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by

J. G. Ramos and A. A. Gomes

CENTRO BRASILEIRO DE PESQUISAS FÍSICAS

Av. Wenceslau Braz, 71

RIO DE JANEIRO

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REMARKS ON THE RETARDED AND ADVANCED GREEN'S FUNCTIONS

J. G. Ramos and A. A. Gomes
Centro Brasileiro de Pesquisas Físicas

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ABSTRACT: The connection between time correlation and retarded, advanced Green's functions is dicussed in a systematic way. The occurence of a time independent contribution to the time correlation function is connected to commutator defined Green's function, and a simple rule is given for its calculation when a suitable decoupling is available.

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I. INTRODUCTION

The method of double-time Green's functions has been widely used in solid state physics, and excellent reviews such as Zubarev's [1] have shown how powerful the method is. Recently, Stevens and Toombs [2] pointed out that special care should be taken when calculating time correlation functions from previously determined Green's functions. Their main point is that if one defines the Green's function through a commutator, sometimes a constant [3] should be added to the usual expression for the time correlation function as given in terms of the jump of the propagator on the real axis [1]. The purpose of this paper is to dicuss in a systematic way why this constant should be included, and how this is correlated to the structure of the commutator Green's function. Our main point is that the commutator Green's function for two operators A and B involves only off-diagonal matrix elements ($E_n \neq E_m$) of these operators, whereas the time correlation function involves also the diagonal ones ($E_n = E_m$). Consequently the usual spectral representation technique [1] for calculating the time correlation function is not in general sufficient to determine it completely. It follows also from these remarks that the commutator Green's function has no pole at frequency $E = 0$, while the anticommutator Green's function may have a pole at this frequency and its residue is directly connected to the constant discussed above (thus providing an unique determination of it). We have also verified that for both types of Green's functions the physical considerations used in the decoupling procedures are the same and this provides a simple method for the complete determination of the correlation functions. Finaly, the regularity of the commutator Green's function for zero frequency introduces restrictions on the possible decoupling schemes. This regularity is an essential feature since if it is not verified, the calculation of the correlation functions from the Green's function are entirely misleading.

II. RETARDED AND ADVANCED GREEN'S FUNCTIONS

The commutador and anticommutador, retarded and advanced Green's functions are defined as usually:

$$\langle\langle A(t); B(t')\rangle\rangle_r^{(\mp)} = -i\theta(t-t')\langle [A(t), B(t')]_{\mp} \rangle , \qquad (1\text{-}a)$$

$$\langle\langle A(t); B(t')\rangle\rangle_a^{(\mp)} = -i\theta(t'-t)\langle [A(t), B(t')]_{\mp} \rangle , \qquad (1\text{-}b)$$

where $\theta(t)$ is the Heaviside's function, (-) is for commutator, (+) is for anticommutator and

$$\langle \ldots \rangle = \frac{1}{Z} Tr(e^{-H\beta} \ldots),$$

where Z is the partition function and $\beta = (k_B T)^{-1}$. In any case, the explicit structure of (1-a) and (1-b) involves the form of the time correlation functions $\langle A(t) B(t')\rangle$ and $\langle B(t') A(t)\rangle$. In order to get these time correlation functions in a clear form, let us introduce the complete set $\{|n\rangle\}$ of eigenstates of the Hamiltonian, corresponding to exact eigenvalues E_n. The time correlation functions read:

$$\langle B(t')A(t)\rangle = (1/Z) \sum_{n,m} \langle n|B|m\rangle\langle m|A|n\rangle \; e^{-E_n\beta} \, e^{-i(E_n-E_m)(t-t')} \qquad (2\text{-}a)$$

$$\langle A(t)B(t')\rangle = (1/Z) \sum_{n,m} \langle n|B|m\rangle\langle m|A|n\rangle\, e^{-E_m\beta}\, e^{-i(E_n-E_m)(t-t')} \tag{2-b}$$

Using (2-a) and (2-b) the averages $\left\langle \left[A(t),\, B(t')\right] \right\rangle$ are given by:

$$\left\langle \left[A(t),\, B(t')\right]_- \right\rangle = (1/Z) \sum_{\substack{n,m \\ E_n \neq E_m}} \langle n|B|m\rangle\langle m|A|n\rangle \left(e^{-E_n\beta} - e^{-E_m\beta} \right) e^{-i(E_n-E_m)(t-t')} \tag{3-a}$$

$$\left\langle \left[A(t),\, B(t')\right]_+ \right\rangle = (1/Z) \sum_{n,m} \langle n|B|m\rangle\langle m|A|n\rangle \left(e^{-E_n} + e^{-E_m} \right) e^{-i(E_n-E_m)(t-t')} \tag{3-b}$$

