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Spectral functions and Green's functions: A critique[§]

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Abstract. The various relations linking the spectral functions and the Green's functions e.g., $J_{AB}(\varepsilon) = [\mathrm{Im}\, G^R_{AB}(\varepsilon)]/[1+\gamma e^{-\beta\varepsilon}]$, are usually established via Lehmann's approach. We demonstrate here how the same can be deduced elegantly through their respective superoperator representations. There are contexts in which the said relationships may not be strictly true and have to be modified through a $c\delta(\varepsilon)$ term (c, a constant) e.g., $J_{AB}(\varepsilon) = [\mathrm{Im}\, G^R_{AB}(\varepsilon)]/[1+\gamma e^{-\beta\varepsilon}] + c\delta(\varepsilon)$. The origin and unambiguous analysis of such situations are presented. A proper bilinear form for the causal Green's function is derived.

The 'displaced harmonic oscillator' is analysed in detail, to illustrate the issues raised above.

The superoperator representation of the imaginary time Green functions is also given, in passing.

Keywords. Spectral functions; Green's functions; Lehmann's approach; superoperator representation; displaced harmonic oscillator.

1. Introduction

The Fourier-transforms of the retarded, advanced and causal Green's Functions (GF) are conveniently expressed in terms of superoperator (§2) resolvents. Distinguished by their analytic (or non-analytic) behaviour in the transform variable, such a representation, in turn, motivates different versions of bilinear forms to be defined in the space generated by the superoperator. These bilinear products are convenient for accommodating the commutation or the anti-commutation operations involved in the definitions of GF and the Fermi or Bose character of the operators. A proper bilinear form for the causal GF is derived here and the relationships among the various GF and the spectral functions are established (§3).

In §3, we show that the usual (but incorrect) inner projection form for the real time causal GF

$$\begin{aligned} G^C_{BA}(\varepsilon) &= \left\langle P\frac{1}{\varepsilon-\hat{L}}B,\ A-\gamma A,\ P\frac{1}{\varepsilon-\hat{L}}B\right\rangle \\ &\quad - i\pi\langle \delta(\varepsilon-\hat{L})\,B,\ A+\gamma\, A,\ \delta(\varepsilon-\hat{L})\ B\rangle \\ &= G^{C,\mathrm{I}}_{BA}(\varepsilon) + i\ G^{C,\mathrm{II}}_{BA}(\varepsilon), \end{aligned}$$

[§] Dedicated to Professor K S G Doss on his eightieth birthday.

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enables us to recover only the principal part $G^{C,\mathrm{I}}_{BA}(\varepsilon)$. An appropriate inner projection form for $G^{C,\mathrm{II}}_{BA}(\varepsilon)$ – wherein the bilinear form used is defined as

$$\langle X|Y\rangle = \langle [X^+, Y]_\gamma\rangle,$$

is deduced (§3) by us. The resulting expression is

$$G^{C,\mathrm{II}}_{BA}(\varepsilon) = -\frac{1}{2}\gamma\left[\left\langle A^+\left|\frac{1}{\varepsilon-\hat{L}-i\eta}\right|B\right\rangle - \left\langle A^+\left|\frac{1}{\varepsilon-\hat{L}+i\eta}\right|B\right\rangle\right]. \tag{1}$$

In (§4) we consider some specific cases to demonstrate explicitly the applicability of (1). The systems we have selected for this purpose are:

(1) the grand canonical ensemble of free electrons, and
(2) the displaced harmonic oscillator.

During the course of analysis, the inconsistency of reported superoperator inner projection representation of $G^C_{BA}(\varepsilon)$, viz

$$G^C_{BA}(\varepsilon) = -\gamma\left(A^+\left|\frac{1}{\varepsilon-\hat{L}}\right|B\right);\ (X|Y) = \langle [X^+,Y]_{-\gamma}\rangle$$

vis-a-vis $G^{C,\mathrm{II}}_{BA}(\varepsilon)$ will be illustrated.

The relation between spectral functions and GF, and also between different kinds of GF is usually obtained via the Lehmann approach. Here, one provides a representation of the Hamiltonian in a complete multi-particle space, through appropriate uses of the identity operator. As a result, the algebra becomes tedious. Alternatively, the above mentioned relations can be obtained in an elegant fashion by using the superoperator notion. In §5, we describe the details of this approach.

In certain instances, the relation between the spectral function and GF may involve an additional, additive term $c\,\delta(\varepsilon)$ where the constant c is non-zero. In §6, we consider the origin of such additional terms in the above mentioned relation. The procedure to obtain c has also been delineated.

The superoperator technique has hitherto been used in the context of real time GF (Paul 1982; Mc-Weeny and Pickup 1980). In §7, a superoperator representation for the imaginary time GF, relevant to finite temperature analysis is given.

2. Time Development : the Heisenberg picture and superoperators

(i) While dealing with a many-body system, we formulate the problem in two ways (Abrikasov *et al* 1963; Mattuck 1976): in the first approach, the system is considered to be isolated and N, the total particle number is specified at the beginning. The fixed N acts as an independent variable and the chemical potential μ is subsequently obtained as a function of N. In the second approach, we do not start with an isolated system but describe it using a grand canonical ensemble, wherein particle exchange is permissible. Now, the chemical potential acts as the unknown but fixed independent variable, to be determined finally by setting the total particle number equal to N.

In the first approach, the time development of any operator O in the Heisenberg representation is

$$O_H(t) = e^{iHt}\ O\ e^{-iHt};\ O = O(0), \tag{2}$$

whereas in the second approach, the same is represented as

$$O_K(t) = e^{iKt}\ O\ e^{-iKt}, \tag{2}$$

where

$$K = H - \mu N, \tag{3}$$

is known as the thermodynamic potential operator (Paul 1982, p.109) or the modified Hamiltonian (Mattuck 1976). H refers to the system's Hamiltonian and, now, N is the corresponding total particle number operator.

Since N commutes with H, (2) can be rewritten as*

$$O_K(t) = e^{iHt}\ [e^{-i\mu Nt}\ O\ e^{i\mu Nt}]e^{-iHt} \tag{4}$$

When O is a particle creation operator, say O_1^+, the term inside the bracket in (4) simplifies to $e^{-i\mu t}\ O_1^+$. Similarly, when O is an annihilation operator, say O_1, the same reduces to $e^{i\mu t}O_1$. Consequently, we have

$$O_{1K}^+(t) = e^{-i\mu t}\ O_{1H}^+(t), \tag{5}$$

$$O_{1K}(t) = e^{i\mu t}\ O_{1H}(t). \tag{6}$$

In general, when O is expressed as a product of creation/annihilation operators, the relation between the thermodynamic and ordinary Heisenberg representations [i.e. between $O_K(t)$ and $O_H(t)$] is obtained by appropriate applications of (5) and (6).

(ii) Corresponding to the two approaches discussed earlier for handling the many-body system, the time development of operator O can be formally represented as (Jorgensen and Simons 1981; Paul 1982, p. 245)

$$O_H(t) = e^{-i\hat{H}t}\ O \tag{7}$$

$$O_K(t) = e^{-i\hat{K}t}\ O \tag{8}$$

In the above expressions, we are yet to specify the meaning of the action of operators H and K. To arrive at this specification, we recall the usual time representations given by (2) and (2)'. It follows from these that connections between $\hat{H}$, H and $\hat{K}$, K are provided by

$$\hat{H}\ O = [O, H]_-, \tag{9}$$

$$\hat{K}\ O = [O, K]_-. \tag{10}$$

Since the above expressions specify the mode of action of $\hat{H}$ and $\hat{K}$, these can be considered as the definitions of $\hat{H}$ and $\hat{K}$. As the operands in (9) and (10) are

* This also ensures that H and N have common eigenfunctions.

themselves operators, we call $\hat{H}$ and $\hat{K}$ the respective superoperators corresponding to H and K. For notational convenience we introduce a superoperator $\hat{L}$ as

$$O_L(t) = e^{-i\hat{L}t}\, O; \quad \hat{L}\, O = [O,\, L]_-; \quad O_L(0) = O, \tag{11}$$

and identify $\hat{L}$ with $\hat{H}$ for isolated system and with $\hat{K}$ for grand canonical description. Similarly, L can either be H or K.

When $L = L_1 + L_2$, the corresponding superoperators L_1, L_2 satisfy the following identity

$$\hat{L}\, O = \hat{L}_1\, O + \hat{L}_2 O. \tag{12}$$

Also for operator product $O_1 O_2$,

$$\hat{L}(O_1 O_2) = (\hat{L}O_1)\, O_2 + O_1(\hat{L}O_2). \tag{13}$$

For further details regarding the mathematical structure of superoperators, we may refer to the papers by Lowdin (1982) and Weiner (1983).

