APPLICATION OF THE ORTHOGONAL OPERATOR EXPANSION METHOD TO THE ZERO-FREQUENCY ANOMALY OF THE CORRELATION FUNCTIONS

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The problem of the zero-frequency anomaly is studied by using the orthogonal operator expansion method and superoperators acting in the operator space. The eigen operators of the Hermitian superoperator $\hat{H}^{\times}$ corresponding to the Hamiltonian H are chosen as the basis in the operator space. A useful formal method for testing the zero-frequency anomaly constants is given. As an application of this method the zero-frequency anomaly of the transverse and longitudinal Heisenberg correlation functions are discussed.

1. *Introduction*

We shall give here a brief mathematical background to the method of orthogonal operator expansion. Let $\tilde{\tilde{H}}$ be a linear, finite-dimensional space which consists of the linear operators $A, B, C, \ldots$

These operators $A, B, C, \ldots$ act on the finite-dimensional Hilbert space $\tilde{H}$ of the states of the physical system. Next we define the bracket $(\ldots, \ldots)$ which is a function of the tensor product $\tilde{\tilde{H}} \otimes \tilde{\tilde{H}}$ in the complex plane. We shall assume that it has the usual properties of a scalar product in $\tilde{\tilde{H}}$ space. Several different realizations of the above function will be given in Section 2.

Let us introduce in $\tilde{\tilde{H}}$ the set of operators $\{O_i\}$, which satisfy the relations

$$(O_i, O_j) = \delta_{ij}. \tag{1.1}$$

This set $\{O_i\}$ is called complete, if

$$(A, A) = \sum_j (A, O_j)(O_j, A), \tag{1.2}$$

holds for every operator of $\tilde{\tilde{H}}$. If a set of operators is complete, any operator A of $\tilde{\tilde{H}}$ can be expanded as

$$A = \sum_j a_j^A O_j, \tag{1.3}$$

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where a_j^A are in general complex numbers given by the formula

$$a_j^A = (A, O_j). \tag{1.4}$$

For details, see *e. g.* [4] and [5].

Let us define in $\tilde{\tilde{H}}$ linear superoperators $\hat{A}, \hat{B}, \hat{C}, \dots$. By a superoperator we mean an entity which when acting on a operator of $\tilde{\tilde{H}}$ turns it into another operator.

We have

$$\hat{A}O_i = \sum_j [\hat{A}]_{ij} O_j, \tag{1.5}$$

$$[\hat{A}]_{ij} = (\hat{A}O_i, O_j). \tag{1.6}$$

The product of $\hat{A}$ and $\hat{B}$, denoted by $\hat{A}\hat{B}$, is also a superoperator $\hat{C}$. The matrix element of $\hat{C}$ can be written in the form

$$[\hat{C}]_{ij} = \sum_k [\hat{A}]_{ik}[\hat{B}]_{kj}. \tag{1.7}$$

Let us distinguish a special set of linear superoperators denoted by $\hat{A}^x, \hat{B}^x, \hat{C}^x, \dots$ and defined by the relation

$$\hat{A}^x = [A, \dots]_-. \tag{1.8}$$

The Heisenberg representation of $A(z)$ for any complex parameter z is defined as

$$A(z) = e^{z\hat{H}^x} A(0) = e^{zH} A(0) e^{-zH}, \tag{1.9}$$

where H is the Hamiltonian of the physical system.

In Section 2 we discuss the solution of the eigen-problem, the Hermitian superoperator corresponding to the Hamiltonian, and a method of obtaining the complete operator basis in $\tilde{\tilde{H}}$.

Using the results of Section 2, the problem of the zero-frequency anomaly for the spin correlation functions of the Heisenberg ferromagnet is discussed in Section 3.

