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# A two-particle Green function self-energy expansion

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Abstract. The two-particle self-energy operator is derived. The method is an extension of the Kadanoff and Baym method for the one-particle self-energy operator. The self-energy is then expanded to illustrate the similarities and differences with the one-particle case. An example is used to study the structure of the expansion. In conclusion a brief discussion of the one-particle method to derive the two-particle Green function is given.

## 1. Introduction

In certain systems the single-particle properties are not of primary interest and higher order properties of the system give the information desired. In these cases the use of single-particle perturbation techniques are not germane; however, they have proved convenient because of their calculational simplicity. Thus single-particle properties (eg single-particle energy, lifetimes, etc) have been attributed to systems which are fundamentally collective in nature.

The extension of the single-particle self-energy operator to an n particle form is of interest for these collective systems. The idea is to derive a self-energy operator which is not composed entirely of single-particle functions and in this way the character attributed to the system will not be single-particle in nature, but will describe a collective entity.

In the first section a derivation of the two-particle self-energy operator is presented. This derivation yields an iterative equation for the self-energy operator and it is noted that the expansion of this equation is a functional of a set of functions. These functions can be chosen appropriately to suit the physical conditions of the model being examined.

A discussion showing the similarities and differences of this expansion with the oneparticle expansion is then given. The special case of self-broadening of spectral lines is used to demonstrate the specialized form of the expansion.

In § 4 the extension of this technique to the four-particle Green function is made. The difficulties inherent in this analysis lead to the suggestion of an alternate method. This method uses a functional differential of the two-particle self-energy operator to generate solutions for the four-particle Green function.

The above derivations were preformed under the assumption of an initially diagonal distribution function. In using this approximation the density matrix is assumed to be separable at some arbitrary initial time. This assumption is explored in the next section and new contributions which arise from a generalized initial condition are discussed. In the conclusion, an analysis of the problems that would arise if the one-particle self-energy operator were used to generate solutions of the two-particle Green function is given.

## 1.1. Temperature Green function and the correlation function

The time-correlation function method and certain types of line broadening calculations require the evaluation of correlation functions. These functions can be generally defined as the product of two time-dependent operators A(t), B(t'), whose times are not the same, averaged over some equilibrium ensemble. Thus, the correlation function is defined as

$$\langle A(t)B(t')\rangle$$
 (1.1.1)

where the bracket will denote the average over the grand canonical ensemble. To outline the relationship between this correlation function and the Green function (GF) the occupation number representation is used. Assuming that A and B operate in the same subsystem and are single-particle operators this correlation function can be written

$$\langle A(t)B(t')\rangle = \int_{\alpha\beta\gamma\delta} A_{\alpha\beta}B_{\gamma\delta}\langle \psi_{\alpha}^{+}(t)\psi_{\beta}(t)\psi_{\gamma}^{+}(t')\psi_{\delta}(t')\rangle \qquad (1.1.2)$$

where  $A_{\alpha\beta}$  denotes the matrix element of operator A between the state denoted by  $\alpha$ and that denoted by  $\beta$ . The construction and destruction operators  $\psi_{\alpha}^{+}(t)$  and  $\psi_{\alpha}(t)$ denote the construction and destruction of a particle state characterized by  $\alpha$  at a time t. Clearly,  $\alpha$ ,  $\beta$ , etc can denote internal and external variables that are either continuous or discrete.

Now this new representation of the correlation function can be used to find the correspondence to the real-time two-particle GF,  $G^{II}$ . Then with this correspondence made, it can be shown how  $\mathscr{G}^{II}$ , the temperature Green function ( $\mathscr{GF}$ ) is related by analytic continuation to the real-time functions (Abrikosov *et al* 1961).

Defining the retarded real-time GF,  $G_{\rm R}^{\rm II}$ ,

$$\begin{aligned} G_{\mathsf{R}}^{\mathsf{II}}(\alpha\beta\gamma\delta;t,0) &= -\operatorname{i}(\langle\psi_{\alpha}^{+}(t)\psi_{\beta}(t)\psi_{\gamma}^{+}(0)\psi_{\delta}(0)\rangle \\ &-\langle\psi_{\gamma}^{+}(0)\psi_{\delta}(0)\psi_{\alpha}^{+}(t)\psi_{\beta}(t)\rangle)\Theta(t) \end{aligned}$$
(1.1.3)

where

$$\Theta(t) = \begin{cases} 1 & t > 0 \\ 0 & t < 0 \end{cases}$$

the transform can be taken. Thus

$$\int_{-\infty}^{+\infty} e^{i\omega t} G_{R}^{II}(t) dt = G_{R}^{II}(\omega)$$
$$= -i \int_{-\infty}^{+\infty} e^{i\omega t} \langle \psi_{\alpha}^{+}(t)\psi_{\beta}(t)\psi_{\gamma}^{+}\psi_{\delta} \rangle - \langle \psi_{\gamma}^{+}\psi_{\delta}\psi_{\alpha}^{+}(t)\psi_{\beta}(t) \rangle)\Theta(t) \qquad (1.1.4)$$

and the transform of the second-quantized correlation function can then be defined as

$$\langle \psi_{\alpha}^{+}(t)\psi_{\beta}(t)\psi_{\gamma}^{+}\psi_{\delta}\rangle = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{-i\omega t}J_{\alpha\beta\gamma\delta}(\omega).$$
(1.1.5)

Using the cyclic properties of the trace and the identity

$$\Theta(t) = \lim_{\epsilon \to 0^+} \frac{1}{2\pi i} \int_{-\infty}^{+\infty} d\alpha \frac{e^{i\alpha t}}{\alpha - i\epsilon}$$

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equation (1.1.4) in conjunction with (1.1.5) yields

$$G_{\mathbf{R}}^{\mathbf{II}}(\omega) = \lim_{\epsilon \to 0^+} -\frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega' \frac{J_{\alpha\beta\gamma\delta}(\omega')}{\omega' - \omega - i\epsilon} (1 - e^{-\beta\omega'}).$$
(1.1.6)

This gives the correspondence between the transformed correlation function  $J(\omega)$  and the real-time GF  $G_{R}^{II}$ , that is

$$\operatorname{Im} G_{\mathbf{R}}^{\mathbf{II}}(\omega) = -\frac{1}{2}J(\omega)(1 - e^{-\beta\omega}). \tag{1.1.7}$$

Now from equations (1.1.6) and (1.1.7) it can be demonstrated that

$$\operatorname{Re} G_{\mathbf{R}}^{\mathrm{II}}(\omega) = \frac{1}{\pi} \operatorname{P} \int_{-\infty}^{+\infty} \mathrm{d}\omega' \frac{\operatorname{Im} G^{\mathrm{II}}(\omega')}{\omega' - \omega}$$
(1.1.8)

where the P denotes the principal part of the integral. This equation indicates that the retarded function is an analytic function of the complex variable  $\omega$  in the upper halfplane (this follows from the Cauchy integral representation of analytic functions whose real and imaginary parts are related by (1.1.8)).