3. Green's functions and superoperator representation

Green's function methods provide a systematic approach to describe the equilibrium and non-equilibrium characteristics of many-body systems – both at zero and finite temperatures. We usually come across different types of GF, differing in their analyticity (Economov 1979, pp. 145, 169). Important among them are: (i) retarded GF: G^R, (ii) advanced GF: G^A and, (iii) causal GF: G^C. Though these are defined over different time domains, there exist general relationships (Economou 1979, pp. 145, 169) among them. The retarded/advanced GF appear as the response functions in 'Linear Response Formalism' and hence are directly related to experimentally measurable quantities. The causal GF describes the propagation of disturbance in a system caused by adding (removing) a specific number of particles at a certain instant of time and removing (adding) them at a later instant. One of the important features of G^C is that it leads directly to the 'equal time operator product average' in suitable limiting cases. Further, the singularities in the Fourier transforms of the above GF are related to the energy spectrum of the system.

We define these Green's functions as

(a) Retarded GF

$$\begin{aligned} G^R_{BA}(t) &= -i\theta(t)\langle[B_L(t),\, A_L(0)]_{-\gamma}\rangle \\ &= (i)^\gamma\,\theta(t)\langle[A_L(0),\, B_L(t)]_{-\gamma}\rangle. \end{aligned} \tag{14}$$

(b) Advanced GF

$$\begin{aligned} G^A_{BA}(t) &= i\theta(-t)\langle[B_L(t),\, A_L(0)]_{-\gamma}\rangle \\ &= (-i)^\gamma\,\theta(-t)\langle[A_L(0),\, B_L(t)]_{-\gamma}\rangle. \end{aligned} \tag{15}$$

(c) Causal GF

$$G_{BA}^{C}(t) = -i\langle T\{B_L(t)\ A_L(0)\}\rangle$$
$$= (-i)^{\gamma}\langle T\{A_L(0)\ B_L(t)\}\rangle, \tag{16}$$

where T, the time ordering operator is defined as

$$T\{B_L(t)\ A_L(0)\} = B_L(t)\ A_L(0),\ t > 0$$
$$= \gamma A_L(0)\ B_L(t),\ 0 > \mathrm{t}.$$

Using the above definition, causal GF can be explicitly written as

$$G_{BA}^{C}(t) = -i\theta(t)\langle B_L(t)\ A_L(0)\rangle - i\gamma\,\theta(-t)\langle A_L(0)\ B_L(t)\rangle. \tag{16a}$$

In the above expressions, γ takes the value: (a) -1 when operators A and B have Fermi character and, (b) $+1$ when both of them have Bose character or one of them has Fermi and the other Bose character (Abrikasov *et al* 1963, p. 50; Paul 1982). The quantity $[X_L(t), Y_L(0)]_{-\gamma}$ denotes anti-commutation in the case (a) and commutation in (b). An operator X which contains an odd number of fermion creation/annihilation operators, and also the product of such an X with any number of boson operators have Fermi character. Products of even numbers of fermion creation/annihilation operators, boson operators and their products, and also the products of these two classes of operators have Bose character. The symbol $\langle\ldots\rangle$ denotes the expectation value over the exact normalized ground state wavefunction of the interacting system for zero temperature case, and the statistical average over grand canonical ensemble for finite temperature case. If in the above definitions we replace B by a column vector of operators, say $\bar{B}$, and A by a row vector $\bar{A}$, we obtain the corresponding generalized Green's functions (Linderberg and Ohrn 1973).

It is important to realize that when one of the operators appearing in the expressions (14) to (16) has Fermi character and the other Bose character, the Fermion particle number conservation does not hold good for the product $B_L(t)\ A(0)$, [or $A(0)\ B_L(t)$].* Consequently, the averages of such products become zeros. This feature can be further generalized to include all those cases wherein the required particle number conservation is violated by the operator products appearing inside $\langle\ldots\rangle$ (Bonch-Bruevich and Tyablikov 1962, p. 7).

Imaginary time GF: A different kind of GF, $\overline{G}_{BA}(\tau)$, known as imaginary time (or Matsubara or temperature) GF, is defined for fictitious times $\tau_i = it_j$, $i = \sqrt{-1}$ over the interval $(0,\beta)$ (Fetter and Walecka 1971)

$$\overline{G}_{BA}(\tau_1 - \tau_2) = -\langle T_\tau\{B_K(\tau_1) A_K(\tau_2)\}\rangle$$
$$= i\langle T_\tau\{B_K(\tau_1 - \tau_2) A(0)\}\rangle, \tag{17}$$

* Here we consider the particle number conservation for fermions only because for certain types of bosons having zero mass, e.g. photon, phonons, collective excitations etc., particle number conservation is not required. Also for such systems, chemical potential μ is identically zero. Next, $A(0) \equiv A_L(0)$ (Thouless 1972, p. 208).

wherein we have used a modified Heisenberg representation*

$$O_K(\tau) = e^{K\tau} O e^{-K\tau}. \tag{17a}$$

T_τ is again a time ordering operator [cf. (17)], but now it orders the operators according to their arguments τ_i. $\langle \ldots \rangle$ denotes the average over a grand canonical ensemble and $\tau (= \tau_1 - \tau_2)$ lies within the interval $[-\beta, \beta]$.

From the cyclic property of trace it follows that

$$\overline{G}_{BA}(\tau) = \gamma \overline{G}_{BA}(\tau + \beta);\ 0 < \tau + \beta < 2\beta, \tag{17b}$$

which shows that $\overline{G}_{BA}$ is a periodic/antiperiodic function in the interval $[-\beta, \beta]$ with the period β.

We shall take up the aspects connected with the superoperator representation of imaginary time GF later, in § 7.

Instead of working directly with the GF defined sin time domain, it is often convenient to work with their Fourier transforms. In the Fourier plane, the analytical properties of various GF, their relationships with each other and with spectral density function become more transparent.

We define the Fourier transform (FT) of $X(t)$ as†

$$X(\varepsilon) = \int_{-\infty}^{\infty} e^{i\varepsilon t - \eta|t|} X(t)\, \mathrm{d}t : \eta \to 0^+,\ \varepsilon \text{ real}. \tag{18}$$

The positive infinitesimal η ensures convergence as $t \to \pm\infty$. From (11), (14)–(16) and (18), the FT of various GF are written as

$$G^R_{BA}(\varepsilon) = \left\langle \frac{1}{\varepsilon - \hat{L} + i\eta} B,\ A - \gamma A,\ \frac{1}{\varepsilon - \hat{L} + i\eta} B \right\rangle \tag{19}$$

$$G^A_{BA}(\varepsilon) = \left\langle \frac{1}{\varepsilon - \hat{L} - i\eta} B,\ A - \gamma A,\ \frac{1}{\varepsilon - \hat{L} - i\eta} B \right\rangle \tag{20}$$

$$G^C_{BA}(\varepsilon) = \left\langle \frac{1}{\varepsilon - \hat{L} + i\eta} B,\ A - \gamma A,\ \frac{1}{\varepsilon - \hat{L} - i\eta} B \right\rangle \tag{21}$$

The symbol ',' appearing in the above expressions is to remind us that the operator $(\varepsilon - \hat{L} \pm i\eta)^{-1}$ known as superoperator resolvent (SOR), acts only on B. In a special situation corresponding to the zero temperature case, wherein the ground state refers to the true vacuum state, the action of SOR in (19)–(21) is equivalent to that of $(\varepsilon - H \pm i\eta)^{-1}$.

The various GF can be expressed as the appropriate matrix elements of the SOR, thus leading to their superoperator representation. In this subsection, we consider the cases of G^R and G^C.

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* When we consider τ as a complex number and analytically continue it to 'it' in the RHS of (17a), we formally obtain the usual Heisenberg representation.

† Strictly speaking, in the present context, ε and η should be replaced in what follows by $\varepsilon\hat{I}$ and $\eta\hat{I}$ where $\hat{I}$ is an identity operator defined through $\hat{I}X = X$ for any operator X. For notational convenience, we have dropped $\hat{I}$ in these expressions.

