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1969 J. Phys. A: Gen. Phys. 2 503

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Correlation functions and Green functions: zero-frequency anomalies†

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MS. received 15th July 1968, in revised form 24th March 1969

Abstract. Some problems associated with the zero-frequency component of the correlation function $J(0)$, its calculation from thermal Green functions and its physical interpretation are studied. Various proposals for determining $J(0)$, which are not directly obtainable from the Green function, are examined and a new method proposed. The related question of the zero-frequency limit of $J(\omega)$ is also considered.

1. Introduction

Some limitations on the use of two-time 'boson-like' Green functions (Zubarev 1960) in the determination of correlation functions have recently been discussed by several authors (Stevens and Tombs 1965, Fernandez and Gersch 1967, Callen *et al.* 1967). We wish to examine and to extend these discussions with particular emphasis on the physical basis of the problems involved and to propose a new method for their resolution.

Stevens and Tombs (1965) first noted that the zero-frequency component of the spectral distribution function $J(\omega)$ is not in general determined by the Green function method. Fernandez and Gersch (1967) then gave an expression for $J(0)$ in terms of the exact eigenstates of the system. While their expression does not directly relate $J(0)$ to the Green function, they did suggest in the same paper a method which under certain conditions will determine $J(0)$ from the Green function. The method consists of introducing a symmetry breaking term into the Hamiltonian, calculating the correlation function, and then, in the final step, letting the symmetry breaking term go to zero. Their additional suggestion, that, since the correlation function and the Green function satisfy the same differential equation with the exception of an inhomogeneous term, a pole of the Green function for $\omega = 0$ implies the existence of a time-independent constant in the correlation function, does not take into account the fact that the two equations are associated with different boundary conditions. The actual conditions for the existence of the constant are more complicated.

Callen *et al.* (1967) approached the problem from a somewhat different point of view. Noting that the zero-frequency component of the spectral distribution function $J(\omega)$ is associated with the infinite time behaviour of the correlation function, they suggested that $J(0)$ be chosen in such a manner that the correlation function factors for infinite time separation, i.e.

$$\lim_{t' \rightarrow t \rightarrow \infty} \langle B(t')A(t) \rangle = \langle B \rangle \langle A \rangle. \quad (1)$$

This factorized form does not in general agree with the rigorous results given by Fernandez and Gersch but represents an approximation through which irreversibility is introduced into the system. It is subject to the objection that irreversibility is also usually introduced through the truncation of higher-order Green functions and that questions can arise concerning the mutual consistency of the various approximations. Cases also occur in which (1) would not be expected to hold and these would need to be approached by an alternative technique.

† This research was supported by the United States Air Force Office of Scientific Research through a grant No. AFOSR 1075-66.

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§ Supported by United States Air Force of Scientific Research under Grant No. AF 68-1416.

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With these observations we shall consider the following questions:

- (i) Under what conditions are there anomalous contributions to $J(0)$ and what physical interpretation can be ascribed to them? How can they be calculated?
 (ii) What statements can be made about the closely related question of the $\lim_{\omega \rightarrow 0} J(\omega)$.

2. The zero-frequency component

We begin by briefly reviewing the connection between the correlation and the relevant Green functions.

Although a differential equation can be derived for the correlation function

$$\langle B(t')A(t) \rangle = \int_{-\infty}^{\infty} d\omega J_{AB}(\omega) \exp\{-i\omega(t-t')\} \quad (2)$$

the boundary conditions are difficult to satisfy and one generally obtains the correlation function by first determining a related Green function, the analytic properties of which lead to considerably simpler boundary conditions. The retarded Green function is defined by the relation

$$G_{A,B}(t-t') = \langle\langle A(t); B(t') \rangle\rangle = -i\theta(t'-t) \langle [A(t), B(t')] \rangle \quad (3)$$

where $\theta(t)$ is a step function, the angular brackets represent an average over a grand canonical ensemble, $A(t)$ and $B(t')$ are operators in the Heisenberg picture, and the expression in square brackets is a commutator. The retarded Green function may also be defined in terms of an anticommutator, but we are concerned here with boson-like operators for which it is more convenient to use a commutator. If we define an effective density of states $\rho(\omega)$ by the relation

$$\rho(\omega) = i\{G_{A,B}(\omega + i\delta) - G_{A,B}(\omega - i\delta)\} \quad (4)$$

we may then determine $J(\omega)$ for $\omega \neq 0$ from the expression

$$\rho(\omega) = (e^{\beta\omega} - 1)J(\omega), \quad \omega \neq 0 \quad (5)$$

However, $J(0)$ is not determined by the Green function.

