

Undetermined-constant method in the boson Green's-function theory

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It is shown in the present paper that if operators of a boson Green's function involve arbitrary c numbers, then the corresponding correlation function obtained from the spectral theorem is independent of the c numbers, which is in contradiction with the definition of the said correlation function. In order to solve this problem we have introduced an undetermined-constant method and applied it to ferromagnetic and ferroelectric systems, respectively. It is pointed out that the introduction of the undetermined constant is an intrinsic characteristic of the boson Green's-function method and that contradictory results can often be obtained if it is not introduced.

I. INTRODUCTION

Since Bogolubov and Tyablikov¹ (hereafter abbreviated as BT) first applied the thermodynamic Green's-function method to study ferromagnetic systems in 1959, a lot of work has been done by using Green's-function methods in researching various systems, such as ferromagnetic and antiferromagnetic systems,²⁻⁴ ferroelectric and antiferroelectric systems,^{5,6} etc., and some interesting results have been obtained.

The main objective of BT's method is to solve directly the motion equation of the Green's function. Since there are two-particle Green's functions in motion equations of one-particle Green's functions, and three- or more-particle Green's functions in two-particle equations, and so on, an infinite chain of motion equations is obtained, which is insolvable. However, if the higher-order Green's functions are resolved into lower-order ones in a certain degree, the chain will be decoupled to form a closed set of equations. The above process is called a decoupling procedure. The needed Green's functions can be found from the solutions of the above equation set and the corresponding correlation functions from the spectral theorem, which makes both kinds of functions related to each other. The required physical quantities can be finally obtained from these correlation functions.

Green's functions can be classified into boson and fermion Green's functions. It is not difficult to establish from the definitions of Green's functions that when arbitrary c numbers are added to the operators of a boson Green's function, the Green's function itself remains unchanged. That causes the corresponding correlation function obtained from the spectral theorem to be also unchanged. But as an assembly average of the product of two operators it must change. Consequently the results, obtained from the spectral theorem by using the boson Green's functions, may be contradictory. This problem has been solved by means of an undetermined-constant method in the present paper. There is no undetermined-constant problem in the fermion Green's-function method.

Applications of the Green's-function method to ferromagnetic and ferroelectric systems are discussed here,

respectively. We have argued that if the undetermined constants are not considered, the results are contradictory, due to the very nature of the boson Green's-function method itself. In BT's work¹ a coincidence between the chosen operators and the chosen decoupling approximation made some, but not all, undetermined constants equal to zero, so that this contradiction was not revealed. Later authors also avoided this contradiction by various means, but their results may be not right. For example, the results of Ganguli *et al.*,⁶ which should be those of a molecular field approximation (MFA), are incorrect by a multiple factor. The reason is that they did not consider the undetermined constants.

II. GREEN'S FUNCTIONS AND CORRELATION FUNCTIONS

The retarded and advanced Green's functions of two operators A and B are defined as¹

$$\langle\langle A(t), B(t') \rangle\rangle^r = -i\Theta(t-t')\langle [A(t), B(t')]_\eta \rangle, \quad (1a)$$

$$\langle\langle A(t), B(t') \rangle\rangle^a = i\Theta(t'-t)\langle [A(t), B(t')]_\eta \rangle, \quad (1b)$$

where $A(t)$ and $B(t')$ are operators in the Heisenberg picture, $[A, B]_\eta = AB - \eta BA$, $\eta = \pm 1$, $\langle \rangle$ is the thermodynamic assembly average, and $\Theta(t)$ is the step function.

