})}{E_{k-w}-E_k+\hbar ws}. \tag{5·36}$$

It is interesting to note that the same equation as (5·36) was derived by Bardeen in a quite different way.[17] Although the nature of the solution of the equation (5·36) was already discussed by him, a more careful investigation of this equation has been made by the present author. The result obtained agrees with that given by Bardeen in its essential point. There exists a solution of (5·36) in which one electron energy E_k has a gap at Fermi surface for sufficiently strong coupling constant. The ground state in which all the states of lower energy are occupied by electrons will correspond to a superconducting state at 0°K. Temperature effect on energy spectrum is easily taken into account in the present method, and it is shown that the energy gap, dependent on temperature, becomes to vanish above a certain temperature. Thus a sort of phase transition is expected. A similar result was worked out by Fröhlich and Kuper[18] with one-dimensional model. The basic idea of the present method resembles rather that of Fröhlich's than Bardeen's. Fröhlich has assumed that a cooperative interaction between electrons and phonons produces such a potential for an electron as to give rise to a splitting of the energy spectrum of the electron. In the present theory, we introduced explicitly a possessing a nature which Fröhlich has assumed, and we have proved in a self-consistent manner that this potential actually gives rise to a splitting in one-electron spectrum even in three dimensional case, and hence brings the assembly of electrons into a special state which we want to call the superconducting state.

§ 6. Extension to Other Systems

The electron-phonon system so far considered is a typical example, to which our method can conveniently be applied. In extending our method to other system, it may happen that some modifications in the formalism are required. In this section we shall show that our method is easily extended to a system in which many particles, obeying Fermi or Bose statistics, are interacting with each other through two-body potential.

In the scheme of second quantization we write the Hamiltonian of a systen in question as

$$\begin{aligned} H&=H_0+H_1, \\ H_0&=\int\psi^*(\boldsymbol{x})\boldsymbol{p}^2/2m\psi(\boldsymbol{x})d^3\boldsymbol{x}, \\ H_1&=\tfrac{1}{2}\iint\psi^*(\boldsymbol{x})\psi^*(\boldsymbol{x}')J(\boldsymbol{x}-\boldsymbol{x}')\psi(\boldsymbol{x}')\psi(\boldsymbol{x})d^3\boldsymbol{x}d^3\boldsymbol{x}', \end{aligned} \tag{6·1}$$

where $J(\boldsymbol{x}-\boldsymbol{x}')$ represents the interaction potential between two particles located at $\boldsymbol{x}$ and $\boldsymbol{x}'$, $\boldsymbol{p}$ the momentum operator of a particle. $\psi^*(\boldsymbol{x})$ and $\psi(\boldsymbol{x})$ can be expanded into Fourier series :

$$\psi^*(\boldsymbol{x})=V^{-1/2}\sum_{\boldsymbol{k}}a_{\boldsymbol{k}}^*e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}, \qquad \psi(\boldsymbol{x})=V^{-1/2}\sum_{\boldsymbol{k}}a_{\boldsymbol{k}}e^{i\boldsymbol{k}\cdot\boldsymbol{x}}, \tag{6·2}$$

in which $a_{\boldsymbol{k}}^*$ and $a_{\boldsymbol{k}}$ are as usual creation and annihilation operators of a particle with wave vector $\boldsymbol{k}$, the commutation relations between them being given by

$$[a_{\boldsymbol{k}},a_{\boldsymbol{k}'}^*]_{\pm}=\delta_{\boldsymbol{k},\boldsymbol{k}'}. \tag{6·3}$$

(+ Fermi, − Bose statistics)

The grand partition function Ξ can be written as

$$\begin{aligned} \Xi/\Xi_0&=1+\xi_1+\xi_2+\xi_3+\cdots \\ &=\exp(C_1+C_2+C_3\cdots) \end{aligned} \tag{6·4}$$

with

$$\begin{aligned} \xi_n&=(-1)^n/n!\int\cdots\int\langle P[H_1(t_1)\cdots H_1(t_n)]\rangle dt_1\cdots dt_n, \\ H_1(t)&=e^{tH_0}H_1e^{-tH_0}, \end{aligned} \tag{6·5}$$