The action of SOR on B generates newer elements of the type

$$[B, L]_-;\ [[B, L]_-, L]_-;\ [[[B, L]_-, L]_-, L]_-;\ \ldots . \tag{22}$$

Using

$$\langle A_L(0) B_L(t) \rangle = \langle A_L(-t) B_L(0) \rangle, \tag{23}$$

in the definitions of GF, we see that $(\varepsilon + \hat{L} \mp i\eta)^{-1} A$, which now appears in the FT of GF, generates operators like

$$[A, L]_-;\ [[A, L]_-, L]_-;\ [[[A, L]_-, L]_-, L]_-;\ \ldots . \tag{24}$$

We define
(a) a linear operator space V containing A, B and all the other operators contained in (22) and (24). In the case when A and B themselves are matrices, say $\bar{A}$ and $\bar{B}$, V contains $\bar{A}$, $\bar{B}$ and elements of the type (22), (24) for each element of $\bar{A}$, $\bar{B}$.
(b) An identity superoperator $\hat{I}$ on V as

$$\hat{I}X = X \qquad \forall X \in V. \tag{25}$$

We note here that the earlier definition of superoperator $\hat{L}$ [cf. (11)] holds for every element in V, i.e.,

$$\hat{L}X = [X, L]_- \qquad \forall X \in V. \tag{11a}$$

The linear space V can be metrized by introducing a proper bilinear product. Depending on the nature of operators, the problem, and also otherwise, more than one type of bilinear form have been reported (Banwell and Primas 1963; Dalgaard and Simons 1977; Löwdin 1982). We give the definitions of some specific bilinear products which are to be used in subsequent analysis* (Paul 1982, p. 245; Bowen 1975; Jorgensen and Simons 1981).

$$\text{(i)}\ \boldsymbol{(}X|Y\boldsymbol{)} = \langle X^\dagger Y \rangle, \tag{26}$$

$$\text{(ii)}\ (X|Y) = \langle [X^\dagger, Y]_{-\gamma} \rangle. \tag{27}$$

For boson operators, the bilinear form (27) is not positive definite. It is obvious that the bilinear form (27) can also be expressed in terms of (26) as

$$(X|Y) = \boldsymbol{(}X|Y\boldsymbol{)} - \gamma \boldsymbol{(}X|Y\boldsymbol{)}, \tag{28}$$

$$\text{(iii)}\ ((X|Y)) = \langle [\hat{L}Y, X^\dagger]_- \rangle. \tag{29}$$

where X and Y have Bose character. It has been shown that bilinear form (29) is positive definite (Bowen 1975). We can also write

$$((X|Y)) = \boldsymbol{(}(L|Y)^\dagger X^\dagger\boldsymbol{)} - \boldsymbol{(}X|\hat{L}Y\boldsymbol{)} \tag{30}$$

Finally, keeping the further development of GF theory in view, we let

$$|\bar{h}) = [\,|h_1),\ |h_2),\ \ldots\ |h_n),\ \ldots\,], \tag{31}$$

be a linearly independent, not necessarily orthogonal, basis for the space V. Then, the identity superoperator admits the following resolution

* With the help of the discussion provided in § (4), these bilinear forms can be shown to be zero when one of the operators has Fermi and the other has Bose character.

$$\hat{I} = |\bar{h})\,(\bar{h}|\bar{h})^{-1}\,(\bar{h}|, \tag{32}$$

where $(\bar{h}|\bar{h})$ refers to any one of the above bilinear products. We also note here that superoperator $\hat{L}$ is hermitian.

Using the bilinear form (27), retarded and advanced GF can be recast as the following matrix elements of SOR

$$G^R_{BA}(\varepsilon) = -\gamma\left(A^\dagger \,\middle|\, \frac{1}{\varepsilon + i\eta - \hat{L}} \,\middle|\, B\right), \tag{33}$$

$$G^A_{BA}(\varepsilon) = -\gamma\left(A^\dagger \,\middle|\, \frac{1}{\varepsilon - i\eta - \hat{L}} \,\middle|\, B\right), \tag{34}$$

Equations (33) and (34) can be viewed as the superoperator representation for G^R and G^A. In principle, we could have also used appropriately the other bilinear forms to express G^R, G^A. For example, when A and B have Bose character G^R is equivalently written as* (Bowen 1975)

$$G^R_{BA}(\varepsilon) = \frac{1}{\varepsilon + i\eta}\langle BA - AB\rangle + \frac{1}{\varepsilon + i\eta}\left(\left(A^\dagger \,\middle|\, \frac{1}{\varepsilon + i\eta - \hat{L}} \,\middle|\, B\right)\right). \tag{35}$$

The above expression can be obtained directly from (33) by using the identity

$$\frac{1}{\varepsilon + i\eta - \hat{L}} = \frac{1}{\varepsilon + i\eta} + \frac{1}{\varepsilon + i\eta}\,\hat{L}\,\frac{1}{\varepsilon + i\eta - \hat{L}} \tag{36}$$

and rewriting the resulting expression in terms of bilinear form (29). This manipulation also brings out an equivalent bilinear form

$$((X|Y)) = \langle\, [\hat{L}Y, X^+]_+ \,\rangle, \tag{37}$$

for operators having Fermi character.

The criteria for using a particular type of bilinear product depend, apart from the structure of the problem, on the associated algebraic structure of various forms. For example, corresponding to Fermi operators A and B, the bilinear form (27) recasts the algebra in terms of a fundamental anti-commutation relationship associated with the bare operators A and B. In contrast, the bilinear product form (37), while retaining the anti-commutation form, employs modified operator $\hat{L}B$, thus making the algebra more cumbersome.

Next we consider the superoperator representation for causal GF. To arrive at the same, the following strategies have been employed in the literature:

1. Dropping the imaginary convergence parameter η altogether (Mc-Weeny and Pickup 1980):

$$G^C_{BA}(\varepsilon) = -\gamma\left(A^+ \left| \frac{1}{\varepsilon - \hat{L}} \right| B\right) \tag{38}$$

2. Not retaining the differences in the sign of η (Paul 1982, p. 245). Then

$$\varepsilon + i\eta \; (= \varepsilon - i\eta) = Z$$

and

$$G^C_{BA} = -\gamma \left(A^+ \left| \frac{1}{Z - \hat{L}} \right| B\right). \tag{39}$$

3. Starting with (38) and finally reintroducing η in a somewhat arbitrary manner (Dalgaard 1977): We see that in the first approach, the criterion for negotiating the singularities in causal GF is completely unspecified; whereas in the second case, depending on whether $Z = \varepsilon + i\eta$, or $\varepsilon - i\eta$, G^C reduces to G^R or G^A. Finally, in the third approach, the process involved in resubstitution of the $i\eta$ term with proper sign has not been discussed and this procedure may become quite confusing for the general case. To avoid these complications, it is important to retain '$i\eta$' properly, right from the beginning, while arriving at the superoperator representation for G^C.

We start with the identity (see, for e.g., Newton 1966, p. 179).

$$\lim_{\eta \to 0^+} \frac{1}{X \pm i\eta} = P\frac{1}{X} \mp i\pi\delta(X) \tag{40}$$

P denotes the principal part and using it, we rewrite the causal GF in the frequency domain as

$$\begin{aligned} G^C_{BA}(\varepsilon) &= \left\langle P\frac{1}{\varepsilon - \hat{L}} B, A - \gamma A, P\frac{1}{\varepsilon - \hat{L}} B\right\rangle \\ &\quad - i\pi\langle \delta(\varepsilon - \hat{L})B, A + \gamma A, \delta(\varepsilon - \hat{L})B\rangle \\ &= G^{C,\mathrm{I}}_{BA}(\varepsilon) + iG^{C,\mathrm{II}}_{BA}(\varepsilon). \end{aligned} \tag{41}$$

It is clear that whereas $G^{C,\mathrm{I}}_{BA}(\varepsilon)$ can be expressed in terms of bilinear form (27) (used for G^R, G^A), i.e.,

$$G^{C,\mathrm{I}}_{BA}(\varepsilon) = -\gamma \left(A^+ \left| P\frac{1}{\varepsilon - \hat{L}} \right| B\right), \tag{42}$$

the same is not the case with $G^{C,\mathrm{II}}_{BA}(\varepsilon)$. Instead, we have to employ the following bilinear form for $G^{C,\mathrm{II}}_{BA}(\varepsilon)$

$$\langle X | Y\rangle = \langle [X^+, Y]_\gamma\rangle \tag{43}$$

$$= (X|Y) + \gamma(X|Y). \tag{43A}$$

Using (42) and (43) in (41), we write the proper super-operator representation for the causal GF as

$$G^C_{BA}(\varepsilon) = -\gamma \left(A^+ \left| P\frac{1}{\varepsilon - \hat{L}} \right| B\right) - i\pi\gamma\langle A^+ | \delta(\varepsilon - \hat{L}) | B\rangle. \tag{44}$$

A more symmetric representation for the second term on the RHS of the above equation is*

$$iG^{C,\mathrm{II}}_{BA}(\varepsilon) = -\frac{1}{2}\gamma \lim_{\eta \to 0^+} \left[\left\langle A^+ \left| \frac{1}{\varepsilon - i\eta - \hat{L}} \right| B \right\rangle - \left[\left\langle A^+ \left| \frac{1}{\varepsilon + i\eta - \hat{L}} \right| B \right\rangle \right]. \right. \tag{45}$$