Customarily a Green's function is called a boson Green's function if $\eta = +1$ or a fermion Green's function if $\eta = -1$. The Fourier-transformed Green's function satisfies the motion equation

$$\langle\langle A, B \rangle\rangle_\omega = \frac{1}{2\pi} \langle [A, B]_\eta \rangle + \langle\langle [A, H], B \rangle\rangle_\omega, \quad (2)$$

where H is the Hamiltonian of the systems and

$$\langle\langle A, B \rangle\rangle_\omega = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \langle\langle A(t), B(t') \rangle\rangle e^{i\omega(t-t')} dt. \quad (3)$$

A correlation function is defined as an assembly average of the product of two operators. The relation between the correlation function $\langle BA \rangle$ and the related Green's function $\langle\langle A, B \rangle\rangle$ is given by the spectral theorem, i.e.,

$$\langle B(t')A(t) \rangle = i \int \frac{\langle\langle A, B \rangle\rangle_{\omega+i0^+} - \langle\langle A, B \rangle\rangle_{\omega-i0^+}}{e^{\beta\omega} - \eta} \times e^{-i\omega(t-t')} d\omega. \quad (4)$$

Since there is no symbol to indicate whether A and B are boson or fermion operators in the definition of the Green's function, and the above formulas are not restricted by the statistical characters, there are no inner links between boson or fermion Green's functions and boson or fermion statistics. In principle, the parameter η may be arbitrarily chosen as $+1$ or -1 as long as it is convenient. However, it is necessary to pay attention to the fact that if the Green's functions have zero-frequency poles, the integral in Eq. (4) will be divergent if $\eta = +1$ because of the factor $1/(e^{\beta\omega} - 1)$. The boson Green's function cannot be used under this circumstance.

It is very easy to show from the definition of the Green's function that if there are arbitrary c numbers in the operators forming a Green's function, the following relations hold:

$$\langle\langle A + \gamma, B + \gamma' \rangle\rangle \begin{cases} \neq \langle\langle A, B \rangle\rangle & \text{if } \eta = -1 \\ = \langle\langle A, B \rangle\rangle & \text{if } \eta = +1, \end{cases} \quad (5)$$

where γ and γ' are c numbers. Since a correlation function is an assembly average of the product of two operators, it follows that

$$\langle (B + \gamma')(A + \gamma) \rangle = \langle BA \rangle + \gamma \langle B \rangle + \gamma' \langle A \rangle + \gamma\gamma' \neq \langle BA \rangle. \quad (6)$$

But from (4) and (5) one calculates

$$\langle (B + \gamma')(A + \gamma) \rangle = \langle BA \rangle \quad \text{if } \eta = +1. \quad (7)$$

This is obviously incorrect. This problem has been solved by using an undetermined-constant method in this paper, i.e., the γ 's are introduced as undetermined constants. They (together with the required physical quantities) are determined by solving the equations of correlation functions.

III. GREEN'S-FUNCTION METHOD IN THE FERROMAGNETIC SYSTEM WITH SPIN $\frac{1}{2}$

In zero external field the Heisenberg Hamiltonian of a ferromagnetic system is

$$H = -J \sum_{i,a} \mathbf{S}_i \cdot \mathbf{S}_{i+a} = -J \sum_{i,a} [(S_i^+ S_{i+a}^- + S_i^- S_{i+a}^+) / 2 + S_i^z S_{i+a}^z], \quad (8)$$

where $S_i^\pm = S_i^x \pm iS_i^y$, J is an exchange integral, i is the lattice site position vector, and $i+a$ that of the nearest neighbor of site i .

The spin operators $\mathbf{S}_i = (S_i^x, S_i^y, S_i^z)$ satisfy the commutation rules of ordinary angular momentum operators, i.e.,

$$\begin{aligned} \mathbf{S}_i \times \mathbf{S}_j &= i \mathbf{S}_i \delta_{ij}, \quad [S_i^\pm, S_j^\pm] = \mp S_i^\pm \delta_{ij}, \\ [S_i^+, S_j^-] &= 2S_i^z \delta_{ij}, \quad \mathbf{S}_i \cdot \mathbf{S}_i = S(S+1), \\ [S_i^+, S_j^+] &= [S_i^-, S_j^-] = [S_i^z, S_j^z] = 0. \end{aligned} \quad (9)$$