One would like to determine $J(\omega)$ from a sum rule on $J(\omega)$, but the natural sum rule is for $\rho(\omega)$

$$\int_{-\infty}^{\infty} d\omega \rho(\omega) = \langle [A, B] \rangle \quad (6)$$

and we can only re-express this in terms of $J(\omega)$ for $\omega \neq 0$, since (5) is only valid in that range.

If $J(\omega)$ is bounded in the neighbourhood of $\omega = 0$, we see from (2) that the correlation function $\langle B(t')A(t) \rangle$ vanishes in the limit of infinite times.

If, on the other hand, $J(\omega)$ had the form

$$J(\omega) = \bar{J}(\omega) + c\delta(\omega) \quad (7)$$

then the delta function gives rise to a constant contribution to the correlation function, and hence to an infinite time behaviour. $\bar{J}(\omega)$ can also contribute to the infinite time behaviour if it is sufficiently singular at the origin. If, for example, $\bar{J}(\omega)$ should go as c'/ω , this would contribute to the infinite time behaviour. In this case the prescription of Callen *et al.* would consist of setting the constant c in (7) equal to $\langle A \rangle \langle B \rangle$ and subtracting the infinite time contribution from $\bar{J}(\omega)$ from the general equation (2), since they would discard all but the factored result.

The simplest case in which $J(\omega)$ has a delta-function singularity is that in which $A = B = Q$, where Q is a constant of the motion; then $Q(t') = Q(t) = Q$, and hence, since $G_{Q,Q}$ is defined in terms of a commutator

$$G_{Q,Q}(t-t') = \langle\langle Q(t); Q(t') \rangle\rangle = 0 \quad (8)$$

so that

$$J(\omega) = 0 + Q^2\delta(\omega). \quad (9)$$

We notice that for this case the criterion of Fernandez and Gersch which states that a singularity in $J(\omega)$ will appear if, and only if, $G(\omega)$ has a pole at $\omega = 0$ does not apply, since the Green function is identically zero.

One can easily generalize the above discussion to operators of the form $A = A_1 + A_2$, where A_1 is a constant of the motion. We will give an example of this form below.

3. The correlation function for density-density fluctuations

In this section we will consider the problem of density-density fluctuations in a non-interacting electron gas in order to establish a basis for the new method of determining $J(0)$ in the next section. We present results in terms of this simple example since they are in fact typical of many 'normal' systems, such as the high-density electron gas.

Omitting the spin for simplicity, we consider the Green function $\langle\langle \rho_q; \rho_q^+ \rangle\rangle$, where ρ_q is the density fluctuation operator defined by

$$\rho_q = \sum_k c_{k+q}^+ c_k \tag{10}$$

and the c_k and c_k^+ are the usual electron annihilation and creation operators.

We first note that ρ_0 is equal to the number operator N for the system and is therefore a constant of the motion. Hence, by our previous discussion, the Green function is identically zero. As a possible way out of this dilemma, we consider the Green function for $q \neq 0$, calculate the correlation function and then take the limit $q \rightarrow 0$. Carrying through the calculation, we find

$$\lim_{q \rightarrow 0} \langle \rho_q^+ \rho_q \rangle = \sum_k f_k (1 - f_k) = \langle N^2 \rangle - \langle N \rangle^2 \tag{11}$$

where

$$f_k = \{ \exp(\beta \epsilon_k) + 1 \}^{-1} \tag{12}$$

the Fermi distribution function f_k being expressed in terms of the energy ϵ_k which is measured with respect to the Fermi energy. The second equality can be confirmed by direct calculation.

On the other hand, identifying $\langle \rho_0^+ \rho_0 \rangle$ with N^2 , we find by direct calculation that

$$\langle \rho_0^+ \rho_0 \rangle = \langle N^2 \rangle = \left(\sum_k f_k \right)^2 + \sum_k f_k (1 - f_k). \tag{13}$$

Thus we find

$$\langle \rho_0^+ \rho_0 \rangle \neq \lim_{q \rightarrow 0} \langle \rho_q^+ \rho_q \rangle \tag{14}$$

although the fluctuation term is contained in both.

We see therefore that by considering an alternative Green function to that which one would naturally tend to consider and then using a limiting process we obtain the correct fluctuations in N^2 although we are still lacking the term $\langle N \rangle^2$.

If we could directly identify the constants of motion, we could use this method to calculate the fluctuations and add the square of thermal average of the constants of motion. We cannot always do this since quantities which are approximate constants of motion (frequently S^2 operators), or as noted above of the type $A = A_1 + A_2$, where A_1 is a constant of motion, lead to difficulties. This latter case also causes problems with the application of the Fernandez and Gersch approach.