2. *The eigen-problem of the Hamiltonian superoperator* $\hat{H}^x$

We consider a finite-dimensional linear space $\tilde{\tilde{H}}$ and determine the subspace invariant under the action of the superoperator $\hat{H}^x$ which corresponds to the Hamiltonian H of the physical system. This is equivalent to solving the system of eigen-equations [1, 2, 7, 9]

$$\hat{H}^x O_i = \omega_i O_i. \tag{2.1}$$

In general there is degeneracy in the equations (2.1). To the eigen-value $\omega_i = 0$ belong all the constants of motion and functions of those and to $\omega_i \neq 0$ belong also the operators obtained by multiplication to the right or left of O_i by arbitrary functions of the constants of motion. The solutions of Eq. (2.1) have a simple physical interpretation which will be given below.

Let $\{\hat{P}_i\}$ be a complete set of Hermitian superoperators acting in $\tilde{\tilde{H}}$ space which commute with one another and with the superoperator $\hat{H}^x$

$$[\hat{H}^x, \hat{P}_i]_- = 0, \quad i = 1, 2, \ldots, s, \tag{2.2}$$

$$[\hat{P}_i, \hat{P}_j]_- = 0, \quad i, j = 1, 2, \ldots, s. \tag{2.3}$$

It is always possible to find such set $\hat{H}^x, \hat{P}_1, \ldots, \hat{P}_s$. The basis operators in $\tilde{\tilde{H}}$ are then determined by the solutions of the eigen-equations

$$\hat{H}^x O_{\omega_k, P'_1, \ldots, P'_s} = \omega_k O_{\omega_k, P'_1, \ldots, P'_s}, \tag{2.4}$$

$$\hat{P}_i O_{\omega_k, P'_1, \ldots, P'_s} = P'_i O_{\omega_k, P'_1, \ldots, P'_s}, \tag{2.5}$$

where

$$(O_{\omega_k, P'_1, \ldots, P'_s}, O_{\omega_r, P''_1, \ldots, P''_s}) = \delta_{\omega_k, \omega_r} \delta_{P'_1, P''_1} \ldots \delta_{P'_s, P''_s}. \tag{2.6}$$

From (2.4) and from $H = H^+$ one obtains the eigen-equations for the Hermitian conjugate operators with the eigen-values $-\omega_k$

$$\hat{H}^x O^+_{\omega_k, P'_1, \ldots, P'_s} = -\omega_k O^+_{\omega_k, P'_1, \ldots, P'_s}. \tag{2.7}$$

Using the equations (2.4) and (2.7) one obtains the relation

$$\hat{H}^x [O_{\omega_i, P'_1, \ldots, P'_s}, O^+_{\omega_j, P''_1, \ldots, P''_s}]_\alpha = (\omega_i - \omega_j) [O_{\omega_i, P'_1, \ldots, P'_s}, O^+_{\omega_j, P''_1, \ldots, P''_s}]_\alpha, \tag{2.8}$$

where

$$[A, B]_\alpha = AB + \alpha BA, \quad \alpha = 0, \pm 1. \tag{2.9}$$

In a particular case $\omega_i = \omega_j$ we conclude from (2.8) that

$$[O_{\omega i, P'_1, \ldots, P'_s}, O^+_{\omega_i, P''_1, \ldots, P''_s}]_\alpha = \sum_{\{P'''_i\}} L^{P'''_1, \ldots, P'''_s; \alpha}_{P'_1, \ldots, P'_s, P''_1, \ldots, P''_s} O_{0, P'''_1, \ldots, P'''_s}, \tag{2.10}$$

where on the right-hand side of Eq. (2.10) we have a linear combination of all the constants of motion. The equation (2.10) is a generalization of the well-known Bose and Fermi commutation relations. To the eigenvalue $\omega = 0$ belong all the operators which are diagonal in the energy representation (all constants of motion), and to the eigenvalues $\omega \neq 0$ belong all the operators which have no diagonal part in the energy representation.