Using Eqs. (8) and (9), we find

$$\begin{aligned} [S_i^z, H] &= -J \sum_a (S_i^+ S_{i+a}^- - S_{i+a}^+ S_i^-), \\ [S_i^\pm, H] &= \mp 2J \sum_a (S_i^z S_{i+a}^\pm - S_{i+a}^z S_i^\pm). \end{aligned} \quad (10)$$

Let us now choose operators $A, B = S_i^z, S_i^\pm$ to construct boson Green's functions. By substituting Eq. (10) into the motion equation (2) we obtain

$$\begin{aligned} \omega \langle\langle S_i^z, S_j^n \rangle\rangle &= \frac{\langle [S_i^z, S_j^n] \rangle}{2} - J \sum_a (\langle\langle S_i^+ S_{i+a}^-, S_j^n \rangle\rangle - \langle\langle S_{i+a}^+ S_i^-, S_j^n \rangle\rangle), \\ \omega \langle\langle S_i^\pm, S_j^n \rangle\rangle &= \frac{\langle [S_i^\pm, S_j^n] \rangle}{2} \mp 2J \sum_a (\langle\langle S_i^z S_{i+a}^\pm, S_j^n \rangle\rangle - \langle\langle S_{i+a}^z S_i^\pm, S_j^n \rangle\rangle), \end{aligned} \quad (11)$$

where $n = z, +, -$. Using the symmetric decoupling approximation (12) and the lattice Fourier transformation (13),

$$\langle\langle S_i^m S_i^{m'}, S_j^n \rangle\rangle \cong \langle S_i^{m'} \rangle \langle\langle S_i^m, S_j^n \rangle\rangle + \langle S_i^m \rangle \langle\langle S_i^{m'}, S_j^n \rangle\rangle, \quad (12)$$

$$\langle\langle S_i^m, S_j^n \rangle\rangle = \frac{1}{N} \sum_K G_K^{mn} e^{i\mathbf{K} \cdot (\mathbf{i} - \mathbf{j})}, \quad (13)$$

we obtain the equations satisfied by the Green's functions, i.e.,

$$\begin{pmatrix} \omega & \langle S^- \rangle \xi_K & -\langle S^+ \rangle \xi_K \\ 2\langle S^+ \rangle \xi_K & \omega - 2\langle S^z \rangle \xi_K & 0 \\ -2\langle S^- \rangle \xi_K & 0 & \omega + 2\langle S^z \rangle \xi_K \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \frac{1}{2\pi} \begin{pmatrix} G_K^{zz} \\ G_K^{+z} \\ G_K^{-z} \\ G_K^{z+} \\ G_K^{+-} \\ G_K^{z-} \\ G_K^{+-} \\ G_K^{--} \end{pmatrix} = \frac{1}{2\pi} \begin{pmatrix} 0 \\ -\langle S^+ \rangle \\ \langle S^- \rangle \\ \langle S^+ \rangle \\ 0 \\ 2\langle S^z \rangle \\ -\langle S^- \rangle \\ 2\langle S^z \rangle \\ 0 \end{pmatrix}, \quad (14)$$

where $\xi_K = J(0) - J(\mathbf{K})$, $J(\mathbf{K}) = J \sum_a e^{i\mathbf{K}\cdot\mathbf{a}}$, and \mathbf{K} is the wave vector.