We wish to emphasize that even in the case of degenerate levels, all the diagonal ($E_n = E_m$) contributions in (3-a) are canceled out by the difference of exponentials, while the diagonal ($E_n = E_m$) contributions are also included in (3-b). Thus the analysis in terms of exact eigenstates enables us to conclude that in the commutator Green's function only off-diagonal ($E_n \neq E_m$) matrix elements of the operators A and B are involved, while in the anticommutator Green's functions all matrix elements are present. In this connection, it may be mentioned that the response to an external perturbation (generalized susceptivility) is given by a commutator Green's function [4], and consequently involves only off-diagonal ($E_n \neq E_m$) matrix elements. Then we can say that the commutator Green's function describes how transitions between eigenstates induced by the "external" operator B modify the thermal average of an observable A. Finally, one concludes that the usual linear response method can be applied only to cases where one knows that the representative operators have only non-vanishing the off-diagonal ($E_n \neq E_m$) matrix elements [5].

We introduce now the Fourier transforms $\langle\langle A;B\rangle\rangle^{(\mp)}_{E,a,r}$ suitably extended to complex energies by [1]:

$$\langle\langle A;B\rangle\rangle^{(\mp)}_{E,a,r} = (1/2\pi)\int_{-\infty}^{+\infty} \langle\langle A(t);B(t')\rangle\rangle^{(\mp)}_{a,r}\, e^{iE(t-t')}\, d(t-t')\ , \quad (4)$$

where in order that (4) have meaning the following conditions should hold:

$$\begin{aligned} &\langle\langle A;B\rangle\rangle^{(\mp)}_{E,r} \quad \text{defined for } \operatorname{Im} E > 0\ , \\ &\langle\langle A;B\rangle\rangle^{(\mp)}_{E,a} \quad \text{defined for } \operatorname{Im} E < 0\ . \end{aligned} \qquad (5)$$

These relations define analytical functions $\langle\langle A;B\rangle\rangle^{(\mp)}_{E}$, which coincide with those defined in (5) in the respective half-planes. Using the above equations one obtains:

$$\langle\langle A;B\rangle\rangle^{(-)}_{E} = \frac{1}{2\pi Z} \sum_{\substack{n,m \\ E_n \neq E_m}} \frac{\langle n|B|m\rangle\langle m|A|n\rangle}{E + E_n - E_m} \left(e^{-E_n\beta} - e^{-E_m\beta}\right) \qquad (6)$$

and

$$\langle\langle A;B\rangle\rangle^{(+)}_{E} = \frac{1}{2\pi Z} \sum_{n,m} \frac{\langle n|B|m\rangle\langle m|A|n\rangle}{E + E_n - E_m} \left(e^{-E_n\beta} + e^{-E_m\beta}\right) \qquad (7)$$

In the explicit forms (6) and (7) one sees that the functions $\langle\langle A;B\rangle\rangle^{(\mp)}_{E}$ are analytic functions for $\operatorname{Im} E \neq 0$, with singularities on the real axis, corresponding to the excitations of the system [6]. It follows also from equation (6) that the limit for $E \to 0$ (in the complex plane) exists, is well defined and given by:

$$\lim_{E \to 0} \langle\langle A;B \rangle\rangle_E^{(-)} = \frac{1}{2\pi Z} \sum_{\substack{n,m \\ E_n \neq E_m}} \frac{\langle n|B|m\rangle\langle m|A|n\rangle}{E_n - E_m} \left(e^{-E_n\beta} - e^{-E_m\beta}\right) , \quad (8)$$

and this limit is adopted as the definition of the Green's function at origin. The regularity of the commutator Green's function can be stated in an equivalent form:

$$\lim_{E \to 0} \left\{ E \langle\langle A;B \rangle\rangle_E^{(-)} \right\} = 0 . \quad (9)$$

The situation is rather different for anticommutator Green's funåtions; quite similarly it can be shown that:

$$\lim_{E \to 0} \left\{ E \langle\langle A;B \rangle\rangle_E^{(+)} \right\} = C/\pi , \quad (10\text{-a})$$

where

$$C = 1/Z \sum_{\substack{n,m \\ E_n = E_m}} \langle n|B|m\rangle \langle m|A|n\rangle e^{-E_n\beta} . \quad (10\text{-b})$$

These expressions mean that if C is non-zero, the anticommutator Green's function has a pole at E=0 and conversely if the Green's function $\langle\langle A;B \rangle\rangle_E^{(+)}$ has a pole at E=0 the corresponding residue is C/π. These remarks will be of fundamental importance in the determination of the time correlation functions. In this connection, we should mention that Callen et al.[7] discussed the problem of the determination of the constant C. Their results will be critically analyzed within the framework of spectral representations.