Further, using the identity (40) we also get [cf. (19), (20)]

$$\begin{aligned} G^R_{BA}(\varepsilon) &= \left\langle P\frac{1}{\varepsilon - \hat{L}} B, A - \gamma A, P\frac{1}{\varepsilon - \hat{L}} B \right\rangle \\ &\quad - i\pi\langle \delta(\varepsilon - \hat{L}) B, A - \gamma A, \delta(\varepsilon - \hat{L}) B \rangle \\ &\equiv G^{R,\mathrm{I}}_{BA}(\varepsilon) + iG^{R,\mathrm{II}}_{BA}(\varepsilon). \end{aligned} \tag{46}$$

$$\begin{aligned} G^A_{BA}(\varepsilon) &= \left\langle P\frac{1}{\varepsilon - \hat{L}} B, A - \gamma A, P\frac{1}{\varepsilon - \hat{L}} B \right\rangle \\ &\quad + i\pi\langle \delta(\varepsilon - \hat{L}) B, A - \gamma A, \delta(\varepsilon - \hat{L}) B \rangle \\ &\equiv G^{A,\mathrm{I}}_{BA}(\varepsilon) + iG^{A,\mathrm{II}}_{BA}(\varepsilon). \end{aligned} \tag{47}$$

From (41), (46) and (47), we have the following relations (see also appendix A)

$$G^{C,\mathrm{I}}_{BA} = G^{R,\mathrm{I}}_{BA} = G^{A,\mathrm{I}}_{BA} \tag{48}$$

$$G^{R,\mathrm{II}}_{BA} = -G^{A,\mathrm{II}}_{BA} \neq G^{C,\mathrm{II}}_{BA} \tag{49}$$

4. Applicability of the new superoperator inner projection form for $G^{C,\mathrm{II}}(\varepsilon)$: some illustrations

4.1 *Grand canonical ensemble of free electrons*

The Hamiltonian for the present system is given as

$$L = K = \sum_i (\varepsilon_i - \mu) c_i^+ c_i \tag{50}$$

and the Fourier transform of single particle causal GF corresponding to state 'a', viz

$$G^C_{aa}(t) = -i\langle T\{C_a(t) C_a^+(0)\}\rangle, \tag{51}$$

is written as (Bonch–Bruevich and Tyablikov 1962, p. 7)

* The analytical properties of the auxiliary functions appearing on the right hand side of (45) are similar to that of G^R or G^A.

$$G^{C}_{aa^{\cdot}}(\varepsilon) = \frac{n_F(a)}{\varepsilon - (\varepsilon_a - \mu) - i\eta} + \frac{1 - n_F(a)}{\varepsilon - (\varepsilon_a - \mu) + i\eta}, \tag{52}$$

we consider $G^{C,\mathrm{II}}_{aa^{\cdot}}(\varepsilon)$ which is equal to Im $G^{C}_{aa^{\cdot}}(\varepsilon)$. We employ (45) which contains the modified inner projection form and obtain

$$\mathrm{Im}\; G^{C}_{aa^{\cdot}}(\varepsilon) = \pi[2(n_F(a)) - 1]\,\delta(\varepsilon - \varepsilon_a + \mu), \tag{53}$$

where

$$n_F(a) = \langle C_a^+ C_a \rangle = [1 + e^{\beta(\varepsilon_a - \mu)}]^{-1}. \tag{54}$$

[Note:

When the usual superoperator representation (38) is employed, we have

$$G_{aa^{\cdot}}(\varepsilon) = \left(C_a \,\middle|\, \frac{1}{\varepsilon - \hat{K}} \,\middle|\, C_a\right) = \frac{1}{\varepsilon - (\varepsilon_a - \mu)}, \tag{55}$$

which obviously differs from the exact expression (52). We note that whereas (52) contains the thermal parameter β, $G^{C}_{aa^{\cdot}}(\varepsilon)$ obtained from (56) is temperature independent! In fact, it is not difficult to verify that, provided we take ε as $\varepsilon + i\eta$, (56) is the Fourier transform of the retarded GF.

Comparing (52) and (55) we also see that the principal parts of $G^{C}_{aa^{\cdot}}(\varepsilon)$ and $G^{R}_{aa^{\cdot}}(\varepsilon)$ are identical [cf. (48)]**]**.

4.2 *Displaced harmonic oscillator* ($T = 0$)

The Hamiltonian for a displaced harmonic oscillator is given as (Haken 1976, p. 13)

$$H = \omega_0 b^+ b + \lambda(b + b^+). \tag{56}$$

and the causal GF corresponding to the displacement operator

$$\phi = b + b^+ = \phi^+ \tag{57}$$

is defined as (Abrikasov *et al* 1963)

$$D^{C}_{\phi\phi}(t) = -i\langle \psi_0 |\, T\{\phi(t)\,\phi(0)\} \,| \psi_0 \rangle. \tag{58}$$

Direct evaluation of (58) is possible via canonical transformation

$$S = e^{(b - b^+)\lambda/\omega_0}, \tag{59}$$

which diagonalizes H as

$$S^{-1} H S = H' = \omega_0 b^+ b - \frac{\lambda^2}{\omega_0} \tag{60}$$

The exact ground state wavefunction, $|\psi_0\rangle$ of H can now be represented in terms of ground state wavefunction $|0\rangle$ of canonically transformed Hamiltonian H', i.e.,

$$|\psi_0\rangle = S|0\rangle \tag{61}$$

Substitution of (61) in (58), and use of the identity (Fong 1975)

$$e^{\xi M} N e^{-\xi M} = N + \xi[M, N] + \frac{\xi^2}{\lfloor 2}[M, [M, N]_-]_- + \dots \tag{62}$$

(ξ is c-number; M, N are operators) finally leads to

$$D^C_{\phi\phi}(t) = -i\theta(t)\left[e^{-i\omega_0 t} + \frac{4\lambda^2}{\omega_0}\right] - i\theta(-t)\left[e^{i\omega_0 t} + \frac{4\lambda^2}{\omega_0}\right]. \tag{63}$$

or

$$D^C_{\phi\phi}(\varepsilon) = \left[\frac{1}{\varepsilon - \omega_0 + i\eta} - \frac{1}{\varepsilon + \omega_0 - i\eta}\right] - \frac{8\pi i\lambda^2}{\omega_0^2}\delta(\varepsilon). \tag{64}$$

[**Note:**

When we evaluate the $D^C_{\phi\phi}(\varepsilon)$ from the wrong expression (38) by using either the EOM method or the superoperator inner projection technique, we obtain

$$D^C_{\phi\phi}(\varepsilon) = \frac{2\omega_0}{\varepsilon^2 - \omega_0^2}. \tag{65}$$

Comparing (65) with the exact $D^C_{\phi\phi}(\varepsilon)$ from (64), we observe that the two expressions are not identical. Whereas the exact result contains the parameter λ, (65) is independent of λ! Indeed it can be seen that when ε is replaced by $\varepsilon + i\eta$, ($\eta \to 0^+$), the right hand side of (65) is the Fourier transform of retarded GF

$$D^R_{\phi\phi}(t) = -i\theta(t)\langle[\phi(t), \phi(0)]_-\rangle, \tag{66}$$]

We shall now use the equation of motion (EOM) approach to show that the correct result for $D^{C,\text{II}}_{\phi\phi}(\varepsilon) = \text{Im } D^C_{\phi\phi}(\varepsilon)$ can only be obtained by employing (45). We write

$$-\text{Im } D^C_{\phi\phi}(\varepsilon) = \frac{1}{2i}\lim_{\eta\to 0^+}\left[\left\langle \phi \left| \frac{I}{\varepsilon - \hat{H} - i\eta} \right| \phi \right\rangle - \left\langle \phi \left| \frac{1}{\varepsilon + \hat{H} - i\eta} \right| \phi \right\rangle\right] \tag{67}$$

The EOM for $\langle\phi|1/(\varepsilon - \hat{H})|\phi\rangle$ leads to the following set of equations (appendix B)

$$\varepsilon d_{\phi\phi}(\varepsilon) = 2\langle\phi^2\rangle + \omega_0 d_{\pi\phi}(\varepsilon), \tag{68}$$

$$\varepsilon d_{\pi\phi}(\varepsilon) = \omega_0 d_{\phi\phi}(\varepsilon) + \frac{4\lambda\langle\phi\rangle}{\varepsilon}, \tag{69}$$

where

$$d_{BA}(\varepsilon) = \left\langle A^+ \left| \frac{1}{\varepsilon - \hat{H}} \right| B \right\rangle. \tag{70}$$