Solving Eq. (14), we obtain the energy spectrum

$$\begin{aligned} \omega_K^2 &= 4(\langle S^+ \rangle \langle S^- \rangle + \langle S^z \rangle^2) \xi_K^2 \\ &= 4(\langle S^x \rangle^2 + \langle S^y \rangle^2 + \langle S^z \rangle^2) \xi_K^2 = 4\langle \mathbf{S} \rangle^2 \xi_K^2 \end{aligned} \quad (15)$$

and the Green's functions are

$$\begin{aligned} G_K^{zz} &= \frac{2\langle S^+ \rangle \langle S^- \rangle}{2\pi} \frac{\xi_K}{\omega^2 - \omega_K^2}, \\ G_K^{+z} &= -\frac{\langle S^+ \rangle}{2\pi} \frac{\omega + 2\langle S^z \rangle \xi_K}{\omega^2 - \omega_K^2}, \\ G_K^{-z} &= \frac{\langle S^- \rangle}{2\pi} \frac{\omega - 2\langle S^z \rangle \xi_K}{\omega^2 - \omega_K^2}, \\ G_K^{z+} &= \frac{\langle S^+ \rangle}{2\pi} \frac{\omega - 2\langle S^z \rangle \xi_K}{\omega^2 - \omega_K^2}, \\ G_K^{+ +} &= -\frac{2\langle S^+ \rangle^2}{2\pi} \frac{\xi_K}{\omega^2 - \omega_K^2}, \\ G_K^{z-} &= -\frac{\langle S^- \rangle}{2\pi} \frac{\omega + 2\langle S^z \rangle \xi_K}{\omega^2 - \omega_K^2}, \\ G_K^{- -} &= -\frac{2\langle S^- \rangle^2}{2\pi} \frac{\xi_K}{\omega^2 - \omega_K^2}, \\ G_K^{- +} &= -\frac{2}{2\pi} \frac{\langle S^z \rangle \omega - (2\langle S^z \rangle^2 + \langle S^+ \rangle \langle S^- \rangle) \xi_K}{\omega^2 - \omega_K^2}, \\ G_K^{+ -} &= \frac{2}{2\pi} \frac{\langle S^z \rangle \omega + (2\langle S^z \rangle^2 + \langle S^+ \rangle \langle S^- \rangle) \xi_K}{\omega^2 - \omega_K^2}. \end{aligned} \quad (16)$$

Introducing undetermined constants γ_1 , γ_2 , and γ_3 through

$$S^+ \sim S^+ + \gamma_1, \quad S^- \sim S^- + \gamma_2, \quad S^z \sim S^z + \gamma_3, \quad (17)$$

the correlation functions are found by using Eqs. (16), (17), and (4) in the form

$$\begin{aligned} \langle (S^z + \gamma_3)(S^z + \gamma_3) \rangle &= \langle (S^z)^2 \rangle + 2\gamma_3 \langle S^z \rangle + \gamma_3^2 \\ &= \langle S^+ \rangle \langle S^- \rangle D, \end{aligned} \quad (18a)$$

$$\begin{aligned} \langle (S^z + \gamma_3)(S^+ + \gamma_1) \rangle &= \langle S^z S^+ \rangle + \gamma_3 \langle S^+ \rangle \\ &\quad + \gamma_1 \langle S^z \rangle + \gamma_1 \gamma_3 \\ &= \frac{\langle S^+ \rangle}{2} - \langle S^+ \rangle \langle S^z \rangle D, \end{aligned} \quad (18b)$$

$$\begin{aligned} \langle (S^z + \gamma_3)(S^- + \gamma_2) \rangle &= \langle S^z S^- \rangle + \gamma_3 \langle S^- \rangle \\ &\quad + \gamma_2 \langle S^z \rangle + \gamma_2 \gamma_3 \\ &= -\frac{\langle S^- \rangle}{2} - \langle S^- \rangle \langle S^z \rangle D, \end{aligned} \quad (18c)$$

$$\begin{aligned} \langle (S^+ + \gamma_1)(S^z + \gamma_3) \rangle &= \langle S^+ S^z \rangle + \gamma_3 \langle S^+ \rangle \\ &\quad + \gamma_1 \langle S^z \rangle + \gamma_1 \gamma_3 \\ &= -\frac{\langle S^+ \rangle}{2} - \langle S^+ \rangle \langle S^z \rangle D, \end{aligned} \quad (18d)$$