The function  $\mathscr{G}^{II}$ , which is defined by

$$\mathscr{G}_{c}^{II}(\alpha\beta\gamma\delta;t_{1}t_{2}) = \langle T_{t}(\psi_{\alpha}^{+}(t_{1})\psi_{\gamma}^{+}(t_{2})\psi_{\beta}(t_{1})\psi_{\delta}(t_{2})) \rangle$$

(where  $T_{\tau}$  orders the imaginary times), is related to  $G_{R}^{II}$  by

$$\mathscr{G}_{c}^{II}(\alpha\beta\gamma\delta;\omega) \rightarrow \text{analytic continuation} \rightarrow G_{R}^{II}(\alpha\beta\gamma\delta;\omega+i\epsilon)$$

if  $\omega$  is positive.

## 1.2. The equation of motion for $\mathscr{G}_{c}^{II}$

The connection has been made between the correlation function and  $\mathscr{G}_{c}^{II}$ , now a method for extracting the information in this function is necessary. In order to do this the equation of motion for an operator C acting on a system characterized by a Hamiltonian  $H_{\text{total}}$  will be used

$$i\frac{\partial}{\partial t}C_{\rm op} = [C_{\rm op}, H_{\rm total}].$$
(1.2.1)

Therefore

$$\begin{split} \mathbf{i} \frac{\partial}{\partial t_1} \mathcal{G}^{\mathrm{ll}}_{\mathbf{c}}(\alpha\beta\gamma\delta; t_1 t_2) &= \mathbf{i} \frac{\partial}{\partial t_1} (\langle \psi^+_{\alpha}(t_1)\psi_{\beta}(t_1)\psi^+_{\gamma}(t_2)\psi_{\delta}(t_2)\rangle \Theta(t_1 - t_2) \\ &+ \langle \psi^+_{\gamma}(t_2)\psi_{\delta}(t_2)\psi^+_{\alpha}(t_1)\psi_{\beta}(t_1)\rangle \Theta(t_2 - t_1)) \end{split}$$

and, since theta functions have derivatives proportional to delta functions, one obtains

$$i\frac{\partial}{\partial t_{1}}\mathscr{G}^{\mathrm{H}}(\alpha\beta\gamma\delta;t_{1}t_{2}) = \langle T_{\mathrm{r}}([\psi_{\alpha}^{+}(t_{1})\psi_{\beta}(t_{1}),H_{\mathrm{total}}]\psi_{\gamma}^{+}(t_{2})\psi_{\delta}(t_{2}))\rangle + i\delta(t_{1}-t_{2})(\langle\psi_{\alpha}^{+}(t_{1})\psi_{\beta}(t_{1})\psi_{\gamma}^{+}(t_{2})\psi_{\delta}(t_{2})\rangle - \langle\psi_{\gamma}^{+}(t_{2})\psi_{\delta}(t_{2})\psi_{\alpha}^{+}(t_{1})\psi_{\beta}(t_{1})\rangle).$$
(1.2.2)

By using commutation rules for the field operators the second term in (1.2.2) becomes

$$-\mathrm{i}(\langle \psi_{\gamma}^{+}(t_{1})\psi_{\beta}(t_{1})\rangle\delta_{\alpha\delta}-\langle \psi_{\alpha}^{+}(t_{1})\psi_{\delta}(t_{1})\rangle\delta_{\beta\gamma})\delta(t_{1}-t_{2}).$$

Then, defining the one-particle temperature Green function as

$$\mathscr{G}_{c}^{l}(\alpha\beta;t_{1}t_{2}) = -i\langle T_{c}(\psi_{\alpha}^{+}(t_{1})\psi_{\beta}(t_{1}))\rangle$$
(1.2.3)

the equation of motion becomes

$$\begin{split} & \mathrm{i}\frac{\partial}{\partial t_{1}}\mathscr{G}_{\mathbf{c}}^{\mathrm{II}}(\alpha\beta\gamma\delta;t_{1}t_{2}) + \langle T_{\mathrm{t}}([H_{\mathrm{total}},\psi_{\alpha}^{+}(t_{1})\psi_{\beta}(t_{1})]\psi_{\gamma}^{+}(t_{2})\psi_{\delta}(t_{2}))\rangle \\ & = \mathscr{G}^{\mathrm{I}}(\gamma\beta;t_{1})\delta_{\alpha\delta}\delta(t_{1}-t_{2}) - \mathscr{G}^{\mathrm{I}}(\alpha\delta;t_{1})\delta_{\beta\gamma}\delta(t_{1}-t_{2}). \end{split}$$
(1.2.4)

To calculate the equation of motion the  $H_{\text{total}}$  must be specified. For simplicity a two-component system will be used; although all of what follows can be tediously extended to any number of components. The two components will be labelled by A and B with A's subsystem being represented by the operators  $\psi^+$ ,  $\psi$  and B's subsystem being represented by the operators will have internal states and all the interactions will be present. Thus

$$H_{\text{total}} = H_{A}^{0} + H_{B}^{0} + V^{AB} + V^{AA} + V^{BB} + V^{A} + V^{B}$$
(1.2.5)

where  $H^0$  represents the free Hamiltonian and  $V^{AB}$  is the interaction potential of the superscripted subsystems. Note that the  $V^{B(A)}$  has been added and that it is a fictitious potential which acts only on the B(A) subsystem. This is a purely formal device and when the limit  $V^{B(A)} \rightarrow 0$  is taken the  $\mathscr{GF}$  returns to its usual definition.

Using the occupation number representation of  $H_{\text{total}}$  the commutator of (1.2.4) yields, if  $V^{AA}$  is symmetrized

$$\left( i\frac{\partial}{\partial t} + H^{0}_{A}(\alpha) - H^{0}_{A}(\beta) \right) \mathscr{G}^{H}_{AA}(\alpha\beta\gamma\delta; t_{1}t_{2})$$

$$+ \int d3V^{A}_{3\alpha}\mathscr{G}^{H}_{AA}(3\beta\gamma\delta; t_{1}t_{2}) - \int d3V^{A}_{\beta\beta3}\mathscr{G}^{H}_{AA}(\alpha3\gamma\delta; t_{1}t_{2})$$

$$- \int d123V^{AA}_{\beta123}\mathscr{G}^{H}_{AAA}(\alpha3\gamma\delta12; t_{1}t_{2}t_{1}) + \int d123V^{AA}_{321\alpha}\mathscr{G}^{HI}_{AAA}(3\beta\gamma\delta12; t_{1}t_{2}t_{1})$$

$$- \int d123V^{AB}_{312\alpha}\mathscr{G}^{HI}_{AAB}(3\beta\gamma\delta12; t_{1}t_{2}t_{1}) + \int d123V^{AB}_{\beta123}\mathscr{G}^{HI}_{AAB}(\alpha3\gamma\delta12; t_{1}t_{2}t_{1})$$

$$= \mathscr{G}^{I}_{A}(\gamma\beta; t_{1})\delta(t_{1}-t_{2})\delta(\alpha-\delta) - \mathscr{G}^{I}_{A}(\alpha\delta; t_{1})\delta(t_{1}-t_{2})\delta(\gamma-\beta).$$

$$(1.2.6)$$

In this equation no assumptions have been made on the form of any of the potentials and the new temperature  $\mathscr{GF}$  is a three-particle function defined by

$$\mathscr{G}_{AAB}^{III}(\alpha\beta\gamma\delta12;t_{1}t_{2}t_{1}) = \langle T_{t}(\psi_{\alpha}^{+}(t_{1})\phi_{1}^{+}(t_{1})\psi_{\gamma}^{+}(t_{2})\psi_{\beta}(t_{1})\phi_{2}(t_{1})\psi_{\delta}(t_{2}))\rangle. \quad (1.2.7)$$

The two-particle self-energy operator is introduced by redefining the terms which contain the high order Green functions. This step will help avoid the usual hierarchy of equations that would be obtained if the solution for  $\mathscr{G}^{III}$  is attempted by another equation of motion.