Solving (68) and (69) for $d_{\phi\phi}(\varepsilon)$, we obtain:

$$d_{\phi\phi}(\varepsilon)=\frac{2\varepsilon\langle\phi^2\rangle}{\varepsilon^2-\omega_0^2}+\frac{4\lambda\omega_0\langle\phi\rangle}{(\varepsilon^2-\omega_0^2)\varepsilon}. \tag{71}$$

Evaluating $\langle\phi^2\rangle$ and $\langle\phi\rangle$ by using (61), we have

$$\langle\phi^2\rangle=1+\frac{4\lambda^2}{\omega_0^2};\ \langle\phi\rangle=-\frac{2\lambda}{\omega_0}. \tag{72}$$

From (71) and (72)

$$d_{\phi\phi}(\varepsilon)=\frac{2\varepsilon}{\varepsilon^2-\omega_0^2}+\frac{8\lambda^2}{\omega_0^2}\frac{1}{\varepsilon}. \tag{73}$$

Substituting (73) (with proper '$i\eta$' terms) in (65)

$$\begin{aligned}\operatorname{Im} D^C_{\phi\phi}(\varepsilon)&=-\frac{1}{2i}\lim_{\eta\to 0^+}\left[\frac{2(\varepsilon-i\eta)}{(\varepsilon-i\eta)^2-\omega_0^2}-\frac{2(\varepsilon+i\eta)}{(\varepsilon+i\eta)^2-\omega_0^2}\right.\\&\qquad\left.+\frac{8\lambda^2}{\omega_0^2}\left(\frac{1}{\varepsilon-i\eta}-\frac{1}{\varepsilon+i\eta}\right)\right]\\&=-\pi[\delta(\varepsilon-\omega_0)+\delta(\varepsilon+\omega_0)]-\frac{8\pi\lambda^2}{\omega_0^2}\delta(\varepsilon).\end{aligned} \tag{74}$$

Comparing (74) with exact $\operatorname{Im} D^C_{\phi\phi}(\varepsilon)$ obtained from (64), we see that the equation of motion approach for evaluating the expression (67) yields the correct result.

Lastly, we consider the superoperator inner projection technique for evaluating $\operatorname{Im} D^C_{\phi\phi}(\varepsilon)$, or more specifically, the auxiliary function $d_{\phi\phi}(\varepsilon)$.

The auxiliary function $d_{BA}(\varepsilon)$ [cf. (70)] is written in the superoperator inner projection form as

$$d_{BA}(\varepsilon)=\langle A^+|\bar{h}\rangle\langle\bar{h}|\varepsilon-\hat{H}|\bar{h}\rangle^{-1}\langle\bar{h}|B\rangle, \tag{75}$$

where $\bar{h}$ is the basis set spanning the space $\langle\hat{H}^nA\cup\hat{H}^nB\}_{n=0}^{\infty}$. To arrive at (75), we have used the following representation of the identity superoperator

$$\hat{I}=|\bar{h}\rangle\langle\bar{h}|\bar{h}\rangle^{-1}\langle\bar{h}|. \tag{76}$$

Substituting in (75) $A=B=\phi$ and the basis set $\bar{h}$ as $[\phi,\pi,1]$, we once again obtain the exact expression (73) for $d_{\phi\phi}(\varepsilon)$. For the details of various steps involved, we may refer to appendix C.

5. Interrelation among spectral functions: a superoperator approach

Here, we consider the relation between the spectral functions $J_{BA}(\varepsilon)$, and $J_{AB}(\varepsilon)$, which are defined as the Fourier transforms of the time correlation functions

$\langle B_L(t)A(0)\rangle$ and $\langle A(0)\,B_L(t)\rangle$ respectively. Writing $B_L(t)$ in terms of superoperator $\hat{L}$, viz, $B_L(t)=e^{-i\hat{L}t}B(0)$, we have*

$$J_{BA}(\varepsilon)=\int_{-\infty}^{\infty}\langle B_L(t)A(0)\rangle e^{i\varepsilon t}\,\mathrm{d}t$$
$$=2\pi\langle\delta(\varepsilon-\hat{L})B,A\rangle, \tag{77}$$

$$J_{AB}(\varepsilon)=\int_{-\infty}^{\infty}\langle A(0)B_L(t)\rangle e^{i\varepsilon t}\,\mathrm{d}t$$
$$=2\pi\langle A,\,\delta(\varepsilon-\hat{L})B\rangle. \tag{78}$$

Here $A=A(0)$, $B=B(0)$.
Since

$$e^{-\beta L}\,\delta(\varepsilon-\hat{L})B,\,A=e^{-\beta L}\,(\varepsilon-\hat{L})Be^{\beta L},\;e^{-\beta L}A$$
$$=e^{\beta\hat{L}}\,\delta(\varepsilon-\hat{L})B,e^{-\beta L}A\ \text{: using the definition of the superoperator,}$$
$$=e^{\beta\varepsilon}\;\delta(\varepsilon-\hat{L})B,e^{-\delta L}A\ \text{: from the property of the } \delta \text{ function,} \tag{79}$$

we have

$$J_{BA}(\varepsilon)=2\pi e^{\beta\varepsilon}\mathrm{Tr}\{\delta(\varepsilon-\hat{L})B,e^{-\beta L}A\}/\mathrm{Tr}\,e^{-\beta L}. \tag{80}$$

From the cyclic property of trace,

$$J_{BA}(\varepsilon)=2\pi e^{\beta\varepsilon}\mathrm{Tr}\{e^{-\beta L}A,\delta(\varepsilon-\hat{L})B\}/\mathrm{Tr}\,e^{-\beta L}, \tag{81}$$

or, from (78) and (81)

$$J_{BA}(\varepsilon)=e^{\beta\varepsilon}J_{AB}(\varepsilon). \tag{82}$$

The above expression denotes the fundamental relation (Lehmann 1954) between J_{BA} and J_{AB}. Further, since the different types of GF in the time domain are defined as appropriate linear combinations of time correlation functions† [cf. §3] the relation between J_{BA} and J_{AB} also determines the interrelation between different GF.

6. The "$C\delta(\varepsilon)$" term in $J_{BA}(\varepsilon)$ and illustrations

The expressions relating the imaginary parts of various GF and the spectral function J_{AB} are generally valid, as shown through the analysis in appendix A and § 5. But, as mentioned in passing in a footnote by Bonch–Bruevich [1962] (p.7) these equations, viz, (A 19) and (A 20) are not strictly true, always. The exception arises for the retarded and advanced GF when we deal with boson operators, and for the

* ',' in (77) reminds us that $\hat{L}$ acts only on B. Further ',' commutes with the operator $\hat{L}$ [cf. (80). Also, for the notational convenience, we have dropped the identity superoperator $\hat{I}$ appearing with ε.
† It may be noted that coefficients of the linear combinations are generalized function $\theta(t)$ and $\theta(-t)$.

causal GF when A and B are fermion operators. Under these conditions, it can be shown that instead of (A 19) and (A 20), the exact expressions are

$$J_{BA} = \frac{-2}{1-e^{-\beta\varepsilon}} \; G_{BA}^{R,\mathrm{II}} + c\,\delta(\varepsilon) = \frac{2}{1-e^{-\beta\varepsilon}} \; G_{BA}^{A,\mathrm{II}} + c\delta(\varepsilon) \quad \text{(for bosons)}, \tag{83}$$

$$J_{BA} = \frac{-2}{1-e^{-\beta\varepsilon}} \; G_{BA}^{C,\mathrm{II}} + c\,\delta(\varepsilon) \quad \text{(for fermions)}. \tag{84}$$

We can prove that (83) and (84) are indeed true and the presence of the δ function centred at $\varepsilon = 0$ has its origin at the inversion stage [refer to (A 14), (A 15) and (A 17)].

The fact that arbitrary c-numbers in (83) and (84) occur, does not necessarily mean that $c \neq 0$ and this does not imply either that c is arbitrary or undetermined, for, the identity

$$\langle B(0)\; A(0) \rangle = \langle BA \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} J_{BA}(\varepsilon)\mathrm{d}\varepsilon \tag{85}$$

can be used to determine c in terms of $\langle BA \rangle$.

Illustrations

(i) Grand canonical ensemble of electrons

In §4 we have already considered the problem of the grand canonical ensemble of electrons. Substituting $B = c_a$, $A = c_a^+$ and the relations (84), (53) in (85) and solving the resulting expression for c, it can be shown that in the present case, the constant c is identically zero.