or more formally as

$$\Xi/\Xi_0=\langle P[\mathfrak{S}]\rangle,$$

where

$$\mathfrak{S}=\exp\left[-\int H_1(t)\,dt\right].$$

First we consider the case of Fermi particles. In applying the computation rules derive in § 3 to the present case, a difficulty arises from the interaction term

$$\int H_1(t)\,dt=\tfrac{1}{2}\iint\psi^*(\boldsymbol{x},\,t)\,\psi^*(\boldsymbol{x}',\,t)J(\boldsymbol{x}-\boldsymbol{x}')\,\psi(\boldsymbol{x}',\,t)\,\psi(\boldsymbol{x},\,t)\,d^3\boldsymbol{x}d^3\boldsymbol{x}'dt, \tag{6·7}$$

which prevents us from accomplishing in a simple manner the t-ordering indicated in the right hand side of (6·5). The problem can, however, be solved by rewriting (6·7) in the form

$$\int H_1(t)\,dt=\tfrac{1}{2}\iint T[\psi^*(x)\,\psi(x)J(x-x')\,\psi^*(x')\,\psi(x')]dxdx'$$

$$-\tfrac{1}{2}J(0)\int\psi^*(x)\,\psi(x)\,dx, \tag{6·8}$$

in which $J(x-x')$ is defined by

$$J(x-x')=J(\boldsymbol{x}-\boldsymbol{x}')\,\delta(t-t'). \tag{6·9}$$

That (6·8) equals (6·7) is easily verified by a short calculation. Then, noting that for arbitrary T-products $T[A]$, $T[B]$,$\cdots$

$$[T[A],T[B],\,\cdots]=T[A,\,B,\,\cdots],$$

we obtain, in place of (6·6),

$$\Xi/\Xi_0=\langle T[\mathfrak{S}]\rangle$$

with (6·10)

$$\mathfrak{S}=\exp[-\tfrac{1}{2}\iint\psi^*(x)\,\psi(x)J(x-x')\,\psi^*(x')\,\psi(x')\,dxdx'$$

$$+\tfrac{1}{2}J(0)\int\psi^*(x)\,\psi(x)\,dx],$$

to which all the rules established in § 3 are now applicable.

We have no trouble with the case of Bose particles. We do not want to repeat here a long analysis, so that we give below only the lemma II modified so as to hold for both statistics.

Lemma III For any product of $\psi^*(x)$ and $\psi(x)$ denoted by $\mathfrak{H}(\psi^*,\,\psi)$, it holds that

$$T[\mathfrak{H}(\psi^*,\,\psi)]=N[\mathfrak{H}(\psi^{*\prime},\,\psi')],$$

in which $T=(\mp1)^PP$ and $\psi'^*(x)$ and $\psi'(x)$ are defined by

$$\psi^{*\prime}(x)=\psi^*(x)+\int dx'S(x-x')\,\delta/\delta\psi(x'),$$

$$\psi'(x)=\psi(x)\mp\int dx'S(x'-x)\,\delta/\delta\psi^*(x'),$$

respectively. $\delta/\delta\psi^*(x)$ and $\delta/\delta\psi(x)$ satisfy the following commution relations:

$$[\delta/\delta\psi(x),\,\psi(x')]_\pm=[\delta/\delta\psi^*(x),\,\psi^*(x')]_\pm=\delta(x-x'),$$

$$[\delta/\delta\psi(x),\,\psi^*(x')]_\pm=[\delta/\delta\psi^*(x),\,\psi(x')]_\pm=0.$$

$S(x-x')$ is given by

$$S(x-x')=\begin{cases} V^{-1}\sum_k f_k e^{-ik\cdot(x-x')+\varepsilon_k(t-t')} & t>t' \\ V^{-1}\sum_k (f_k\mp 1)\, e^{-ik\cdot(x-x')+\varepsilon_k(t-t')} & t<t' \end{cases}$$