$$\begin{aligned} \langle (S^+ + \gamma_1)(S^+ + \gamma_1) \rangle &= \langle (S^+)^2 \rangle + 2\gamma_1 \langle S^+ \rangle + \gamma_1^2 \\ &= -\langle S^+ \rangle^2 D, \end{aligned} \quad (18e)$$

$$\begin{aligned} \langle (S^+ + \gamma_1)(S^- + \gamma_2) \rangle &= \langle S^+ S^- \rangle + \gamma_1 \langle S^- \rangle \\ &\quad + \gamma_2 \langle S^+ \rangle + \gamma_1 \gamma_2 \\ &= \langle S^z \rangle + (2\langle S^z \rangle^2 + \langle S^+ \rangle \langle S^- \rangle) D, \end{aligned} \quad (18f)$$

$$\begin{aligned} \langle (S^- + \gamma_2)(S^z + \gamma_3) \rangle &= \langle S^- S^z \rangle + \gamma_2 \langle S^z \rangle + \gamma_3 \langle S^- \rangle + \gamma_2 \gamma_3 \\ &= \frac{\langle S^- \rangle}{2} - \langle S^- \rangle \langle S^z \rangle D, \end{aligned} \quad (18g)$$

$$\begin{aligned} \langle (S^- + \gamma_2)(S^+ + \gamma_1) \rangle &= \langle S^- S^+ \rangle + \gamma_2 \langle S^+ \rangle \\ &\quad + \gamma_1 \langle S^- \rangle + \gamma_1 \gamma_2 \\ &= -\langle S^z \rangle + (2\langle S^z \rangle^2 \\ &\quad + \langle S^+ \rangle \langle S^- \rangle) D, \end{aligned} \quad (18h)$$

$$\begin{aligned} \langle (S^- + \gamma_2)(S^- + \gamma_2) \rangle &= \langle (S^-)^2 \rangle + 2\gamma_2 \langle S^- \rangle + \gamma_2^2 \\ &= -\langle S^- \rangle^2 D, \end{aligned} \quad (18i)$$

where

$$D = \frac{1}{N} \sum_K \frac{\xi_K}{\omega_K} \coth \left[\frac{\beta \omega_K}{2} \right].$$

When spin $S = \frac{1}{2}$, we have

$$(S^z)^2 = \frac{1}{4}, \quad (S^+)^2 = (S^-)^2 = 0, \quad (19)$$

$$S^+ S^- + S^- S^+ = 1, \quad S^z = S^+ S^- - \frac{1}{2} = \frac{1}{2} - S^- S^+,$$

so that

$$\begin{aligned} \langle S^z S^+ \rangle &= -\langle S^+ S^z \rangle = \langle S^+ \rangle / 2, \\ \langle S^z S^- \rangle &= -\langle S^- S^z \rangle = -\langle S^- \rangle / 2, \\ \langle S^+ S^- \rangle &= \langle S^z \rangle + \frac{1}{2}, \quad \langle S^- S^+ \rangle = \frac{1}{2} - \langle S^z \rangle. \end{aligned} \quad (20)$$

Substituting Eqs. (20) to Eqs. (18), we get

$$\frac{1}{4} + 2\gamma_3 \langle S^z \rangle + \gamma_3^2 = \langle S^+ \rangle \langle S^- \rangle D, \quad (21a)$$

$$\gamma_3 \langle S^+ \rangle + \gamma_1 \langle S^z \rangle + \gamma_1 \gamma_3 = -\langle S^+ \rangle \langle S^z \rangle D, \quad (21b)$$

$$\gamma_3 \langle S^- \rangle + \gamma_2 \langle S^z \rangle + \gamma_2 \gamma_3 = -\langle S^- \rangle \langle S^z \rangle D, \quad (21c)$$

$$2\gamma_1 \langle S^+ \rangle + \gamma_1^2 = -\langle S^+ \rangle^2 D, \quad (21d)$$

$$\begin{aligned} \frac{1}{2} + \gamma_1 \langle S^- \rangle + \gamma_2 \langle S^+ \rangle + \gamma_1 \gamma_2 \\ = (2\langle S^z \rangle^2 + \langle S^+ \rangle \langle S^- \rangle) D, \end{aligned} \quad (21e)$$

$$2\gamma_2\langle S^- \rangle + \gamma_2^2 = -\langle S^- \rangle^2 D. \quad (21f)$$