(ii) *Displaced harmonic oscillator*

The constant c appearing in the spectral function-retarded (advanced) GF relation [cf. (83)] can be obtained in a straightforward manner by using (85). Substituting $B = A = \phi$ in (85), and using the relations† (83), (72) and

$$D_{\phi\phi}^{R,\mathrm{II}} = \mathrm{Im}\; D_{\phi\phi}^{R} = -\pi[\delta(\varepsilon - \omega_0) + \delta(\varepsilon + \omega_0)], \tag{86}$$

we obtain

$$1 + \frac{4\lambda^2}{\omega_0^2} = \int_{-\infty}^{\infty} \frac{1}{1-e^{-\beta\varepsilon}} [\delta(\varepsilon - \omega_0) + \delta(\varepsilon + \omega_0)]\mathrm{d}\varepsilon + \frac{c}{2\pi} \tag{87}$$

Solving the above expression for c, we obtain a non-zero value of c in the present case, viz,

$$c = (8\pi\lambda^2)/\omega_0^2 \,. \tag{88}$$

† Presently, we consider only the retarded GF. The c appearing in advanced GF can be obtained in a similar fashion.

It is interesting to note that in the case $\lambda = 0$, $c = 0$ [refer to (88)] which means that the $c\delta(\varepsilon)$ correction becomes unnecessary for a simple harmonic oscillator (i.e. $\lambda = 0$)!

7. Superoperator representation of imaginary time GF

We have already introduced the imaginary time GF, $\overline{G}_{BA}(\tau)$ in §3 [equation (17)]. Presently, we consider the superoperator inner projection representation of frequency* GF, $\overline{G}_{BA}(\varepsilon_n)$, obtained from the Fourier series expansion of $\overline{G}_{BA}(\tau)$

$$\overline{G}_{BA}(\tau) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} e^{-i\varepsilon_n\tau}\overline{G}_{\mathrm{BA}}(\varepsilon_n) \; . \tag{89}$$

We write $\overline{G}_{BA}(\varepsilon_n)$ as

$$\overline{G}_{BA}(\varepsilon_n) = \int_0^\beta e^{i\varepsilon_n\tau}\, \overline{G}_{\mathrm{BA}}(\tau)\, \mathrm{d}\tau \tag{90}$$

$$\begin{aligned} \varepsilon_n &= (2n+1)\pi/\beta \text{ for fermions,} \\ &= 2n\pi/\beta \text{ for bosons.} \end{aligned} \tag{91}$$

Obviously superoperator representation for $\overline{G}_{BA}(\tau)$ follows from that of $\overline{G}_{BA}(\varepsilon_n)$ via (89). Substituting $\overline{G}_{BA}(\tau)$ from (17) in (90), we get

$$\begin{aligned} \overline{G}_{BA}(\varepsilon_n) &= -\int_0^\beta \mathrm{d}\tau e^{i\varepsilon_n\tau}[\theta(\tau)\langle B_K(\tau)A(0)\rangle \\ &\quad + \gamma\theta(-\tau)\langle A(0)B_K(\tau)\rangle]\mathrm{d}\tau \\ &= -\int_0^\beta \mathrm{d}\tau e^{i\varepsilon_n\tau}\langle B_K(\tau)A(0)\rangle \end{aligned} \tag{92}$$

Substituting [cf. (11), (17a)]

$$B_K(\tau) = e^{-\hat{K}\tau}B, \; B = B(0), \tag{93}$$

in (92), we get*

$$\begin{aligned} \overline{G}_{BA}(\varepsilon_n) &= -\int_0^\beta \mathrm{d}\tau \langle e^{(i\varepsilon_n-\hat{K})}B,A\rangle \mathrm{d}\tau \\ &= -\mathrm{Tr}\left\{e^{-\beta K}\int_0^\beta \mathrm{d}\tau e^{(i\varepsilon_n-\hat{K})}B,A\right\}\Big/ Z; \end{aligned}$$

---

*'Frequency dependent GF' according to Mahan (1981, p. 123).

*Refer footnote on p. 320 for ',' symbol in (94)–(102).

$$|Z = \mathrm{Tr}\{e^{-\beta K}\}| \tag{94}$$

$$= -\,\mathrm{Tr}\left\{e^{-\beta K}\left|\,\frac{e^{i\varepsilon_n\tau - \hat{K}\tau}}{i\varepsilon_n - \hat{K}}\,\right|_0^\beta B,\ A\right\}\Big/ Z. \tag{95}$$

From (91) it can easily be seen that

$$e^{i\varepsilon_n\beta} = \gamma, \tag{96}$$

where $\gamma = -1$, when A, B have Fermi character, and $\gamma = +1$ when they have Bose character [cf. §3, above]. As a result, we have

$$\overline{G}_{BA}(\varepsilon_n) = -\,\mathrm{Tr}\left\{e^{-\beta K}\left(\frac{\gamma e^{-K\beta}}{i\varepsilon_n - \hat{K}} B,\ A - \frac{1}{i\varepsilon_n - \hat{K}}\ B,\ A\right)\right\}\Big/ Z \tag{97}$$

Next, let

$$X = \mathrm{Tr}\left\{e^{-\beta K}\ e^{-\hat{K}\beta}\ \frac{\gamma}{i\varepsilon_n - \hat{K}}\ B,\ A\right\},\ \text{which we can rewrite as}$$

$$X = \mathrm{Tr}\left\{e^{-\beta K}\ e^{\beta K}\ \frac{\gamma}{i\varepsilon_n - \hat{K}}\ Be^{-\beta K},\ A\right\}, \tag{98}$$

Since ' , ' restricts the action of superoperator $\hat{K}$ only, we have

$$X = \mathrm{Tr}\left\{\frac{\gamma}{i\varepsilon_n - \hat{K}}\ B,\ e^{-\beta K},\ A\right\}, \tag{99}$$

or, from the cyclic property of the trace

$$X = \mathrm{Tr}\left\{e^{-\beta K}\ A,\ \frac{\gamma}{i\varepsilon_n - \hat{K}}\ B\right\}, \tag{100}$$

Substituting (100) in (97), we get

$$\overline{G}_{BA}(\varepsilon_n) = -\gamma\,\mathrm{Tr}\left\{e^{-\beta K}\left(A,\ \frac{1}{i\varepsilon_n - \hat{K}}\ B - \gamma\frac{1}{i\varepsilon_n - \hat{K}}\ B,\ A\right)\right\}\Big/ Z \tag{101}$$

Finally, using the bilinear form defined by (45), $\overline{G}_{BA}(\varepsilon_n)$ is written as

$$\overline{G}_{BA}(\varepsilon_n) = -\,\gamma\left(A^{\dagger}\,\middle|\,\frac{1}{i\varepsilon_n - \hat{K}}\,\middle|\,B\right), \tag{102}$$

which is the superoperator representation for frequency GF.

8. Summary and conclusions

(1) a correct superoperator representation of the causal Green's function–requiring

a bilinear form different from the usual ones used for advanced and retarded GF is given;
(2) the correctness of such a representation is demonstrated through its application to (a) a free-electron system, and (b) displaced harmonic oscillator, and comparing the same with the exact results;
(3) the well-known relations between the spectral functions and the various GF are deduced through their superoperator representations, thus by-passing the apparently more tedious Lehman approach;
(4) the problem of the 'the $c\delta(\varepsilon)$ ambiguity' as pointed out in connection with relating the spectral J_{AB} and Green's functions G^{i}_{AB} (i = causal, when A, B are Fermions and i = advanced/retarded when A, B are Bosons) is analysed in detail. An unambiguous method of determining the coefficient c is outlined. Both the possibilities viz. $c = 0$, $c \neq 0$, are illustrated through the Fermi gas and the displaced harmonic oscillator models;
(5) finally, the superoperator representation for the imaginary time causal GF is derived.

Appendix A. Relation between Green's functions and spectral functions

Spectral functions are directly associated with time correlation functions and represent their Fourier transforms. The spectral function corresponding to the time correlation function $\langle A(0)\, B_L(t) \rangle$ is defined as:

$$J_{AB}(\varepsilon) = \int_{-\infty}^{\infty} e^{i\varepsilon t} \langle A(0)\, B_L(t) \rangle \mathrm{d}t. \tag{A1}$$

Similarly,

$$J_{BA}(\varepsilon) = \int_{-\infty}^{\infty} e^{i\varepsilon t} \langle B_L(t)\, A(0) \rangle \mathrm{d}t\,. \tag{A2}$$

For further discussion, it is important to obtain the relation between J_{BA} and J_{AB}. We consider here $T \neq 0$ case. The zero temperature result can be obtained from it by taking appropriate limits.