III. SPECTRAL REPRESENTATIONS

We now discuss how these results affect the usual theory of spectral representations.

First we define as in [1] the spectral density:

$$J(\omega) = 1/Z \sum_{n,m} \langle n|B|m\rangle \langle m|A|n\rangle \; e^{-E_n\beta} \delta(\omega - E_n + E_m) \, . \qquad (11)$$

The time correlations functions are connected to $J(\omega)$ by [1]:

$$\langle B(t')\, A(t)\rangle = \int_{-\infty}^{+\infty} J(\omega)\, e^{-i\omega(t-t')}\, d\omega \qquad (12\text{-a})$$

$$\langle A(t)\, B(t')\rangle = \int_{-\infty}^{+\infty} J(\omega)\, e^{\omega\beta}\, e^{-i\omega(t-t')}\, d\omega \qquad (12\text{-b})$$

Comparison of equations (10-b) and (11) suggests us to divide the spectral density in two contributions:

$$J(\omega) = J_o(\omega) + J'(\omega) \, , \qquad (13)$$

where

$$J_o(\omega) = C\, \delta(\omega) \qquad (13\text{-b})$$

and

$$J'(\omega) = 1/Z \sum_{\substack{n,m \\ E_n \neq E_m}} \langle n|B|m\rangle \langle m|A|n\rangle \; e^{-E_n\beta} \delta(\omega - E_n + E_m) \, . \qquad (13\text{-c})$$

The definition (13-c) implies that $J'(0) = 0$, and this means that in $J'(\omega)$ only the excitation spectrum is included. From (13) and (12) one gets:

$$\langle B(t') A(t)\rangle = C + \int_{-\infty}^{+\infty} J'(\omega)\, e^{-i\omega(t-t')}\, d\omega \qquad (14\text{-a})$$

$$\langle A(t) B(t')\rangle = C + \int_{-\infty}^{+\infty} J'(\omega)\, e^{\omega\beta} e^{-i\omega(t-t')}\, d\omega . \qquad (14\text{-b})$$

These expressions show that π times the residue at origin (when the pole exists) of the anticommutator Green's functions gives the time independent part of the time correlation functions.

Using equations (14) and the definitions (1) and (4) it is easily shown that:

$$\langle\langle A;B\rangle\rangle_E^{(-)} = 1/2\pi \int_{-\infty}^{+\infty} (e^{\omega\beta} - 1)\, J'(\omega)\, d\omega/E-\omega, \qquad (15\text{-a})$$

$$\langle\langle A;B\rangle\rangle_E^{(+)} = 1/2\pi \int_{-\infty}^{+\infty} (e^{\omega\beta} + 1)\, J(\omega)\, d\omega/E-\omega . \qquad (15\text{-b})$$

We wish to emphasize that in the commutator Green's function (15-a) only the $J'(\omega)$ part of the spectral density contributes to the spectral representation, since the constant C of (14) cancels out; in the anticommutator Green's functions however the complete spectral density is present. These spectral representations provide a useful way for determining $J'(\omega)$ or $J(\omega)$ from the corresponding Green's functions [1]:

$$J'(\omega) = \frac{i}{e^{\omega\beta}-1} \lim_{\epsilon\to 0} \left\{ \langle\langle A;B\rangle\rangle^{(-)}_{\omega+i\epsilon} - \langle\langle A;B\rangle\rangle^{(-)}_{\omega-i\epsilon} \right\} \quad (16\text{-a})$$

and

$$J(\omega) = \frac{i}{e^{\omega\beta}+1} \cdot \lim_{\epsilon\to 0} \left\{ \langle\langle A;B\rangle\rangle^{(+)}_{\omega+i\epsilon} - \langle\langle A;B\rangle\rangle^{(+)}_{\omega-i\epsilon} \right\} \quad (16\text{-b})$$