where

$$f_k=(e^{\alpha+\beta\varepsilon_k}\pm 1)^{-1}.$$

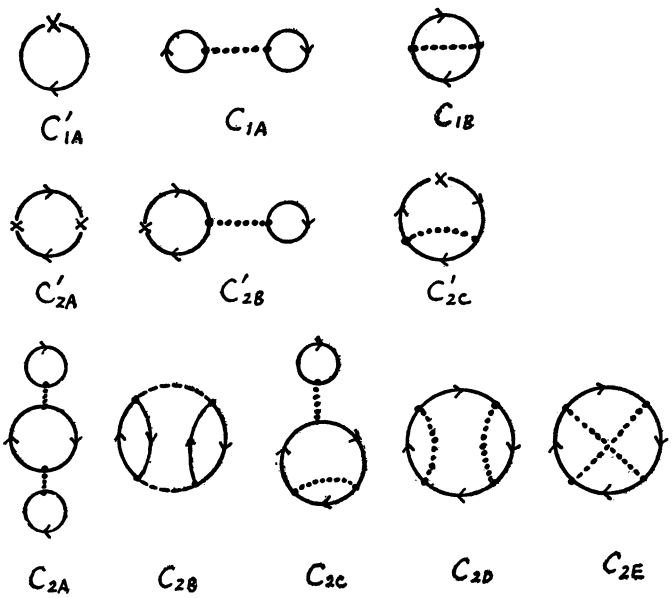

Fig. 3. Various Feynman graphs appearing in C_1 and C_2. Dotted line $x\cdots\cdots x'$ corresponds to $J(x-x')$. Directed line $x\rightarrow x'$ corresponds to $S(x-x')$. $\times$ represents self energy $J(0)$.

All the upper signs or doubled signatures correspond to Fermi case and lower signs to Bose case.

We can analyze $\hat{\xi}_n$ or C_k into Feynman graphs by drawing a directed (particle) line for every factor $S(x-x')$ from x to x', and a dotted line connecting the points x and x' for every factor $J(x-x')$. In the present case a particle line may join a point to itself. In Fig. 3 the Feynman graphs appearing in the lower order terms of C_k's are shown.

It will be worth while to compare the results derived from Fig. 3 with that of Ichimura's calculation. In the notation adopted here, the results for C_k's obtained by Ichimura by his own method are written as follows:[6]

$$C_1=-\tfrac{1}{2}\beta V^{-1}\sum_{k}\sum_{\neq l}(J_0\mp J_{k-l})f_k f_l \tag{6·11a}$$

$$\begin{aligned} C_2=&\tfrac{1}{2}\beta^2 V^{-2}\sum_{k}\sum_{\neq l}\sum_{\neq m} f_k(1\mp f_k)f_l f_m(J_0\mp J_{k-l})(J_0\mp J_{k-m}) \\ &+\tfrac{1}{4}\beta V^{-2}\sum_{k}\sum_{l}\sum_{m}\sum_{n}{}' \frac{(J_{k-m}\mp J_{k-n})^2}{\varepsilon_k+\varepsilon_l-\varepsilon_m-\varepsilon_n}(1\mp f_k)(1\mp f_l)f_m f_n, \end{aligned} \tag{6·11b}$$

$k+l=m+n$

where J_k is the Fourier component of $J(x)$ defined by

$$J_k=\int J(x)e^{ik\cdot x}d^3x.$$

We will show that (6·11) are in complete agreement with our results. Inspecting Fig. 3,

our expression for C_1 is readily written down as

$$C_1=\tfrac{1}{2}J(0)\int S(0)\,dx-\tfrac{1}{2}\iint J(x_1-x_2)\,\{S(0)\}^2 dx_1dx_2$$
$$\pm\tfrac{1}{2}\iint J(x_1-x_2)S(x_1-x_2)S(x_2-x_1)\,dx_1dx_2. \qquad (6\cdot12)$$

Noting that

$$S(0)=V^{-1}\sum_k f_k$$
$$S(x-x')S(x'-x)=-V^{-2}\sum_k\sum_{k'} f_k(1\mp f_{k'})\,e^{i\{(k-k')\cdot(x-x')-(\varepsilon_{k'}-\varepsilon_k)|t-t'|}$$
$$J(0)=V^{-1}\sum_k J_k, \qquad \int J(x-x')\,dx=J_0,$$