It has been shown that for real ε, spectral functions are real quantities. From the knowledge of spectral functions, time correlation functions are obtained by using the inverse FT

$$\langle B_L(t)\, A(0) \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\varepsilon t} J_{BA}(\varepsilon)\, \mathrm{d}\varepsilon\,, \tag{A3}$$

$$\langle A(0)\, B_L(t) \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\varepsilon t} J_{AB}(\varepsilon)\, \mathrm{d}\varepsilon\,,$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\varepsilon t}\, e^{-\beta\varepsilon}\, J_{BA}(\varepsilon)\, \mathrm{d}\varepsilon\,, \tag{A4}$$

Also,

$$\langle B(0)\ A(0)\rangle = \langle BA\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty} J_{BA}(\varepsilon)\ \mathrm{d}\varepsilon\ , \tag{A5}$$

Here, we note that the expectation value of equal time operator product can be directly obtained from causal GF. From (16a)

$$\langle AB\rangle = i\gamma \lim_{t\to 0^-} G^C_{BA}(t) \tag{A6}$$

Our next step is to consider the relation between various GFS and spectral functions. Employing the inverse FT and the relation $J_{BA}(\varepsilon) = e^{\beta\varepsilon} J_{AB}(\varepsilon)$ as well as (14)–(16), (A1) and (A2),

$$G^R_{BA}(t) = -i\theta(t)\int_{-\infty}^{\infty} e^{-i\varepsilon' t}\,[1-\gamma e^{-\beta\varepsilon'}]\ J_{BA}(\varepsilon')\ \frac{\mathrm{d}\varepsilon'}{2\pi}, \tag{A7}$$

$$G^A_{BA}(t) = i\theta(-t)\int_{-\infty}^{\infty} e^{-i\varepsilon' t}\,[1-\gamma e^{-\beta\varepsilon'}]\ J_{BA}(\varepsilon')\ \frac{\mathrm{d}\varepsilon'}{2\pi}, \tag{A8}$$

$$G^C_{BA}(t) = -i\theta(t)\int_{-\infty}^{\infty} e^{-i\varepsilon' t}\ J_{BA}(\varepsilon')\ \frac{\mathrm{d}\varepsilon'}{2\pi}$$

$$-\,i\gamma\theta(-t)\int_{-\infty}^{\infty} e^{-i\varepsilon' t}\ J_{AB}(\varepsilon')\ \frac{\mathrm{d}\varepsilon'}{2\pi}, \tag{A9}$$

Alternatively [Bonch–Bruevich and Tyblikov 1962]

$$G^R_{BA}(\varepsilon) = \frac{1}{2\pi}\int_{-\infty}^{\infty}(1-\gamma e^{-\beta\varepsilon'})\ \frac{J_{BA}(\varepsilon')}{\varepsilon-\varepsilon'+i\eta}\ \mathrm{d}\varepsilon' \tag{A10}$$

$$G^A_{BA}(\varepsilon) = \frac{1}{2\pi}\int_{-\infty}^{\infty}(1-\gamma e^{-\beta\varepsilon'})\ \frac{J_{BA}(\varepsilon')}{\varepsilon-\varepsilon'-i\eta}\ \mathrm{d}\varepsilon' \tag{A11}$$

$$G^C_{BA}(\varepsilon) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\left(\frac{1}{\varepsilon-\varepsilon'+i\eta} - \gamma\frac{e^{-\beta\varepsilon'}}{\varepsilon-\varepsilon'-i\eta}\right) J_{BA}(\varepsilon')\ \mathrm{d}\varepsilon'\ . \tag{A12}$$

Thus, in the complex ε plane (i.e. in z)

$$\frac{1}{2\pi i}\int_{-\infty}^{\infty}(1-\gamma e^{-\beta\varepsilon'})\ \frac{iJ_{BA}(\varepsilon')\ \mathrm{d}\varepsilon'}{z-\varepsilon'\ \ 2\pi} = \begin{cases} G^R_{BA}(z), & \mathrm{Im}\, z>0 \\ G^A_{BA}(z), & \mathrm{Im}\, z<0 \end{cases} \tag{A13}$$

In fact, G^R and G^A together can be considered as a single analytical function $G(z)$, defined over the whole complex plane except on the real axis, where it has singularities (either isolated poles or branch cut, depending on the spectrum of L)

[Ter Haar 1962, p. 119]. When we approach the real axis from the upper or lower sides, we have

$$G_{BA}(\varepsilon+i\eta) \equiv G^R_{BA}(\varepsilon) = P\int_{-\infty}^{\infty}(1-\gamma e^{-\beta\varepsilon'})\frac{J_{BA}(\varepsilon')}{\varepsilon-\varepsilon'}\frac{d\varepsilon'}{2\pi} - \frac{i}{2}(1-\gamma e^{-\beta\varepsilon})J_{BA}(\varepsilon) \tag{A14}$$

or

$$G_{BA}(\varepsilon-i\eta) \equiv G^A_{BA}(\varepsilon) = P\int_{-\infty}^{\infty}(1-\gamma e^{-\beta\varepsilon'})\frac{J_{BA}(\varepsilon')}{i\varepsilon-\varepsilon'}\frac{d\varepsilon'}{2\pi} + \frac{i}{2}(1-\gamma e^{-\beta\varepsilon})J_{BA}(\varepsilon) \tag{A15}$$

From (A14) and (A15), we obtain the following important relation

$$J_{BA}(\varepsilon) = \frac{i}{1-\gamma e^{-\beta\varepsilon}}[G^R_{BA}(\varepsilon) - G^A_{BA}(\varepsilon)], \tag{A16}$$

which in conjunction with (A3)–(A5) can be used to obtain various observables. From (A9), we can write the FT of causal GF as

$$G^C_{BA}(\varepsilon) = P\int_{-\infty}^{\infty}(1-\gamma e^{-\beta\varepsilon'})\frac{J_{BA}(\varepsilon')}{\varepsilon-\varepsilon'}\frac{d\varepsilon'}{2\pi} - \frac{i}{2}(1+\gamma e^{-\beta\varepsilon})J_{BA}(\varepsilon). \tag{A17}$$

Causal GF is non-analytical in the complex plane [Mattuck 1976]. This can be ascertained from the fact that real and imaginary parts of causal GF do not satisfy the dispersion relation associated with analytical functions.

From the above discussion [cf. (48), (A14)–(A17)], it also follows that

$$G^{i,I}_{BA}(\varepsilon) = P\int_{-\infty}^{\infty}(1-e^{-\beta\varepsilon'})\frac{J_{BA}(\varepsilon')}{\varepsilon-\varepsilon'}\frac{d\varepsilon'}{2\pi}, \tag{A18}$$

where $i = [R,A,C]$
and*

* In the case of a minus sign appearing in the denominators of (A19), (A20), the RHS of these expressions can contain a term $c\,\delta(\varepsilon)$ also where c is a constant (§6). We note (cf. §3) that a minus sign will appear in the denominator of (A19) when A and B are Boson operators and in the denominator of (A20) when A and B have Fermi characteristics.

$$J_{BA}(\varepsilon) = -\frac{2}{1-\gamma e^{-\beta\varepsilon}} G_{BA}^{R,II}(\varepsilon)$$
$$= \frac{2}{1-\gamma e^{-\beta\varepsilon}} G_{BA}^{A,II}(\varepsilon). \tag{A19}$$

From (41) and (A17), $J_{BA}(\varepsilon)$ can also be written in terms of causal GF as

$$J_{BA}(\varepsilon) = -\frac{2}{1+\gamma e^{-\beta\varepsilon}} G_{BA}^{C,II}(\varepsilon). \tag{A20}$$

Finally we notice that when $J_{BA}(\varepsilon)$ is real

$$G_{BA}^{i,I}(\varepsilon) = \mathrm{Re}\, G^{i}_{BA}(\varepsilon), \tag{A21}$$

and

$$G_{BA}^{i,II}(\varepsilon) = \mathrm{Im}\, G^{i}_{BA}(\varepsilon). \tag{A22}$$

Needless to say that, in general, the expressions (A18)–(A20) can be used to generate the other GFS from the knowledge of any particular type of Green's function.

Appendix B. Evaluation of (30) and (31)

(a) EOM for $d_{\phi\phi}$ is

$$\left\langle \phi \middle| \frac{1}{\varepsilon-\hat{H}} \middle| \phi \right\rangle = \frac{1}{\varepsilon}\left\langle \phi \middle| \phi \right\rangle + \frac{1}{\varepsilon}\left\langle \phi \middle| \frac{1}{\varepsilon-\hat{H}}\hat{H} \middle| \phi \right\rangle. \tag{B1}$$

Next

$$\langle \phi|\phi\rangle = \langle \phi^{+}\phi + \phi\,\phi^{+}\rangle = 2\langle \phi^2\rangle \qquad \text{[cf. (2)]}, \tag{B2}$$

and $$\hat{H}\phi = \omega_0 \pi. \tag{B3}$$

From (B1) – (B3)

$$\varepsilon d_{\phi\phi} = 2\langle \phi^2\rangle + \omega_0 d_{\pi\phi}, \tag{B4}$$

which is (30).