Substituting (16-a) in (14-a), for instance, one gets the expression first derived by [2]:

$$\langle B(t')A(t)\rangle = C + \lim_{\epsilon\to 0} i \int_{-\infty}^{+\infty} \frac{\langle\langle A;B\rangle\rangle^{(-)}_{\omega+i\epsilon} - \langle\langle A;B\rangle\rangle^{(-)}_{\omega-i\epsilon}}{e^{\omega\beta}-1} e^{-i\omega(t-t')} d\omega \quad (17)$$

One should note that the integrand of equation (17) is perfectly defined at $\omega = 0$, since the condition $J'(0) = 0$ must be satisfied, and except for the exponential $e^{-i\omega(t-t')}$ this integrand is precisely equation (16-a). In this connection, (16-a) provides a restriction for the decoupling schemes to break the infinite chain of equations associated with the determination of $\langle\langle A;B\rangle\rangle^{(-)}_{E}$: the acceptable schemes are such that the commutator Green's function has no pole at $E = 0$ and $J'(0) = 0$. This restriction can be put in a more explicit form using equation (16-a); in order to have $J'(0) = 0$ the Green's function must satisfy:

$$\lim_{\omega\to 0} J'(\omega) = i \lim_{\omega\to 0} \frac{\frac{d}{d\omega} \lim_{\epsilon\to 0} \left\{ \langle\langle A;B\rangle\rangle^{(-)}_{\omega+i\epsilon} - \langle\langle A;B\rangle\rangle^{(-)}_{\omega-i\epsilon} \right\}}{\frac{d}{d\omega}(e^{\omega\beta}-1)} = 0. \quad (18)$$

Equation (18) can be used as a simple algorithm to check the suitability of the decoupling scheme.

In conclusion, one sees that commutator Green's functions should be handled carefully when calculating time correlation functions, and depending on the nature of the problem, the constant C may play a fundamental role [8]. However the problem of knowing "a priori", if the constant C is zero or not, still remains. This problem in general cannot be solved because the exact eigenstates are not known, but the above equations provide a simple trick to check the doubtful cases. In fact, the physical considerations involved in the decoupling procedures do not depend on the definition of the Green's functions, as one verifies easily by inspection of the equations of motion. In this way, using the same approximations, one calculates the anticommutator Green's function, and if it admits a pole at $E = 0$, the constant C is π times the residue at this pole.

Now the results of Callen et al. [7] will be discussed in the light of the present formulation. These authors define new operators $\tilde{A} = A - \langle A \rangle$ and $\tilde{B} = B - \langle B \rangle$, and introduce new Green's functions $G_{\tilde{A}\tilde{B}}$, which are identical to our $G^{(-)}_{AB}$. As a consequence of this fact, equation (16-a) implies that:

$$J'_{\tilde{A}\tilde{B}}(\omega) = J'_{AB}(\omega) , \tag{19}$$

showing that the same physical information is contained in both formulations.

The same procedure can be used to define a constant $\tilde{C}$ (in complete analogy to (10-b), the A and B operators being replaced by $\tilde{A}$ and $\tilde{B}$). After algebraic manipulation of this formula it can be shown that:

$$\tilde{C} = C - \langle A\rangle\langle B\rangle \, . \tag{20}$$

Expression (20) has two fundamental implications: first it provides a connection between the two constants; second, this connection is precisely the difference between the usually defined time correlation function $\langle B(0)\, A(t)\rangle$ and the new definition $\langle \tilde{B}(0)\, \tilde{A}(t)\rangle$. In fact, using (19), (17) and the modified version of (17) for the $\tilde{A}$ and $\tilde{B}$ operators it follows that:

$$\langle\tilde{B}(0)\tilde{A}(t)\rangle = \langle B(0)A(t)\rangle + \tilde{C} - C = \langle B(0)\, A(t)\rangle - \langle A\rangle\langle B\rangle \tag{21}$$

These expressions show that, although the constants are different, the same formal expression can be used for the time correlation functions as given in terms of Green's functions (in terms of A, B operators or $\tilde{A}$, $\tilde{B}$ operators), and the relation between these constants is provided by (20).

If A and B operate in independent subsystems, from (10-b) and from the fact that the partition function in this case is a product of the partition function of each subsystem it follows that the constant C is precisely $\langle A\rangle\langle B\rangle$. Finally, applications of this method to particular systems will be presented in a forthcoming publication.

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