Thus, defining the self-energy operator by

$$\int_{0}^{-i\beta} \mathrm{d}3\,\mathrm{d}4\,\mathrm{d}t_{3}\,\Sigma_{AA}^{2}\,(\alpha\beta34;t_{1}t_{3})\mathscr{G}_{AA}^{II}(34\gamma\delta;t_{3}t_{2}) = \int\,\mathrm{d}124V_{\beta124}^{AA}\mathscr{G}_{AAA}^{II}(\alpha4\gamma\delta12;t_{1}t_{2}t_{1})$$
(1.2.8)

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with three others of similar form, gives a new equation of motion. Thus

$$\left( i\frac{\partial}{\partial t_{1}} + H^{0}_{A}(\alpha) - H^{0}_{A}(\beta) \right) \mathscr{G}^{II}_{AA}(\alpha\beta\gamma\delta; t_{1}t_{2}) + \int d3V^{A}_{3\alpha} \mathscr{G}^{II}_{AA}(3\beta\gamma\delta; t_{1}t_{2}) - \int d3V^{A}_{\beta3} \mathscr{G}^{II}_{AA}(\alpha3\gamma\delta; t_{1}t_{2}) + \int d3 d4 dt_{3} \Sigma_{\text{total}}(\alpha\beta34; t_{1}t_{3}) \mathscr{G}^{II}_{AA}(34\gamma\delta; t_{3}t_{2}) = \mathscr{G}^{I}_{A}(\gamma\beta; t_{1})\delta(t_{1}-t_{2})\delta_{\alpha\delta} - \mathscr{G}^{I}_{A}(\alpha\delta; t_{1})\delta(t_{1}-t_{2})\delta_{\gamma\beta}.$$
(1.2.9)

Here the  $\Sigma_{\text{total}}$  is the sum of all the self-energy operators of the type in (1.2.8). Hence, the left hand side is entirely dependent on  $\mathscr{G}_{AA}^{II}$  which is precisely the situation desired. The only quantity to be determined is  $\Sigma_{\text{total}}$ ; now a method will be introduced to generate solutions for this self-energy operator.

#### 1.3. The iterative equation for the self-energy operator

Now the problem is to find a form for the self-energy operator that yields a well defined expansion. For simplicity the derivation of the self-energy equation will be carried out for only the one  $\Sigma$  in equation (1.2.8). The derivation for all the self-energy operators is similar; the differences will be pointed out as the derivation proceeds.

The first step in the derivation is to rewrite the  $\mathscr{G}^{III}$  using the functional derivative (see Appendix). This gives

$$\mathscr{G}_{\mathbf{A}\mathbf{A}\mathbf{A}}^{\mathbf{I}\mathbf{I}}(\alpha\beta\gamma\delta\mathbf{1}\mathbf{2};t_{1}t_{2}t_{1}) = -\mathbf{i}\left(\mathscr{G}_{\mathbf{A}}^{\mathbf{I}}(\mathbf{1}\mathbf{2};t_{1}) - \frac{\delta}{\delta V_{\mathbf{1}\mathbf{2}}^{\mathbf{A}}(t_{1})}\right)\mathscr{G}_{\mathbf{A}\mathbf{A}}^{\mathbf{I}\mathbf{I}}(\alpha\beta\gamma\delta;t_{1}t_{2}). \quad (1.3.1)$$

Thus, yielding for (1.2.8)

$$\int_{0}^{-i\beta} d3 d4 dt_{3} \Sigma_{AA}^{2} (\alpha\beta 34; t_{1}t_{3}) \mathscr{G}_{AA}^{II} (34\gamma\delta; t_{3}t_{2})$$
  
=  $-i \int d123 V_{312\alpha}^{AA} \left( \mathscr{G}_{A}^{I} (12; t_{1}) - \frac{\delta}{\delta V_{12}^{A} (t_{1})} \right) \mathscr{G}_{AA}^{II} (3\beta\gamma\delta; t_{1}t_{2}).$  (1.3.2)

To solve this equation for  $\sum_{AA}^2$  a matrix inverse of  $\mathscr{G}_{AA}^{II}$  is defined. This definition is purely formal and the inverse will eventually be eliminated.

$$\int_{0}^{-i\beta} \mathrm{d}3\,\mathrm{d}4\,\mathrm{d}t_{3}\mathscr{G}_{\mathbf{A}\mathbf{A}}^{\mathbf{I}}(\alpha\beta34;t_{1}t_{3})\mathscr{G}_{\mathbf{A}\mathbf{A}}^{\mathbf{I}_{1}-1}(\gamma\delta34;t_{2}t_{3}) = \delta_{\gamma\alpha}\delta_{\beta\delta}\delta(t_{1}-t_{2}). \quad (1.3.3)$$

Operating on the right of equation (1.3.2) with  $\mathscr{G}_{AA}^{II-1}(56\gamma\delta; t_3t_2)$  and integrating over 5, 6 and  $t_2$  yields

$$\Sigma_{AA}^{2} (\alpha \beta \gamma \delta; t_{1}t_{2}) = -i \int d1 \ d2 V_{\gamma 12\alpha}^{AA} \mathscr{G}_{A}^{I} (12; t_{1}) \delta(t_{1} - t_{2}) \delta_{\beta \delta}$$
$$- \int_{0}^{-i\beta} d(1-5) \ dt_{3} V_{312\alpha}^{AA} \mathscr{G}_{AA}^{II} (3\beta 45; t_{1}t_{3})$$
$$\times \frac{\delta}{\delta V_{12}^{A}(t_{1})} \mathscr{G}_{AA}^{II-1} (\gamma \delta 45; t_{2}t_{3}).$$
(1.3.4)

Here the fact that the functional derivative of equation (1.3.3) is equal to zero was used, and the convention that the indices  $\alpha\beta\gamma\delta$  are not variable is introduced.

The only term in (1.3.4) which is not known is the functional derivative of the inverse  $\mathscr{G}^{II-1}$ . This can now be expressed in terms of the self-energy operators so that the expansion will be closed in the self-energy operator.