(b) EOM for $d_{\pi\phi}$ is

$$\left\langle \phi \middle| \frac{1}{\varepsilon-\hat{H}} \middle| \pi \right\rangle = \frac{1}{\varepsilon}\left\langle \phi \middle| \pi \right\rangle + \frac{1}{\varepsilon}\left\langle \phi \middle| \frac{1}{\varepsilon-\hat{H}}\hat{H} \middle| \pi \right\rangle. \tag{B5}$$

Since

$$\hat{H}\pi = [\pi, \omega_0 b^+ b + \lambda\phi]_-$$
$$= \omega_0\phi + \lambda(\pi\phi - \phi\pi). \tag{B6}$$

We have

$$\left\langle \phi \left| \frac{1}{\varepsilon - \hat{H}} \hat{H} \right| \pi \right\rangle = \omega_0 \left\langle \phi \left| \frac{1}{\varepsilon - \hat{H}} \right| \phi \right\rangle + \lambda \left\langle \phi \left| \frac{1}{\varepsilon - \hat{H}} \right| \pi\phi - \phi\pi \right\rangle. \tag{B7}$$

Further using (13)

$$\hat{H}(\pi\phi - \phi\pi) = (\hat{H}\pi)\phi + \pi(\hat{H}\phi) - (\hat{H}\phi)\pi - \phi(\hat{H}\pi) = 0. \tag{B8}$$

From (B7) and (B8)

$$\left\langle \phi \left| \frac{1}{\varepsilon - \hat{H}} \right| \pi\phi - \phi\pi \right\rangle = \frac{1}{\varepsilon} \left\langle \phi \left| \pi\phi - \phi\pi \right. \right\rangle. \tag{B9}$$

Now,

$$\langle \phi | \pi\phi - \phi\pi \rangle = \langle \phi^+ \pi\phi + \pi\phi\phi^+ \rangle - \langle \phi^+ \phi\pi + \phi\pi\phi^+ \rangle$$
$$= \langle \pi\phi\phi - \phi\phi\pi \rangle. \tag{B10}$$

Substituting the identity

$$\phi\pi - \pi\phi = -2, \tag{B11}$$

obtained from the commutation $[\phi, \pi]_-$, in (B10), we get

$$\langle \phi | \pi\phi - \phi\pi \rangle = 4\langle \phi \rangle. \tag{B12}$$

From (B9) and (B12)

$$\left\langle \phi \left| \frac{1}{\varepsilon - \hat{H}} \right| \pi\phi - \phi\pi \right\rangle = \frac{4\langle \phi \rangle}{\varepsilon}, \tag{B13}$$

or from (B7) and (B13)

$$\left\langle \phi \left| \frac{1}{\varepsilon - \hat{H}} \hat{H} \right| \pi \right\rangle = \omega_0 \left\langle \phi \left| \frac{1}{\varepsilon - \hat{H}} \right| \phi \right\rangle + \frac{4\lambda\langle \phi \rangle}{\varepsilon} \quad . \tag{B14}$$

Next,

$$\langle \phi | \pi \rangle = \langle \phi^+ \pi + \pi\phi^+ \rangle = \langle \phi\pi + \pi\phi \rangle, \tag{B15}$$

which using (B11) can be rewritten as

$$\langle \phi | \pi \rangle = 2 + 2\langle \phi\pi \rangle. \tag{B16}$$

Now using (23) and (24), we have

$$\langle \phi\pi \rangle = \langle \psi_0 | \phi\pi | \psi_0 \rangle = \langle 0 | S^{-1}\phi S S^{-1}\pi S | 0 \rangle$$

$$= \left\langle 0 \left| (\phi - \frac{2\lambda}{\omega_0})\pi \right| 0 \right\rangle = -1. \tag{B17}$$

Substituting (B17) in (B16)

$$\langle \phi | \pi \rangle = 0. \tag{B18}$$

Finally, (B5), (B14) and (B18) leads to

$$\varepsilon \left\langle \phi \left| \frac{1}{\varepsilon - \hat{H}} \right| \pi \right\rangle = \omega_0 \left\langle \phi \left| \frac{1}{\varepsilon - \hat{H}} \right| \phi \right\rangle + \frac{4\lambda \langle \phi \rangle}{\varepsilon} ,$$

which is (31).

Appendix C. Evaluation of $d_{\phi\phi}$ via superoperator inner projection method

Before proceeding for the derivation of $d_{\phi\phi}$, we evaluate certain relevant bilinear products.

(1) $$\langle \pi | \phi \rangle = \langle \pi^+ \phi + \phi \pi^+ \rangle. \tag{C1}$$

Since $\pi^+ = (b - b^+)^+ = -(b - b^+) = -\pi$

$$\langle \pi | \phi \rangle = -\langle \pi\phi + \phi\pi \rangle = -\langle \phi | \pi \rangle ,$$

or from (B18)

$$\langle \pi | \phi \rangle = \langle \phi | \pi \rangle = 0. \tag{C2}$$

(2) $$\langle \pi | \pi \rangle = \langle \pi^+ \pi + \pi\pi^+ \rangle = -2\langle \pi^2 \rangle.$$

From (23)

$$\langle \pi | \pi \rangle = -2\langle 0 | S^{-1}\pi^2 S | 0 \rangle = 2. \tag{C3}$$

(3) $$\langle \pi | \pi\phi - \phi\pi \rangle = \langle -\pi\pi\phi - \pi\phi\pi \rangle - \langle -\pi\phi\pi - \phi\pi\pi \rangle$$

$$= \langle -\pi\pi\phi + \phi\pi\pi \rangle. \tag{C4}$$

From the above expression and (B11)

$$\langle \pi | \pi\phi - \phi\pi \rangle = -4\langle \pi \rangle.$$

using (23) to evaluate $\langle \pi \rangle$, we get

$$\langle \pi | \pi\phi - \phi\pi \rangle = 0. \tag{C5}$$

(4) $$\langle 1 | A \rangle = 2\langle A \rangle , \tag{C6}$$

$$\langle A | 1 \rangle = 2\langle A^+ \rangle , \tag{C7}$$

for any operator A.

Now, from (37) and (A4)

$$d_{\phi\phi} = \langle\phi|\bar{h}\rangle\langle\bar{h}|\varepsilon-\hat{H}|\bar{h}\rangle^{-1}\langle\bar{h}|\phi\rangle$$

$$=[\langle\phi|\phi\rangle\langle\phi|\pi\rangle\langle\phi|1\rangle]$$

$$\begin{bmatrix}\langle\phi|\varepsilon-\hat{H}|\phi\rangle & \langle\phi|\varepsilon-\hat{H}|\pi\rangle & \langle\phi|\varepsilon-\hat{H}|1\rangle\\ \langle\pi|\varepsilon-\hat{H}|\phi\rangle & \langle\pi|\varepsilon-\hat{H}|\pi\rangle & \langle\pi|\varepsilon-\hat{H}|1\rangle\\ \langle 1|\varepsilon-\hat{H}|\phi\rangle & \langle 1|\varepsilon-\hat{H}|\pi\rangle & \langle 1|\varepsilon-\hat{H}|1\rangle\end{bmatrix}^{-1}\begin{bmatrix}\langle\phi|\phi\rangle\\ \langle\pi|\phi\rangle\\ \langle 1|\phi\rangle\end{bmatrix} \tag{C8}$$

Using (B2), (B3), (B6), (B12), (C2), (C3),(C5)–(C7) and

$$\hat{H}1 = 0;\ \langle 1|1\rangle = 2, \tag{C9}$$

the expression (C8) is written as

$$d_{\phi\phi} = [2\langle\phi^2\rangle\ 0\ 2\langle\phi\rangle]$$

$$\begin{bmatrix}2\varepsilon\langle\phi^2\rangle & -2\omega_0\langle\phi^2\rangle-4\lambda\langle\phi\rangle & 2\varepsilon\langle\phi\rangle\\ -2\omega_0 & 2\varepsilon & -2\varepsilon\langle\pi\rangle\\ 2\varepsilon\langle\phi\rangle & 2\varepsilon\langle\pi\rangle & 2\varepsilon\end{bmatrix}^{-1}\begin{bmatrix}-2\langle\phi^2\rangle\\ 0\\ 2\langle\phi\rangle\end{bmatrix} \tag{C10}$$

Substituting $\langle\phi\rangle$ and $\langle\phi^2\rangle$ from (34) and [cf.(23)]

$$\langle\pi\rangle = 0, \tag{C11}$$

in (C10), we get

$$d_{\phi\phi} = \frac{2\varepsilon}{\varepsilon^2-\omega_0^2} + \frac{8\lambda^2}{\omega_0^2}\frac{1}{\varepsilon} \tag{C12}$$

which is (35) of the text.

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