(6·12) can be reduced to

$$C_1/\beta V=-\tfrac{1}{2}V^{-2}\sum_k\sum_{k'}\{-J_kf_{k'}+J_0f_kf_{k'}\mp J_{k'-k}f_k(f_{k'}\mp1)\}$$
$$=-\tfrac{1}{2}V^{-2}\sum_k\sum_{k'}(J_0\mp J_{k'-k})f_kf_{k'},$$

which is just equal to (6·11a). It is seen from the above calculation that the term $J(0)\int\psi^*(x)\psi(x)\,dx$ in $\mathfrak{S}$ so behaves as to subtract the self-energy from the final results. We may, therefore, disregard this term hereafter, provide we keep in mind that the self-energy parts are always to be subtracted. Then C_2 is shown to consist of five integrals:

$$C_2=\mp4C_{2A}+2C_{2B}+8C_{2C}\mp4C_{2D}\mp2C_{2E},$$

$$C_{2A}=\tfrac{1}{4}\int\cdots\int\{S(0)\}^2J(x_1-x_2)S(x_2-x_3)S(x_3-x_2)J(x_3-x_4)\,dx_1\cdots dx_4$$
$$=\tfrac{1}{4}\beta^2V^{-2}J_0^2\sum_k\sum_l\sum_m f_k(f_k\mp1)f_lf_m,$$

$$C_{2B}=\tfrac{1}{4}\int\cdots\int S(x_1-x_2)S(x_2-x_1)S(x_3-x_4)S(x_4-x_3)J(x_1-x_3)J(x_2-x_4)\,dx_1\cdots dx_4$$
$$=\tfrac{1}{2}\beta V^{-2}\sum_k\sum_l\sum_m\sum_n{}'\frac{(J_{k-m})^2}{\varepsilon_k+\varepsilon_l-\varepsilon_m-\varepsilon_n}(f_k\mp1)(f_l\mp1)f_mf_n,$$

where $\sum'$ denotes $k+l=m+n$.

$$C_{2C}=\tfrac{1}{4}\int\cdots\int S(0)J(x_1-x_2)S(x_2-x_3)S(x_3-x_4)S(x_4-x_2)J(x_3-x_4)\,dx_1\cdots dx_4$$
$$=\tfrac{1}{4}\beta^2V^{-2}\sum_k\sum_l\sum_m J_0J_{k-l}f_k(f_k\mp1)f_lf_m,$$

$$C_{2D}=\tfrac{1}{4}\int\cdots\int S(x_1-x_2)S(x_2-x_3)S(x_3-x_4)S(x_4-x_1)J(x_1-x_2)J(x_3-x_4)\,dx\cdots dx_4$$
$$=\tfrac{1}{4}\beta^2V^{-2}\sum_k\sum_l\sum_m J_{k-l}J_{k-m}f_k(f_k\mp1)f_lf_m,$$

$$C_{2E}=\tfrac{1}{4}\int\cdots\int S(x_1-x_2)S(x_2-x_3)S(x_3-x_4)S(x_4-x_1)J(x_1-x_3)J(x_2-x_4)dx_1\cdots dx_4$$

$$=\tfrac{1}{2}\beta V^{-2}\sum_{k}\sum_{\substack{l\\ k+l=m+n}}\sum_{m}\sum_{n}\frac{J_{k-m}J_{k-n}}{\varepsilon_k+\varepsilon_l-\varepsilon_m-\varepsilon_n}(f_k\mp 1)\,(f_l\mp 1)f_m f_n.$$

As to the evaluation of the above integrals, see appendix *B*. The summation of these five integrals with given numerical coefficients immediately leads us to (6·11b), apart from the self-energy parts which can be cancelled out by the integrals corresponding to the graphs C'_{2A}, C'_{2B} and C'_{2C} in Fig. 3.

An application of the method of partial summation over certain special Feynman graphs, which was proved useful in § 4, gives rise to an interesting result for the electrons interacting with coulomb potential. It is suggested from Feynman graph analysis that the interaction potential $J(x-x')$ has better to be replaced by

$$J^*(x-x')=J(x-x')+2\int\int J(x-x_1)S(x_1-x_2)S(x_2-x_1)J(x_2-x')dx_1dx_2$$

$$+2^2\int\cdots\int J(x-x_1)S(x_1-x_2)S(x_2-x_1)J(x_2-x_3)S(x_3-x_4)S(x_4-x_3)J(x_3-x')dx\cdots dx_4+\cdots \tag{6·13}$$