Returning to the equation of motion (1.2.9) and operating with the appropriate inverse yields

$$\left( i\frac{\partial}{\partial t_1} + H^0_{\mathsf{A}}(\alpha) - H^0_{\mathsf{A}}(\beta) \right) \delta_{\alpha\gamma} \delta_{\beta\delta} \delta(t_1 - t_2) + V^{\mathsf{A}}_{\gamma\alpha}(t_1) \delta_{\beta\delta} \delta(t_1 - t_2) - V^{\mathsf{A}}_{\beta\delta}(t_1) \delta_{\alpha\gamma} \delta(t_1 - t_2) + \Sigma_{\text{total}} \left( \alpha \beta \gamma \delta ; t_1 t_2 \right) = \mathscr{G}^{11-1}(\gamma \delta \beta \alpha ; t_2 t_1) (n(\beta) - n(\alpha)).$$

$$(1.3.5)$$

Here the inhomogeneous term has been evaluated according to the condition that the subsystems are initially unperturbed. The  $n(\alpha)$  represents the occupation number of the state denoted by the label  $\alpha$  (DeBoer and Uhlenbeck 1965). This approximation will be discussed in § 5. Hence the functional derivative of this equation produces

$$\delta_{\beta\delta}\delta_{1\gamma}\delta_{2\alpha}\delta(t_1-t_3)\delta(t_1-t_2) - \delta_{\gamma\alpha}\delta_{1\beta}\delta_{2\delta}\delta(t_1-t_3)\delta(t_1-t_2) + \frac{\delta\sum_{\text{total}} (\alpha\beta\gamma\delta; t_1t_2)}{\delta V_{12}^A(t_3)}$$
$$= \frac{\delta\mathcal{G}_{AA}^{\text{ll}-1}(\gamma\delta\beta\alpha; t_2t_1)}{\delta V_{12}^A(t_3)}(n(\beta)-n(\alpha)). \tag{1.3.6}$$

So that

$$\begin{split} \Sigma_{AA}^{2} \left( \alpha \beta \gamma \delta ; t_{1} t_{2} \right) &= -i \int d1 \ d2 V_{\gamma 12\alpha}^{AA} \mathscr{G}_{A}^{I} (12 ; t_{1}) \delta(t_{1} - t_{2}) \delta_{\beta \delta} \\ &- \int d1 \ d2 V_{\gamma 12\alpha}^{AA} \frac{\mathscr{G}_{AA}^{II} (1\beta \delta 2 ; t_{1} t_{2})}{n(2) - n(\delta)} \delta(t_{1} - t_{2}) \\ &+ \int d1 \ d2 V_{12\delta \alpha}^{AA} \frac{\mathscr{G}_{AA}^{II} (1\beta 2\gamma ; t_{1} t_{2})}{n(\gamma) - n(2)} \delta(t_{1} - t_{2}) \\ &- \int_{0}^{-i\beta} d(1 - 5) \ dt_{3} V_{312\alpha}^{AA} \frac{\mathscr{G}_{AA}^{II} (3\beta 45 ; t_{1} t_{3})}{n(5) - n(4)} \\ &\times \frac{\delta}{\delta V_{12}^{A} (t_{1})} \Sigma_{\text{total}} (45\gamma \delta ; t_{2} t_{3}). \end{split}$$
(1.3.7)

This is the equation of interest. The first terms on the right hand side and the last term compose the self-energy operator for the interactions  $V^{AB}$ . Thus

$$\Sigma_{AB}^{2} (\alpha \beta \gamma \delta; t_{1}t_{2}) = -i \int d1 \ d2 V_{\gamma 1 2 \alpha}^{AB} \mathscr{G}_{B}^{I}(12; t_{1}) \delta(t_{1} - t_{2}) \delta_{\beta \delta}$$
$$- \int_{0}^{-i\beta} d(1-5) \ dt_{3} V_{312 \alpha}^{AB} \frac{\mathscr{G}_{AA}^{II}(3\beta 45; t_{1}t_{3})}{n(5) - n(4)}$$
$$\times \frac{\delta}{\delta V_{12}^{B}(t_{1})} \Sigma_{\text{total}} (45\gamma \delta; t_{2}t_{3}).$$
(1.3.8)

The difference in the two is the exclusion of the second and third terms in (1.3.7).

## 2. The self-energy contributions

Now that the equations for the self-energy operators have been derived some general properties of these equations can be studied. This is most easily done by examining equations (1.3.7) and (1.3.8).

First it is obvious that in the event that interactions were not present in the system  $\Sigma_{total}$  would be identically zero. This gives rise to the noninteracting two-particle Green function, not the product of two single-particle Green functions. The difference between the  $\mathscr{G}_0^{II}$  and  $\mathscr{G}^{I}\mathscr{G}^{I}$  is important because it is an indication of the difference between the usual graphical expansions (Ross 1966) of the two-particle Green function and the method used here. For in most graphical expansions the quantity of interest is the single-particle Green function and its self-energy operator, which modifies the single-particle properties of the system.

The initial term of the self-energy equation is a Hartree-type term. It can be represented graphically as



where the broken line is the interaction and the full line is a single-particle Green function. The squares are the delta functions of the states in (1.3.7) and (1.3.8). This term is local in space and therefore will affect only one of the two members of the two-particle function. There are four of these terms in  $\Sigma_{total}$ , two for each of the interactions possible.

In equation (1.3.7), the self-energy equation arising from the interaction  $V^{AA}$  contains an additional term. In the case of a one-particle Green function and its self-energy operator, this contribution would be the exchange part of the Hartree–Fock approximation. In the two-particle case this 'exchange' contribution appears not as a  $V^{AA}G^{I}_{A}$  but as a  $V^{AA}G^{II}_{AA}$ . Obviously this exchange term is the only structural difference between the identical and nonidentical particle self-energy expansions, (1.3.7) and (1.3.8) respectively. Moreover, if  $\Sigma_{total}$  were iterated repeatedly these two contributions arising from the two subsystems A and B would mix. However, the contributions arising from the exchange term ( $V^{AA}G^{II}_{AA}$ ) would not mix with the Hartree or direct terms.

Upon a single iteration the terms of the Hartree type yield in a matrix notation

$$\Sigma \simeq V V \mathscr{G}^{\mathrm{II}} \mathscr{G}^{\mathrm{II}}.$$
(2.2)

These are now analysed by treating different subsystems separately. In the case of the B subsystems perturbations (2.2) becomes

$$V^{AB}V^{AB}\mathscr{G}^{II}_{AA}\mathscr{G}^{II}_{BB}.$$
(2.3)

This represents a generalization of the usual Born approximation defined in the oneparticle case by

$$V^{AB}V^{AB}\mathcal{G}^{I}_{A}\mathcal{G}^{I}_{B}\mathcal{G}^{I}_{B}.$$

$$(2.4)$$

This form also arises when the Hartree terms from subsystem A are iterated. In the two-particle self-energy operator these terms are not constrained to the case where the

 $\mathscr{G}^{\mu}$  is approximated by two single-particle Green functions. Indeed, if this were the case the usefulness of this two-particle technique would be restricted.