Suppose we add a BCS-type pairing term

$$\lambda \sum_k (a_k^+ a_{-k}^+ + a_{-k} a_k)$$

to the Hamiltonian; $\rho_0 = N$ is then no longer a constant of the motion. A calculation of the $\lambda \rightarrow 0$ limit of $\langle \rho_0^+ \rho_0 \rangle_\lambda$ from the Green function again does not correctly determine $\langle \rho_0^+ \rho_0 \rangle$. The source of the error is that in terms of the operators which diagonalize $H\lambda$, ρ_0 still contains a part which commutes with $H\lambda$.

4. Alternative Green functions

We shall now discuss a method for calculating $J(0)$ by means of alternative Green functions which has a wide range of applicability. For definiteness and simplicity we consider the density-density fluctuation problem $\mathbf{q} = 0$. The more general case is also easily treated.

We recall that $J(\omega)$ is completely determined by the Green function except for $\omega = 0$. Inserting the expression for $J(\omega)$ from (7) into (2) we find

$$\langle B(t')A(0) \rangle = \int_{-\infty}^{\infty} d\omega \bar{J}(\omega) \exp(-i\omega t) + c \quad (13)$$

and therefore that

$$c = \langle B(0)A(0) \rangle - \int_{-\infty}^{\infty} d\omega \bar{J}(\omega) \quad (14)$$

so that, if we can calculate $\langle B(0)A(0) \rangle$ by some means, we can then obtain the complete correlation function $\langle B(t)A(0) \rangle$.

Now in the case of density-density fluctuations we defined our Green function in terms of a commutator rather than an anticommutator because the density fluctuation operators $\rho_{\mathbf{q}}, \rho_{\mathbf{q}}^+$ are 'boson-like' and the calculation is greatly simplified. Had we only been interested in the average

$$\langle \rho_0^2 \rangle = \langle N^2 \rangle \quad (15)$$

and not in the general correlation function we could equally well have considered Green functions of the form

$$\sum_{\mathbf{k}'} \langle\langle c_{\mathbf{k}'} \rho_0; c_{\mathbf{k}'}^+ \rangle\rangle.$$

The operators are then 'Fermi-like' and we can use conveniently Green functions defined in terms of anticommutators rather than commutators. For these Green functions (5) is replaced by

$$\rho(\omega) = \{e^{\beta\omega} + 1\}J(\omega) \quad (16)$$

and the problem at $\omega = 0$ does not arise.

For the general case we can then calculate $J(\omega)$ for $\omega \neq 0$ by 'boson' Green functions and for $\omega = 0$ by 'fermion' Green functions. In each case the natural choice, commutators or anticommutators, is used.

For the simple case under consideration one readily finds that $J(\omega) = 0$ and we correctly obtain

$$c = \left(\sum_{\mathbf{k}} f_{\mathbf{k}} \right)^2 + \sum_{\mathbf{k}} f_{\mathbf{k}}(1-f_{\mathbf{k}}). \quad (17)$$

The general approach is also useful in spin- $\frac{1}{2}$ problems in which one can replace S^z by $\frac{1}{2}(S^-S^+ + S^+S^-)$ and put the S^+ and S^- in opposite terms in the Green function. In this method the problem of consistency also arises since results depend on the use of two different Green functions.

5. The zero-frequency limit

Let us finally turn our attention to the examination of the zero-frequency limit of $J(\omega)$. The three characteristic types of results which we consider illustrate that the anomalies associated with the calculation of $J(0)$ are intimately connected with other long-time or in some cases long-range behaviour such as characteristically occur for ordered systems.

We first consider the case for which in the macroscopic limit $J(\omega)$ is continuous for ω in the neighbourhood of $\omega = 0$. In this case, only the term in (7) containing a delta function contributes to the infinite time behaviour. If $c = 0$ we then find a normal behaviour for $J(\omega)$, as discussed by Abrikosov *et al.* (1963), for which $\lim_{\omega \rightarrow 0} J(\omega) = \text{constant}$, giving no in-

finite time contribution. Thus, for example, for density-density fluctuations we find for

small q in a non-interacting system $\rho_q(\omega) \sim \omega$, but

$$\lim_{q \rightarrow 0} \rho_q(\omega) = \sum_k f_k(1-f_k)\delta(\omega)\beta\omega \tag{18}$$

and therefore for small ω we find

$$\lim_{q \rightarrow 0} J_q(\omega) = \rho_q(\omega)(e^{\beta\omega} - 1)^{-1} \sum_k f_k(1-f_k)\delta(\omega). \tag{19}$$

An evaluation for the high-density electron gas leads to a similar result. The infinite time behaviour, if any, is then given exclusively by the constant, while the rest is obtained from the usual Green function method.