For coulomb potential $J(x-x')=e^2/|\boldsymbol{x}-\boldsymbol{x}'|\delta(t-t')$, the Fourier transform of (6·13), integrated over t, becomes

$$J^*(\boldsymbol{k})=\frac{4\pi e^2}{k^2}\left\{1+\frac{4\pi e^2}{k^2}\Lambda(\boldsymbol{k})+\left(\frac{4\pi e^2}{k^2}\Lambda(\boldsymbol{k})\right)^2+\cdots\right\}$$

$$=\frac{4\pi e^2}{k^2-4\pi e^2\Lambda(\boldsymbol{k})},$$

$$\Lambda(\boldsymbol{k})=\frac{2}{V}\sum_{k'}\int S(k';-t)S(k'-k;t)dt=\frac{2}{V}\sum_{k'}\left(\frac{f_{k'}-f_{k'-k}}{\varepsilon_{k'}-\varepsilon_{k'-k}}\right). \tag{6·14}$$

This result shows us that the coulomb interaction between electrons is to be screened (as $1/r\to e^{-\lambda r}/r$), the screening constant λ being roughly estimated as

$$\lambda^2=-4\pi e^2\Lambda(0)=-\frac{8\pi e^2}{V}\sum_{k}\left(\frac{\partial f_k}{\partial\varepsilon_k}\right)\simeq\frac{4\pi e^2 m}{\hbar^2}K_m. \tag{6·15}$$

(K_m=the magnitude of wave vector of electron with Fermi energy).

The same result as (6·15) for the screening effect was derived by Macke by a variational calculation.[19]

Appendix A

A Proof of Lemma I

We shall prove the validity of lemma I by a mathematical induction. Assume that

it is true for some T-product $T[\mathfrak{F}(\varphi)]$, i.e. that

$$T[\mathfrak{F}(\varphi)]=N[\mathfrak{F}(\varphi')]. \tag{A·1}$$

Then if we can prove it for $T[\varphi(x)\mathfrak{F}(\varphi)]$, we can conclude that the statement of lemma I is valid, since for $\mathfrak{F}(\varphi)=1$ and for $\mathfrak{F}(\varphi)=\varphi$ (A·1) is trivially true. Without a loss of generality we can take $\mathfrak{F}(\varphi)$ as a product of n factors; $\varphi(x_1)\varphi(x_2)\cdots\varphi(x_n)$. When

$$t_1>t_2>\cdots\cdots>t_n$$

$T[\mathfrak{F}(\varphi)]$ can be written as

$$T[\mathfrak{F}(\varphi)]=\varphi(x_1)\varphi(x_2)\cdots\cdots\varphi(x_n). \tag{A·2}$$

Now let us assume that

$$t_1>t_2>\cdots t_r>t>t_{r-1}>\cdots>t_n.$$

Then

$$\begin{aligned}T[\varphi(x)\mathfrak{F}(\varphi)]&=\varphi(x_1)\cdots\varphi(x_r)\varphi(x)\varphi(x_{r+1})\cdots\varphi(x_n)\\&\equiv X(\varphi)\varphi(x)\,Y(\varphi).\end{aligned} \tag{A·3}$$

Here we decompose $\varphi(x)$ into two parts according to

$$\varphi(x)=\varphi_+(x)+\varphi_-(x),$$

and transfer $\varphi_-(x)$ to the left through $X(\varphi)$, and $\varphi_+(x)$ to the right through $Y(\varphi)$. The result is conveniently expressed as

$$X(\varphi)\varphi(x)\,Y(\varphi)=\varphi_-(x)\,XY+XY\varphi_+(x)+\int dx'\Delta_1(xx')\,\delta/\delta\varphi(x')\,(XY) \tag{A·4}$$

where

$$\Delta_1(xx')=\begin{cases}[\varphi_+(x),\,\varphi(x')]_- & t>t'\\ -[\varphi_-(x),\,\varphi(x')]_- & t<t'.\end{cases} \tag{A·5}$$