The substitution of the second term in equation (1.3.7) into the functional derivative  $\delta \Sigma / \delta V^A$  leads to an integral containing a three-particle function. This is not present in the first iteration of the self-energy operators of the B subsystem. This exchange term can be cast into the form of the generalized Born approximation by writing the three-particle function to lowest order in  $\mathscr{G}^{II}$ . This is done by using the relationship

$$\frac{\delta \mathscr{G}_{\mathbf{A}\mathbf{A}}^{\mathrm{II}}(\alpha\beta\gamma\delta;t_{1}t_{2})}{\delta V_{12}^{\mathrm{A}}(t_{3})} = \int_{0}^{-i\beta} \mathrm{d}t_{4} \, \mathrm{d}t_{5} \, \mathrm{d}(1-4) \mathscr{G}_{\mathbf{A}\mathbf{A}}^{\mathrm{II}}(\alpha\beta34;t_{1}t_{4}) \\ \times \frac{\delta \mathscr{G}_{\mathbf{A}\mathbf{A}}^{\mathrm{II}-1}(3412;t_{4}t_{5})}{\delta V_{12}^{\mathrm{A}}(t_{3})} \mathscr{G}_{\mathbf{A}\mathbf{A}}^{\mathrm{II}}(\gamma\delta12;t_{2}t_{5}).$$
(2.5)

Examining the functional derivative of the inverse given in equation (1.3.6), the lowest order contribution to  $\delta \mathscr{G}^{II}/\delta V$  using  $\mathscr{G}^{II}$  as an expansion parameter is

$$\frac{\delta \mathscr{G}_{AA}^{II}(\alpha\beta\gamma\delta;t_{1}t_{2})}{\delta V_{12}^{A}(t_{3})} = \int d3 \mathscr{G}_{AA}^{II}(\alpha\beta23;t_{1}t_{3}) \mathscr{G}_{AA}^{II}(\gamma\delta13;t_{2}t_{3})$$
(2.6)

yielding for the self-energy

$$V^{AA}V^{AA}\mathcal{G}^{II}_{AA}\mathcal{G}^{II}_{AA}\mathcal{G}^{II}_{AA}.$$
(2.7)

This along with the Hartree iterations form the first Born approximation for the A subsystem.

In the discussion above no reference was made to the dependence of the two-particle Green functions on the potentials. In fact the self-energy operator is being expanded as a functional of more than the coupling constant. Indeed, for the cases in which the B subsystem's perturbations of A are considered, the mutual interactions of the particles in B are not in any way affected by the expansion techniques. This can be an important point if different situations prevail in the two systems. In particular, it is not necessary to specify an approximation for the particles in B before a calculation is carried out for the A subsystem. This is not the case in some graphical techniques. For in these graphical techniques the approximation for the B subsystem precedes the necessary calculations, and subsequent corrections require a completely new calculation.

The technique derived in this paper also allows freedom in choosing the expansion parameters. The choice of the  $\mathscr{G}^{II}$  and the coupling constant, as is done above, is not the only possibility. The higher order Green functions could be used to generate an expansion in terms of the fluctuations. Also, the use of the coupling constant and the noninteracting two-particle  $\mathscr{GF}$  will allow the comparison of this procedure with the usual coupling constant expansions.

## 3. Comment on the structure of $\Sigma_{total}$

An interesting point arises from the structure of the self-energy expansion in the case where only one species of particles is present. In this case the direct and exchange terms are distinct and to third order in the two-particle Green function they are not mixed. (Mixing of these two contributions would not occur at all if the higher order Green functions were chosen as the expansion parameters. However, by choosing the two-particle function an extra term  $\delta \Sigma / \delta V^A$  is introduced (see equations (2.5) and (1.3.6)).)

This situation is relevant to the self-broadening of spectral lines. Here the twoparticle Green function can be related to the dipole-dipole correlation function and its solution provides the lineshape profile. In the literature Ben-Rueven (1966) and Di Giacomo (1965) have formulated theories for perturbations of a spectral emitter (absorber). In both papers the assertation has been made that by symmetrizing the potentials a foreign gas broadening formulation will properly describe self-broadening.

More recently Bezzerides (1967) has formulated a theory of self-broadening that included both exchange and direct interactions. There a formalism is developed for the use of a T matrix approximation. Both direct and exchange contributions are mixed at the outset by the use of a symmetrized T matrix (Kadanoff and Baym 1961 and 1962).

Bezzerides discusses contributions to the two-particle Green function which are valid only to third order in  $\mathscr{G}_{AA}^{II}$  in the self-energy operator. However, these contributions are of the same graphical form as those that would arise if a foreign gas were perturbing the emitter (Ross 1966). Moreover, if the foreign gas particles had an energy level that was degenerate with the excited level of the emitter the contributions arising from Bezzerides 'exchange' scattering could prove dominant. Hence, this type of 'exchange' does not intrinsically depend on the statistics of the particles.

This pathological example is used to illustrate that the formalism employed by Bezzerides does not correctly deal with the distinguishability of the particles. Indeed, in this example the self- and foreign-broadening would differ only by symmetrizations of the functions concerned.

Now examining the structure of the self-energy operator a completely distinct set of terms arising from self-broadening is found. This set of terms implies that the exchange contributions are quite distinct from those connected with direct interactions. The fact that the two-particle Green function is of interest complicates the seemingly simple task of accounting for the exchange process. That is, in the case of a one-particle Green function to first order in the potential the proper symmetrization of the potential correctly changes the Hartree approximation to the Hartree–Fock (Kadanoff and Baym 1962). However, the self-energy operator for the two-particle function gives rise to exchange terms that are of the form  $V^{AA} \mathscr{G}^{II}_{AA}$ . Hence no possible symmetrization could be used to obtain this term from the Hartree term  $V^{AA} \mathscr{G}^{I}_{A}$ .

Therefore, the broadening due to identical particles will be different than that due to foreign gases and this distinction formally exists no matter what the character of the system of interest, that is, density, temperature etc.

#### 4. The four-particle Green function

The interesting correlation functions are not always the two-particle type. The reason that the two-particle Green function is examined above is that single-particle operators make up the correlation function. If, however, the correlation function under inspection were composed of two-particle operators, the four-particle Green function would be of interest. Illustrating the self-energy expansion technique for the four-particle Green function will serve to expose some of the difficulties in generalizing these techniques further. The equation of motion for the system of identical particles with an interaction potential  $V^{AA}$  is

$$\begin{split} \mathbf{i} \frac{\partial}{\partial t_{1}} \mathscr{G}^{\mathbf{IV}}[\alpha, 1] &= \int \mathrm{d} 5(H_{5\beta} \mathscr{G}^{\mathbf{IV}}(5\alpha\gamma\delta; 1] + H_{5\alpha} \mathscr{G}^{\mathbf{IV}}(5\beta\gamma\delta; 1] \\ &- H_{\delta 5} \mathscr{G}^{\mathbf{IV}}(\alpha\beta\gamma5; 1] - H_{\gamma 5} \mathscr{G}^{\mathbf{IV}}(\alpha\beta\delta5; 1]) \\ &+ \int \mathrm{d} 567(V_{\delta 567} \mathscr{G}^{\mathbf{V}}(\alpha\beta2\gamma3; 1] + V_{56\beta7} \mathscr{G}^{\mathbf{V}}(\alpha567\gamma\delta; 1] \\ &- V_{5\gamma67} \mathscr{G}^{\mathbf{V}}(\alpha\beta5\delta67; 1] - V_{567\alpha} \mathscr{G}^{\mathbf{V}}(567\beta\gamma\delta; 1]) + I. \end{split}$$