The following quantities are obtained by solving Eqs. (21):

$$\gamma_1 = -\langle S^+ \rangle \left[1 \pm \left[1 - \frac{1}{4\langle S \rangle^2} \right]^{1/2} \right], \quad (22a)$$

$$\gamma_2 = -\langle S^- \rangle \left[1 \pm \left[1 - \frac{1}{4\langle S \rangle^2} \right]^{1/2} \right], \quad (22b)$$

$$\gamma_3 = -\langle S^z \rangle \left[1 \pm \left[1 - \frac{1}{4\langle S \rangle^2} \right]^{1/2} \right], \quad (22c)$$

and

$$\langle S \rangle = \left[\frac{2}{N} \sum_K \coth \left(\frac{\beta \omega_K}{2} \right) \right]^{-1}. \quad (23)$$

It is very obvious that when $\langle S^x \rangle = \langle S^y \rangle = 0$, or $\langle S^+ \rangle = \langle S^- \rangle = 0$, BT's result is obtained immediately from Eq. (23).

If the undetermined constants are not considered, i.e., $\gamma_{1,2,3} = 0$, we find that

$$\langle S^+ \rangle \langle S^- \rangle D = \frac{1}{4} \quad (24a)$$

by Eq. (21a);

$$\langle S^+ \rangle \langle S^z \rangle D = \langle S^- \rangle \langle S^z \rangle D = \langle S^+ \rangle^2 D = \langle S^- \rangle^2 D = 0 \quad (24b)$$

by Eqs. (21b)–(21d) and Eq. (21f); and

$$(2\langle S^z \rangle^2 + \langle S^+ \rangle \langle S^- \rangle) D = \frac{1}{2} \quad (24c)$$

by Eq. (21e).

Since $D \neq 0$, Eq. (24b) requires $\langle S^+ \rangle = \langle S^- \rangle = 0$, and is evidently in contradiction with Eq. (24a), so that at least one of the γ 's is not equal to zero.

By comparing the asymmetric decoupling approximation (12) with that of BT,¹ i.e.,

$$\begin{aligned} \langle\langle S_i^z S_{i+a}^\pm, S_j^n \rangle\rangle &\cong \langle S_i^z \rangle \langle\langle S_{i+a}^\pm, S_j^n \rangle\rangle, \\ \langle\langle S_{i+a}^\pm S_i^\pm, S_j^n \rangle\rangle &= \langle S_{i+a}^\pm \rangle \langle\langle S_i^\pm, S_j^n \rangle\rangle, \end{aligned} \quad (25)$$

it is not difficult to establish that Eqs. (25) are special cases of Eq. (12) when $\langle S^+ \rangle = \langle S^- \rangle = 0$. Since BT only discussed the uniaxial ferromagnet, the above conditions evidently exist and under these conditions, γ_1 and γ_2 happen to be zero, but $\gamma_3 \neq 0$. Since BT only chose the operators S^\pm to construct Green's functions, but not S^z , they could also obtain the correct results, which concealed the contradiction in Eq. (24).

If fermion Green's functions are used to investigate the similar system, identical results can be obtained.