In order to obtain the N-product of $X\varphi(x)\,Y$ from (A·4), we have to bring back $\varphi_-(x)$ to the right and $\varphi_+(x)$ to the left, becanse $\varphi_-(x)$ may stand to the left of $\varphi_-(x_1)$, $\varphi_-(x_2)$, $\cdots$ $\varphi_-(x_r)$ and $\varphi_+(x)$ may stand to the right of $\varphi_+(x_{r+1})$, $\cdots$ $\varphi_+(x_n)$. Carrying out rearrangements needed for getting N-product, we can express the result in the form

$$\begin{aligned}\varphi_-(x)\,XY&=N[\varphi_-(x)\,XY]+\int dx'[\varphi_-(x),\,\varphi_-(x')]_-\delta X/\delta\varphi_-(x')\,Y,\\ XY\varphi_+(x)&=N[XY\varphi_+(x)]-\int dx'[\varphi_+(x),\,\varphi_+(x')]_-X\delta Y/\delta\varphi_+(x'),\end{aligned} \tag{A·6}$$

where operators $\delta/\delta\varphi_+(x)$ and $\delta/\delta\varphi_-(x)$ are difined through

$$\begin{aligned}&[\delta/\delta\varphi_+(x),\,\varphi_+(x')]_-=[\delta/\delta\varphi_-(x),\,\varphi_-(x')]_-=\delta(x-x'),\\&[\delta/\delta\varphi_+(x),\,\varphi_-(x')]_-=[\delta/\delta\varphi_-(x),\,\varphi_+(x')]_-=0,\end{aligned} \tag{A·7}$$

namely they represent functional differentiation. Since X and Y contain $\varphi_+(x)$ and $\varphi_-(x)$ as factors through the combined form $\varphi(x)=\varphi_+(x)+\varphi_-(x)$, it follows that

$$\delta X/\delta\varphi_-(x)=\delta X/\delta\varphi(x), \quad \delta Y/\delta\varphi_+(x)=\delta Y/\delta\varphi(x). \tag{A·8}$$

If we define further

$$\Delta_2(xx')=\begin{cases}[\varphi_+(x),\,\varphi_+(x')]_- & t>t'\\ -[\varphi_-(x),\,\varphi_-(x')]_- & t<t',\end{cases} \tag{A·8}$$

then from (A·3)—(A·8) we obtain

$$X\varphi(x)\,Y=N[\{\varphi_+(x)+\varphi_-(x)\}XY]+\int dx'[\Delta_1(xx')-\Delta_2(xx')]\,\delta(XY)/\delta\varphi(x'). \tag{A·10}$$

In view of the first assumption (A·1) and a property of N-product

$$N[\varphi' N[\mathfrak{F}(\varphi')]]=N[\varphi'\mathfrak{F}(\varphi')]$$

(A·10) tells us that

$$T[\varphi(x)\mathfrak{F}(\varphi)]=N[\varphi'(x)\mathfrak{F}(\varphi')]$$

where

$$\varphi(x)=\varphi(x)+\int dx'\{\Delta_1(xx')-\Delta_2(xx')\}\,\delta/\delta\varphi(x').$$

With the help of (A·5) and (A·9) it is easy to show that

$$\begin{aligned}&\Delta_1(xx')-\Delta_2(xx')\\ &\quad=\begin{cases}[\varphi_+(x),\,\varphi(x')]_--[\varphi_+(x),\,\varphi_+(x')]_-=[\varphi_+(x),\,\varphi_-(x')]_- & t>t'\\ [\varphi_-(x),\,\varphi_-(x')]_--[\varphi_-(x),\,\varphi(x')]_-=[\varphi_+(x'),\,\varphi_-(x)]_- & t<t'\end{cases}\\ &\quad=D(x-x),\end{aligned}$$

which is identical with the definition of $D(x-x')$ given by (3·8). Thus our proof is completed. The proof of lemma II can be achieved in quite a similar manner, so that it will be unnecessary to repeat here the similar procedure.

Appendix B

First we shall derive the formula (4·5). For simplicity, we employ hereafter such an unit as to make $s=1$ and $\hbar=1$. Fourier component of $D(x)$ is then expressed as

$$D(\boldsymbol{k},\,t)=\tfrac{1}{2}k\{(N_k+1)e^{-k|t|}+N_k e^{k|t|}\}. \tag{B·1}$$

Now the Fourier transform of (4·4) is given by

$$D^*(\boldsymbol{k},\,t-t')=D(\boldsymbol{k},\,t-t')-2g'\int_0^\beta D(\boldsymbol{k},\,t-t_1)\,D(\boldsymbol{k},\,t_1-t')\,dt_1$$

$$+(2g')^2\int_0^\beta\int_0^\beta D(\boldsymbol{k},\ t-t_1)D(\boldsymbol{k},\ t_1-t_2)D(\boldsymbol{k},\ t_2-t')dt_1dt_2\cdots \qquad (B\cdot 2)$$