$$(4.1.1)$$

where H represents the free Hamiltonian and the fictitious external potential  $V^A$ . The definitions of the Green functions are

$$\mathscr{G}^{\text{IV}}(\alpha\beta\gamma\delta; 1234; t_{1}t_{2}) = \langle T_{\mathfrak{r}}(\psi_{\alpha}^{+}(t_{1})\psi_{\beta}^{+}(t_{1})\psi_{1}^{+}(t_{2})\psi_{2}^{+}(t_{2})\psi_{\gamma}(t_{1})\psi_{\delta}(t_{1})\psi_{3}(t_{2})\psi_{4}(t_{2}))\rangle \qquad (4.1.2a)$$
  
$$\mathscr{G}^{\text{V}}(56\beta7\gamma\delta, 1234; t_{1}t_{2}) = \langle T_{\mathfrak{r}}(\psi_{\gamma}^{+}(t_{1})\psi_{\beta}^{+}(t_{1})\psi_{\beta}^{+}(t_{1})\psi_{1}^{+}(t_{2})\psi_{2}^{+}(t_{2})\psi_{\gamma}(t_{1})$$
  
$$\times \psi_{\gamma}(t_{1})\psi_{\delta}(t_{1})\psi_{3}(t_{2})\psi_{4}(t_{2}))\rangle \qquad (4.1.2b)$$

with  $\alpha\beta\gamma\delta$ ;  $t_1$  and 1234;  $t_2$  being denoted by [ $\alpha$  and 1], respectively.

Now by assuming the distribution is initially diagonal I can be written as

$$I = \delta[\alpha, 1](\langle (n_{\beta}+1)(n_{\delta}+1)(n_{\gamma}+1) \rangle + \langle (n_{\alpha}+1)(n_{\delta}+1)n_{\gamma} \rangle$$
$$- \langle (n_{\alpha}+1)(n_{\beta}+1)n_{\delta} \rangle - \langle (n_{\alpha}+1)(n_{\beta}+1)(n_{\gamma}+1) \rangle)$$
$$= \delta[\alpha, 1]f(\alpha).$$
(4.1.3)

Following the same procedure as outlined in § 1 for the two-particle case, we define and solve for the self-energy operator. The results are, with [A = A, B, C, D; t']

$$\begin{split} \Sigma^{1}\left[\alpha,A\right] &= \mathrm{i} \int \mathrm{d} 67 V_{A67\alpha} \mathscr{G}^{\mathrm{II}}(67;t') \delta_{\beta B} \delta_{\gamma C} \delta_{\delta D} \delta(t_{1}-t') \\ &+ \int \mathrm{d} 57 (\overline{\mathscr{G}}^{\mathrm{IV}}(5\beta\gamma\delta; 6C\beta A;t_{1}t') V_{56D\alpha} \\ &+ \overline{\mathscr{G}}^{\mathrm{IV}}(5\beta\gamma\delta; D6BA;t_{1}t') V_{56C\alpha} \\ &- \overline{\mathscr{G}}^{\mathrm{IV}}(5\beta\gamma\delta; DC7A;t_{1}t') V_{D\beta7\alpha} - \overline{\mathscr{G}}^{\mathrm{IV}}(5\beta\gamma\delta; DCB7;t_{1}t') V_{5A7\alpha}) \\ &+ \int \mathrm{d}(1-7) \, \mathrm{d} t_{2} V_{567\alpha} \overline{\mathscr{G}}^{\mathrm{IV}}(5\beta\gamma\delta;1] \frac{\delta}{\delta V_{67}(t_{1})} \Sigma_{\mathrm{total}}\left[1,A\right] \end{split}$$

$$(4.1.4)$$

where

$$\overline{\mathscr{G}}^{\mathrm{IV}}[\alpha,1] = \frac{\mathscr{G}^{\mathrm{IV}}[\alpha,1]}{f[1]}$$

and  $\Sigma_{total}$  is defined by the equation of motion.

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$$i\frac{\partial}{\partial t_{1}}\overline{\mathscr{G}^{IV}}[\alpha, 1] - \int d5(H_{5\beta}\overline{\mathscr{G}^{IV}}(5\alpha\gamma\delta; 1] + H_{5\alpha}\overline{\mathscr{G}^{IV}}(5\beta\gamma\delta; 1] - H_{\delta5}\overline{\mathscr{G}^{IV}}(\alpha\beta\gamma5; 1] - H_{\gamma5}\overline{\mathscr{G}^{IV}}(\alpha\beta\delta5; 1]) + \int dA] \Sigma_{\text{total}}[\alpha, A]\overline{\mathscr{G}^{IV}}[A, 1] = \delta[\alpha, 1].$$
(4.1.5)

In equation (4.1.4) the first term is the typical Hartree term; this will arise in all orders if the potential is a two-body operator. The next four terms are the effects of the perturbations that occur when similar particles interact. The iterations are straight forward and they provide results similar in structure to the two-particle self-energy operator. It should be noted that the interpretation of these terms is made exceedingly difficult due to the complexity of the four-particle Green function  $\mathscr{G}_{4}^{N}$ .

#### 4.1. Alternative method

An alternative method can be employed. Since a four-point (body or particle) fictitious potential can be introduced to the two-particle Green function, a self-energy operator that is a function of this new external potential can be derived. The derivation follows § 1. In matrix notation

$$(\mathscr{G}_{0}^{\mathrm{II}}(U_{12}) - \Sigma_{\mathrm{total}}(U_{12}, U_{1234}))\widetilde{\mathscr{G}}^{\mathrm{II}} = I.$$

Now expanding the  $\Sigma_{\text{total}}$  to the required approximation by using  $\mathscr{G}^{\text{II}}$  as an expansion parameter, a self-energy which is a function of  $V, \mathscr{G}^{\text{II}}, U_{1234}^{\text{ext}}$ ,  $U_{1234}^{\text{ext}}$  is obtained. Now taking the limit as  $U_{12}^{\text{ext}}$  goes to zero and functionally differentiating the resulting two-particle Green function by  $U_{1234}^{\text{ext}}$  an equation for the four-particle function is obtained

$$\mathcal{G}^{\mathrm{IV}} = \mathcal{G}^{\mathrm{II}} \mathcal{G}^{\mathrm{II}} - \mathcal{G}^{\mathrm{II}} \mathcal{G}^{\mathrm{II}} \frac{\partial \Sigma_{\mathrm{total}}}{\partial \mathcal{G}^{\mathrm{II}}} \mathcal{G}^{\mathrm{II}} \mathcal{G}^{\mathrm{II}} + \mathcal{G}^{\mathrm{II}} \mathcal{G}^{\mathrm{II}} \frac{\partial \Sigma_{\mathrm{total}}}{\partial \mathcal{G}^{\mathrm{II}}} \mathcal{G}^{\mathrm{IV}}.$$
(4.2.2)

Here a generalized chain rule for the functional derivative was used. This equation is closed in  $\mathscr{G}^{IV}$ , under the assumption that the two-particle Green function can be calculated.