IV. THE APPLICATION OF GREEN'S-FUNCTION METHOD TO THE FERROELECTRIC SYSTEM WITH PSEUDOSPIN MODEL

The Hamiltonian of the pseudospin system is

$$H = -\Omega \sum_i S_i^x - \frac{1}{2} \sum_{i,j} J_{ij} S_i^z S_j^z. \quad (26)$$

Choosing the operators $A, B = S_i^x, S_i^y, S_i^z$ to constitute boson Green's functions and using the Tyablikov decoupling approximation⁵ $\langle S^y \rangle = 0$, we get

$$\begin{pmatrix} \omega & -iJ_0\langle S^z \rangle & 0 \\ iJ_0\langle S^z \rangle & \omega & -i\Omega \\ 0 & i\Omega & \omega \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} G^{xx}(\omega) \\ G^{yx}(\omega) \\ G^{zx}(\omega) \\ G^{xy}(\omega) \\ G^{yy}(\omega) \\ G^{zy}(\omega) \\ G^{xz}(\omega) \\ G^{yz}(\omega) \\ G^{zz}(\omega) \end{pmatrix} = \frac{i}{2\pi} \begin{pmatrix} 0 \\ -\langle S^z \rangle \\ 0 \\ \langle S^z \rangle \\ 0 \\ -\langle S^x \rangle \\ 0 \\ \langle S^x \rangle \\ 0 \end{pmatrix}, \quad (27)$$

where

$$G^{mn}(\omega) = \langle\langle S^m, S^n \rangle\rangle_\omega \quad (m, n = x, y, z),$$

$$J_0 = \sum_j J_{ij}.$$

The solutions of Eq. (27) are

$$\omega_p^2 = \Omega^2 + J_0^2 \langle S^z \rangle^2 \quad (28)$$

and

$$\begin{aligned} G^{xx}(\omega) &= \frac{J_0 \langle S^z \rangle}{2\pi} \frac{\langle S^z \rangle}{\omega^2 - \omega_p^2}, & G^{yx}(\omega) &= -\frac{i}{2\pi} \frac{\omega \langle S^z \rangle}{\omega^2 - \omega_p^2}, \\ G^{zx}(\omega) &= -\frac{1}{2\pi} \frac{\Omega \langle S^z \rangle}{\omega^2 - \omega_p^2}, & G^{xz}(\omega) &= -\frac{1}{2\pi} \frac{J_0 \langle S^x \rangle \langle S^z \rangle}{\omega^2 - \omega_p^2}, \\ G^{yz}(\omega) &= \frac{i}{2\pi} \frac{\omega \langle S^x \rangle}{\omega^2 - \omega_p^2}, & G^{zz}(\omega) &= \frac{\Omega}{2\pi} \frac{\langle S^x \rangle}{\omega^2 - \omega_p^2}. \end{aligned} \quad (29)$$

We introduce the undetermined constants as follows:

$$S_i^x \sim S_i^x + \gamma_1, \quad S_i^y \sim S_i^y + \gamma_2, \quad S_i^z \sim S_i^z + \gamma_3. \quad (30)$$

By constituting Eq. (30) and Eqs. (29) into the spectral theorem (4), we find that

$$\frac{1}{4} + 2\gamma_1 \langle S^x \rangle + \gamma_1^2 = J_0 \langle S^z \rangle^2 E, \quad (31a)$$

$$\frac{1}{4} + 2\gamma_3 \langle S^z \rangle + \gamma_3^2 = \langle S^x \rangle E, \quad (31b)$$

$$\gamma_1 \langle S^z \rangle + \gamma_3 \langle S^x \rangle + \gamma_1 \gamma_3 = -\langle S^z \rangle E, \quad (31c)$$

$$\gamma_1 \langle S^z \rangle + \gamma_3 \langle S^x \rangle + \gamma_1 \gamma_3 = -J_0 \langle S^x \rangle \langle S^z \rangle E, \quad (31d)$$