Although $D^*(\boldsymbol{k},\ t)$ can be evaluated by solving an integral equation

$$D^*(\boldsymbol{k},\ t)=D(\boldsymbol{k},\ t)-2g'\int_0^\beta D(\boldsymbol{k},\ t-s)D^*(\boldsymbol{k},\ s)ds, \qquad (B\cdot 3)$$

we shall follow a more direct and elementary method. A short calculation yields that

$$\int_0^\beta D(\boldsymbol{k},\ t-t_1)D(\boldsymbol{k}',\ t_1-t')dt_1=\frac{k^2}{k^2-k'^2}D(\boldsymbol{k},\ t-t')-\frac{k'^2}{k'^2-k^2}D(\boldsymbol{k}',\ t-t') \qquad (B\cdot 4)$$

which is reduced in the limit of $\boldsymbol{k}\to\boldsymbol{k}'$ to

$$\int_0^\beta D(\boldsymbol{k},\ t-t_1)D(\boldsymbol{k},\ t_1-t')dt_1=(1-\tfrac{1}{2}kd/dk)D(\boldsymbol{k},\ t-t')=\Delta_kD(\boldsymbol{k},\ t-t') \qquad (B\cdot 5)$$

where

$$\Delta_k=(1-\tfrac{1}{2}kd/dk). \qquad (B\cdot 6)$$

Using (B·5) in a repeated manner, we can put (B·2) into the form

$$D^*(\boldsymbol{k},\ t)=(1-2g'\Delta_k+(2g'\Delta_k)^2-\cdots)D(\boldsymbol{k},\ t)$$

$$=\frac{1}{1+2g'\Delta_k}D(\boldsymbol{k},\ t),$$

or

$$(1+2g'\Delta_k)D^*(\boldsymbol{k},\ t)=D(\boldsymbol{k},\ t). \qquad (B\cdot 7)$$

It is easy to solve this inhomogeneous linear differential equation of first order with a condition $\lim_{k\to\infty}D^*(\boldsymbol{k},\ t)=0$. The result is

$$D^*(\boldsymbol{k},\ t)=1/g'\int_k^\infty k^{\alpha-1}D(\boldsymbol{k}',\ t)k'^{-\alpha}dk'$$

$$=1/g'\int_1^\infty\xi^{-\alpha}D(\xi\boldsymbol{k},\ t)d\xi \qquad (B\cdot 8)$$

where

$$\alpha=(1+3g')/g'.$$

Thus (4·5) is proved. For the Fourier component of $S(x)$, the following equations are easily proved:

$$\int_0^\beta S(\boldsymbol{k},\ t-t_1)S(\boldsymbol{k}',\ t_1-t')dt_1=\frac{S(\boldsymbol{k},\ t-t')-S(\boldsymbol{k}',\ t-t')}{\varepsilon_k-\varepsilon_{k'}}, \qquad (B\cdot 9)$$

$$\int_0^\beta S(\boldsymbol{k},\ t-t_1)S(\boldsymbol{l},\ t_1-t)S(\boldsymbol{m},\ t_1-t')S(\boldsymbol{n},\ t'-t_1)dt_1$$

$$=(f_m-f_n)/(\varepsilon_l+\varepsilon_m-\varepsilon_k-\varepsilon_n)S(\boldsymbol{k},\ t-t')S(\boldsymbol{l},\ t'-t) \qquad (B\cdot 10)$$

$$-(f_k-f_l)/(\varepsilon_l+\varepsilon_m-\varepsilon_k-\varepsilon_n)S(\boldsymbol{m}, t-t')S(\boldsymbol{n}, t'-t).$$

In particular, in the limit of $\boldsymbol{k}\to\boldsymbol{k}'$, $t\to t'$ (B·9) becomes

$$\int_0^\beta S(\boldsymbol{k}, t-t_1)S(\boldsymbol{k}, t_1-t)dt_1=\frac{\partial}{\partial\varepsilon_k}S(\boldsymbol{k}, 0)=-\beta f_k(1\mp f_k). \qquad \text{(B·11)}$$

(B·9), (B·10) and (B·11) were used in evaluating the integrals C_{2A}—C_{2K} in § 6.

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