Thus, by being able to approximate a self-energy operator for the two-particle system, solutions for the four-particle Green function can be generated. This last approach is especially useful in the cases of higher order Green functions when intuition will not be as helpful as in the lower order cases.

## 5. Initial condition

We have presented the equations of motion using a system that is not initially correlated. This assumption is similar to the condition of initially random phases (Van Hove 1957) and diagonality (Zwanzig 1961) used in the derivation of the master equation.

The inhomogeneous terms contain the explicit contribution of the initial state of the system (see the left hand side of equation (1.2.9)). However, examination of the equations of motion shows that replacing the full Hamiltonian in the density matrix not only effects the inhomogeneous term but *all* the averaged quantities. To discuss these contributions a generalized self-energy operator can be derived.

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The derivation of the equation of motion with generalized initial conditions follows in the same way as the derivation in §2. However, to arrive at an equation for the self-energy operator, the inverse inhomogeneous term  $f^{-1}$  is defined by the equation

$$\int d12f^{-1}(1234)f(1256) = \delta_{35}\delta_{64}$$

where f is the unapproximated inhomogeneous term in equation (1.2.9). With this the equation for  $\sum_{AA}^{2}$  can be written

$$\Sigma_{AA}^{2}(\alpha\beta\gamma\delta;t_{1}t_{2}) = \Sigma_{AA}^{2}(\alpha\beta\gamma\delta;t_{1}t_{2};f(V^{A}=0)) + \Sigma_{AA}^{2}(\alpha\beta\gamma\delta;t_{1}t_{2};f(V^{A})) - \int_{0}^{-i\beta} dt_{3} d(1-4)V_{512\alpha}^{AA}\mathscr{G}_{AA}^{II}(5\beta67;t_{1}t_{3}) \times f^{-1}(8967)\frac{\delta f(89,34)}{\delta V_{12}^{A}(t_{1})}\mathscr{G}_{AA}^{II-1}(\gamma\delta34;t_{2}t_{3}).$$
(5.1)

Here  $\sum_{AA}^{2} (f(V^{A} = 0))$  is of the same form as  $\sum_{AA}^{2}$  of equation (1.3.7) without the diagonalization of f, but with  $V^{A}$  the external potential in f set equal to zero. The  $\sum_{AA}^{2} (f(V^{A} = 0))$ is also of the same form as (1.3.7); however, it is understood that this term contributes only to the first iteration by functional differentiation of  $f(V^{A})$ . With this prescription the self-energy operator becomes separable into two parts, one which depends on the dynamics of the system, that is  $\sum_{AA}^{2} (f(V^{A} = 0))$ , and a part which depends on the initial condition, the second and third terms in equation (5.1).

The separation of the expansion into these two parts can be interpreted in the following manner. The processes which influence the  $\mathscr{G}^{II}$  can be split into those which start at t = 0 and those which start at later times t > 0. Those which do start at t = 0 contribute directly to the second and third terms of (5.1). In the second case the 'collisional' nature of these contributions will be described by  $\sum_{AA}^2 (f(V^A = 0))$ . Note, that the initial condition will affect the terms in  $\sum_{AA}^2 (f(V^A = 0))$  through its functional dependence on the initial distribution.

The choice of initial condition used in §§ 2 and 3 is analogous to the condition used in the calculation of transport coefficients (eg Kadanoff and Baym 1962). Specifically, the choice is that at some time, say t > 0, the perturbations are turned on, but the distribution at t = 0 is described by an equilibrium ensemble. With this choice equation (1.2.9) was derived. However, additional contributions will arise from the same choice of distributions in the generalized regime. Indeed, simple calculations show that these additional terms are not identically zero.

The problem then is to find the effects of these extra terms. Examination of the self-energy equation shows that the terms that arise from  $\sum_{AA}^{2}(f(V^{A}))$  will be of higher order in  $\mathscr{G}^{II}$  than the terms of the  $\sum_{AA}^{2}(f(V^{A} = 0))$  which were discussed above. The contribution from the last term in equation (5.1) is not to be grouped with the 'dynamic' part of the solution for  $\mathscr{G}^{II}$ . This is checked by substituting the  $\sum_{AA}^{2}$  of equation (5.1) into the equation of motion and using the relationship (1.3.3). Then these terms will contribute to the inhomogeneous part and act as 'driving' terms (Bezzerides 1969).

The only one of these new contributions that is of the same order as those discussed in the previous sections arises from the lowest order in the inhomogeneous term correction, that is

$$-\mathrm{i}\int \frac{\mathrm{d}\omega_1}{2\pi}\mathrm{d}[1-4]V^{\mathrm{A}\mathrm{A}}\mathscr{G}^{\mathrm{II}}f^{-1}\mathscr{G}^{\mathrm{II}}.$$

The effect of this term can be estimated when the  $\mathscr{G}^{II}$  are approximated by their unperturbed values. Then the analytic continuations provide the total inhomogeneous term and in the case of a two-level system one obtains

$$n_{(1)} - n_{(0)} \left( 1 - \frac{V_{0101}^{AA}}{\omega - 2\omega_{10}} (n(\omega - \omega_{10}) - n(\omega_{10})) \right)$$
(5.2)

with  $n(\omega_1) = 1/(e^{\beta\omega_1} - 1)$ . Where 1,0 designate the two levels with the energies  $\omega_1$ and  $\omega_0$ , respectively. A calculation using a hydrogen atom with  $\omega_{10}$  being the Lyman  $\alpha$  transition, shows that the correction term is negligible, (ie six orders of magnitude smaller than the original inhomogeneous term) except in a region close to the resonance  $\omega = \omega_{10}$ . However, in this region the assumption of unperturbed energies, manifested by using zeroth order  $\mathscr{G}^{II}$ , breaks down. In fact the addition of perturbations in the  $\mathscr{G}^{II}$  will make this term small for all frequencies. Thus the initial condition chosen in § 2 and used in § 3 will be justified when the system is close to equilibrium. However, these terms will not necessarily be small for all conditions. For instance, this would be the case when the atoms in a plasma are at a temperature low compared to that of the charged perturbers. Then the second term in equation (5.2) will give rise to the absorption (or emission) of radiation in the region of the resonance frequency.

## 6. Conclusion

The method examined above is useful in those cases where two-particle or higher correlations are of primary interest. However, the method outlined in §4.2 as an alternative to generating a four-particle Green function can be used to obtain the two-particle Green function and this method has been used previously (Kadanoff and Baym 1961). In this way, approximation of the single-particle self-energy operator and the subsequent functional differentiation of the one-particle Green function yields an equation for the two-particle Green function.