The second case we consider is that of a bound spectrum of bosons for which the chemical potential is non-zero. In this case one must carefully treat the macroscopic limit. Thus for a system of non-interacting bosons at finite density n , taking $A(0) = a_q(0)$ and $B(t) = a_q^+(t)$ as the boson annihilation and creation operators

$$J(\omega) = \delta\left(\omega - \frac{q}{2m} + \frac{\alpha}{\beta}\right)(e^{\beta\omega} - 1)^{-1}. \tag{20}$$

with the chemical potential being written α/β . For high enough temperatures and finite volume, $\alpha < 0$ and the spectrum has a lower bound $\epsilon_0 > 0$, so that $\rho(\omega = 0) = 0$; for this case no problems arise. However, at a certain temperature for sufficiently large n if we let $V \rightarrow \infty$, keeping n constant, then α goes to zero. In this case $J_0(\omega) = 0$ for $\omega \neq 0$, while $J_0(0)$ is, as always, undetermined by the Green function. Here, however, the presence of the Bose-Einstein condensation requires taking the macroscopic limit with care. One must take α not zero, but of order $1/N$, whence, writing $\alpha = (\alpha N)^{-1}$,

$$J_0(\omega) = (e^{\beta\omega} - 1)^{-1} \delta\left(\omega + \frac{\alpha}{\beta}\right). \tag{21}$$

Thus we obtain a well-defined zero-frequency contribution to $J(0)$ in the macroscopic limit if we define

$$j_0(0) = \lim_{N \rightarrow \infty} \frac{J_0(\omega)}{N} = \lim_{N \rightarrow \infty} \frac{N^{-1}\delta(\omega)}{e^{\alpha} - 1} = a\delta(\omega). \tag{22}$$

Thus in this case the Green function completely determines all results, but only after a careful limiting procedure.

The last example which we shall discuss is one with a bounded spectrum, but with no analogue of the chemical potential present. The case examined is that of spin-wave excitations in a ferromagnet. In the absence of a magnetic field for sufficiently low temperatures, we can take the spin-wave energies to be

$$\epsilon_q = Aq^2. \tag{23}$$

We take $A = S_{-q}^-$ and $B = S_q^+$, and then

$$J_q(\omega) = \delta(\omega - Aq^2)(e^{\beta\omega} - 1)^{-1} \tag{24}$$

and it is most convenient to discuss the results in terms of

$$\langle S_q^+ S_{-q}^- \rangle = \int_{-\infty}^{\infty} d\omega \exp(-i0^+t) J_q(\omega). \tag{25}$$

As we have noted previously, $\langle S_0^+ S_0^- \rangle$ is not determined from the Green functions; the $q \rightarrow 0$ limit of (25) diverges:

$$\lim_{q \rightarrow 0} \langle S_q^+ S_{-q}^- \rangle = \lim_{q \rightarrow 0} \{\exp(-\beta Aq^2) - 1\}^{-1} = \infty. \tag{26}$$

We then include an external magnetic field h in energy units. Then

$$\epsilon_q(h) = Aq^2 + h. \quad (27)$$

We are then able to obtain

$$\langle S_0^+ S_0^- \rangle_h = (e^{\beta h} - 1)^{-1}$$

from the Green function as well as by direct evaluation. The limit of $h \rightarrow 0$ of this expression also diverges. Notice this divergence persists also for a finite system, a $q = 0$ mode corresponding to the rotation of the total spin.[†] The divergence of $J(0)$ (for $h = 0$) is real and is to be identified with the infinite transverse susceptibility associated with the rotation of the whole system. For a macroscopic system this should be excluded either due to (i) astronomically long relaxation times or (ii) the presence of small perturbing fields. Thus either $J(0)$ is to be discarded due to physical exclusion of rotations of the system or one can formally remove $J(0)$ by retaining a field large enough for $e^{\beta h} - 1 \ll N$, but small enough to modify $\sum_{q \neq 0} \langle S_q^+ S_{-q}^- \rangle$ negligibly.

6. Conclusion

In conclusion, we have studied methods of calculating and interpreting $J(0)$ and $\lim_{\omega \rightarrow 0} J(\omega)$. While $J(0)$ is not directly determinable by the Green function method, its contribution to the correlation function can frequently be calculated by considering a suitably defined second Green function. This provides an alternative approach to that suggested by Fernandez and Gersch, in which a symmetry breaking term is added to the Hamiltonian, or to that of Callen *et al.*, in which $J(0)$ is defined so that the correlation function factors for infinite time separation.

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[†] These two limits $\lim_{q \rightarrow 0} \langle S_q^+ S_{-q}^- \rangle$ and $\lim_{q \rightarrow 0} \langle S_0^+ S_0^- \rangle_h$ are physically distinct. The first is integrable in three dimensions and is related to spin-wave instability of the ferromagnetic state in one and two dimensions. The latter relates to instability to rotation of the total moment for vanishing magnetic field (see Kubo 1953).