$$\gamma_2 (\langle S^x \rangle + \gamma_1) = 0, \quad (31e)$$

$$\gamma_2 (\langle S^z \rangle + \gamma_3) = 0, \quad (31f)$$

where

$$E = \frac{1}{2\omega_p} \coth \left[\frac{\beta\omega_p}{2} \right].$$

The γ 's are determined from Eqs. (31), i.e.,

$$\gamma_1 = -\langle S^x \rangle \left[1 \pm \left[1 - \frac{1}{4(\langle S^x \rangle^2 + \langle S^z \rangle^2)} \right]^{1/2} \right], \quad (32a)$$

$$\gamma_2 = 0, \quad (32b)$$

$$\gamma_3 = -S^z \left[1 \pm \left[1 - \frac{1}{4(\langle S^x \rangle^2 + \langle S^z \rangle^2)} \right]^{1/2} \right]. \quad (32c)$$

It can also be seen from Eqs. (31) that for (i) the paraelectric phase

$$\langle S^z \rangle = 0, \quad \langle S^x \rangle = \frac{1}{2} \tanh \left[\frac{\beta\Omega}{2} \right] \quad (33)$$

and (ii) the ferroelectric phase

$$\langle S^x \rangle = \Omega/J_0, \quad \frac{J_0}{2\omega_p} \tanh \left[\frac{\beta\omega_p}{2} \right] = 1. \quad (34)$$

The results of (33) and (34) are just those of the MFA.^{7,8} That is as expected since it is easy to prove that the Tyablikov decoupling approximation is that of MFA. Incidentally the Green's functions with $B = S^y$ only produce three identical equations and all the independent equations can be obtained through the Green's functions with $B = S^x, S^z$.

If the undetermined constants are not introduced (i.e., $\gamma_{1,2,3}$ are set equal to zero), Eqs. (31) give

$$\frac{1}{4} = J_0 \langle S^z \rangle^2 E = \Omega \langle S^x \rangle E, \quad (35a)$$

$$0 = \langle S^z \rangle E = J_0 \langle S^x \rangle \langle S^z \rangle E, \quad (35b)$$

and these are obviously contradictory.

Without considering the undetermined constants, Ganguli *et al.*⁶ used only some of the Green's functions G^{mm} ($m = x, y, z$) to find the correlation functions. In this manner they avoided any obvious contradiction, because only one equation like (35a) may not of itself be contradictory. Considering both the correlation functions to be finite and

$$\langle (S^x)^2 \rangle + \langle (S^y)^2 \rangle + \langle (S^z)^2 \rangle = S(S+1), \quad (36)$$

they obtained the (i) paraelectric phase

$$\langle S^z \rangle = 0, \quad \langle S^x \rangle = \frac{3}{4} \tanh \left[\frac{\beta\Omega}{2} \right] \quad (37)$$

and (ii) the ferroelectric phase

$$\langle S^x \rangle = \Omega/J_0, \quad \frac{3J_0}{4\omega_p} \tanh \left[\frac{\beta\omega_p}{2} \right] = 1. \quad (38)$$

By comparing (37) with (33) and (38) with (34), it is found that the results of Ganguli *et al.* are incorrect by a $\frac{3}{2}$ factor. If the undetermined constants obtained above are introduced to find the correlation functions with Eq. (36), the results of (33) and (34) are obtained immediately.

The application of the Green's-function method to the pseudospin problem is discussed here only in the Tyablikov decoupling approximation. It can also be discussed in the symmetric decoupling approximation (12) with the similar pattern. Results are also very similar in appearance.

V. CONCLUSION

It is shown that when arbitrary c numbers are added to the operators of a boson Green's function, the Green's function itself is unchanged, so that the corresponding correlation function obtained from the spectral theorem is also unchanged. This is in contradiction with the definition of the correlation function, so that the final results may also be contradictory. This difficulty can be overcome by an undetermined-constant method. It can also be shown that the problem of the undetermined constant is an intrinsic attribute of the boson Green's-function method. Specific expressions for the undetermined constants can be determined for specific systems and decoupling approximations.

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