This method contains certain difficulties, essentially because the lower order oneparticle function is used to generate the two-particle function  $\mathscr{G}^{II}$  (Lee 1970). First, the self-energy expansion when functionally differentiated contains terms which are not consistent with a two-particle expansion. These terms can not be neglected by introducing a different set of expansion parameters because they arise in the lowest order. For example, in the case of subsystem B perturbing A a term  $\mathscr{G}^{II}_{AB}$  arises. This introduces a new function that is not one of the original expansion parameters and can not be expressed as a function of these original parameters. That is,  $\mathscr{G}^{II}_{AB}$  is not a functional of  $\mathscr{G}^{II}_{BA}$  or  $\mathscr{G}^{II}_{BB}$ .

Second, the functional differentiation introduces an extraneous time variable, and if the equation of motion is then transformed to frequency space this gives rise to an extraneous frequency. In order to analyse the Green function an integration over this frequency is required. The integration, however, requires the detailed knowledge of the singularities of a function similar to (1.4.7) and this is a very difficult problem.

Therefore, when two-particle correlations are of interest this method provides a viable approach. The use of this self-energy expansion allows the direct examination of the two-body attributes of the system and in this way the collective effects of the system, energy spectrum, lifetime, etc are directly calculated.

The usefulness of this two-particle self-energy expansion can be illustrated by concrete examples. In a following paper (Lee 1972) an application of this method will be used to calculate the lineshape profile for spectral line-broadening in a plasma.

## Appendix 1

In this Appendix the method of functional differentiation will be examined. In order to generate (1.3.1), the two-particle temperature Green function will be used

$$\mathscr{G}_{AA}^{II}(\alpha\beta\gamma\delta;t_{1}t_{2}) = \langle T_{\tau}(\psi_{\alpha}^{+}(t_{1})\psi_{\gamma}^{+}(t_{2})\psi_{\beta}(t_{1})\psi_{\delta}(t_{2}))\rangle.$$
(A.1)

Now writing this in interaction representation with the fictitious potential separated out, one obtains

$$\mathscr{G}_{AA}^{II}(\alpha\beta\gamma\delta;t_{1}t_{2}) = \frac{\langle T_{\tau}(\bar{\psi}_{z}^{+}(t_{1})\bar{\psi}_{\gamma}^{+}(t_{2})\bar{\psi}_{\beta}(t_{1})\bar{\psi}_{\delta}(t_{2})\mathscr{S}_{(\beta)}^{A})\rangle}{\langle \mathscr{S}_{(\beta)}^{A}\rangle}$$
(A.2)

where the time dependence of the interaction representation field operators is determined by  $H = H_A^0 + H_B^0 + V^{BB} + V^{AA} + V^{AB} + V^B$ . Here the imaginary time domain allows the inclusion of all the  $V^A$  into one  $\mathscr{G}^A_{(\beta)}$  matrix. This matrix is given by

$$\mathscr{S}_{(\beta)}^{A} = T_{\tau} \exp\left(-i \int_{0}^{-i\beta} dt \, d1 \, d2 V_{12}^{A} \overline{\psi}_{1}^{+}(t) \overline{\psi}_{2}(t)\right). \tag{A.3}$$

Varying (A.2) with respect to  $V^{A}$  yields

$$\begin{split} \delta\mathscr{G}_{\mathbf{A}\mathbf{A}}^{\mathbf{II}}(\alpha\beta\gamma\delta;t_{1}t_{2}) &= \delta \bigg(\frac{1}{\langle\mathscr{S}_{(\beta)}^{\mathbf{A}}\rangle}\bigg) \langle T_{\mathfrak{r}}(\overline{\psi}_{\alpha}^{+}(t_{1})\overline{\psi}_{\gamma}^{+}(t_{2})\overline{\psi}_{\beta}(t_{1})\overline{\psi}_{\delta}(t_{2}))\rangle \\ &+ \langle T_{\mathfrak{r}}(\overline{\psi}_{\alpha}^{+}(t_{1})\overline{\psi}_{\gamma}^{+}(t_{2})\overline{\psi}_{\beta}(t_{1})\overline{\psi}_{\delta}(t_{1})\delta\mathscr{S}_{(\beta)}^{\mathbf{A}})\rangle \langle \mathscr{S}_{(\beta)}^{\mathbf{A}}\rangle^{-1}. \end{split}$$

Evaluating the first variation on the right

$$\delta\left(\frac{1}{\langle \mathscr{S}^{A}_{(\beta)} \rangle}\right) = -\frac{\langle \delta \mathscr{S}^{A}_{(\beta)} \rangle}{\langle \mathscr{S}^{A}_{(\beta)} \rangle^{2}}$$
(A.4)

and calculating  $\delta \mathscr{G}^{\mathsf{A}}_{(\beta)}$  one obtains

$$\delta \mathscr{S}^{\mathbf{A}}_{(\beta)} = \left( -i \int_{0}^{-i\beta} d1 \, d2 \, dt_1 \overline{\psi}^+_1(t_1) \overline{\psi}_2(t_1) \delta V^{\mathbf{A}}_{12}(t_1) \right) \mathscr{S}^{\mathbf{A}}_{(\beta)}. \tag{A.5}$$

Now using the fact that

$$\frac{\delta V_{12}^{A}(t_{1})}{\delta V_{34}^{A}(t_{2})} = \delta_{12}\delta_{34}\delta(t_{1} - t_{2})$$

the functional derivative can then be obtained. Thus

$$\frac{\delta \mathcal{G}_{AA}^{II}}{\delta V_{12}^{A}(t_{3})} (\alpha \beta \gamma \delta; t_{1}t_{2}) = i \frac{\langle T_{t}(\overline{\psi}_{\alpha}^{+}(t_{1})\overline{\psi}_{\gamma}^{+}(t_{2})\overline{\psi}_{\beta}(t_{1})\overline{\psi}_{\delta}(t_{2})\mathcal{S}_{(\beta)}^{A}) \rangle}{\langle \mathcal{S}_{(\beta)}^{A} \rangle} \frac{\langle T_{t}(\overline{\psi}_{1}^{+}(t_{3})\overline{\psi}_{2}(t_{3})\mathcal{S}_{(\beta)}^{A}) \rangle}{\langle \mathcal{S}_{(\beta)}^{A} \rangle} - i \frac{\langle T_{t}(\overline{\psi}_{\alpha}^{+}(t_{1})\overline{\psi}_{1}^{+}(t_{1})\overline{\psi}_{\gamma}^{+}(t_{2})\overline{\psi}_{\beta}(t_{1})\overline{\psi}_{2}(t_{1})\overline{\psi}_{\delta}(t_{2})\mathcal{S}_{(\beta)}^{A}) \rangle}{\langle \mathcal{S}_{(\beta)}^{A} \rangle}.$$

Recalling the definitions of the various Green functions, the functional derivative yields

$$\frac{\delta \mathscr{G}_{AA}^{II}(\alpha\beta\gamma\delta;t_{1}t_{2})}{\delta V_{12}^{A}(t_{3})} = \mathscr{G}_{AA}^{II}(\alpha\beta\gamma\delta;t_{1}t_{2})\mathscr{G}_{A}^{I}(12;t_{3}) - \mathscr{G}_{AAA}^{III}(\alpha\beta\gamma\delta12;t_{1}t_{2}t_{1}).$$
(A.7)

This, when solved for  $\mathscr{G}^{III}$ , gives the result desired.

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