For any linear operator acting in the $\tilde{H}$ space one can write

$$A = \sum_{\{P'_i\}} \{a^A_{0, P'_1, \ldots, P'_s} O_{0, P'_1, \ldots, P'_s} + \sum_{\omega_i} a^A_{\omega_i, P'_1, \ldots, P'_s} O_{\omega_i, P'_1, \ldots, P'_s}\}, \tag{2.11}$$

where

$$a^A_{0, P'_1, \ldots, P'_s} = (A, O_{0, P'_1, \ldots, P'_s}), \tag{2.12}$$

$$a^A_{\omega_i, P'_1, \ldots, P'_s} = (A, O_{\omega_i, P'_1, \ldots, P'_s}). \tag{2.13}$$

The first term on the right-hand side of equation (2.11) represents the diagonal part of A and the second one the off-diagonal part of A in the energy representation. Let $H, P_1, \ldots, P_s$ be a complete set of commuting observables in $\tilde{H}$ space. The eigen-equations for these operators can be written as

$$H|\varepsilon_k, \tilde{P}'_1, \ldots, \tilde{P}'_s\rangle = \varepsilon_k|\varepsilon_k, \tilde{P}'_1, \ldots, \tilde{P}'_s\rangle, \tag{2.14}$$

$$P_i|\varepsilon_k, \tilde{P}'_1, \ldots, \tilde{P}'_s\rangle = \tilde{P}'_i|\varepsilon_k, \tilde{P}'_1, \ldots, \tilde{P}'_s\rangle, \tag{2.15}$$

for $i = 1, 2, \ldots, s$.

In $\tilde{\tilde{H}}$-space the set $H, P_1, \ldots, P_s$ has the following counterparts

$$H \to \hat{H}^x, \quad P_i \to \hat{P}_i^x, \tag{2.16}$$

for $i = 1, 2, \ldots, s$. The superoperators $\hat{H}^x$ and $\hat{P}_i^x$ also commute with one another. If the set $\hat{H}^x, \hat{P}_1^x, \ldots, \hat{P}_s^x$ is complete set of commuting Hermitian superoperators then the solutions of (2.4) and (2.5) have the form

$$|\varepsilon_k, \tilde{P}'_1, \ldots, \tilde{P}'_s\rangle \langle\varepsilon_i, \tilde{P}''_1, \ldots, \tilde{P}''_s|. \tag{2.17}$$

The operators (2.17) are all eigen-operators with the eigenvalues

$$P'_i = \tilde{P}'_i - \tilde{P}''_i,$$

$$\omega_i = \varepsilon_k - \varepsilon_i. \tag{2.18}$$

The results (2.18) can be obtained from (2.17) and by making use of the definitions $\hat{H}^x, \hat{P}_1^x, \ldots, \hat{P}_s^x$. The operators (2.17) correspond to the $O_{\omega_i, P_1', \ldots, P_s'}$. One can see that $O_{\omega_i, P_1', \ldots, P_s'}$ are transition operators between quantum states, where $\omega_i, P'_1, \ldots, P'_s$ are relevant differences of quantum numbers.

Let us consider the retarded Green function [8],

$$\langle\langle A(t)|B\rangle\rangle = -i\Theta(t)\langle[A(t), B]_-\rangle, \tag{2.19}$$

where

$$\langle\ldots\rangle = \mathrm{Tr}(\varrho\ldots), \quad \varrho = \frac{e^{-\beta H}}{\mathrm{Tr}\, e^{-\beta H}}, \quad \beta = \frac{1}{k_B T}, \tag{2.20}$$

and Θ is the Heaviside step function equal to 1 for $t > 0$ and to 0 for $t < 0$. The equation of motion for the Fourier transform of the function is

$$E\langle\langle A|B\rangle\rangle_E = \frac{1}{2\pi}\langle[A, B]_-\rangle + \langle\langle[A, H]_-|B\rangle\rangle_E. \tag{2.21}$$

The Green function $\langle\langle A|B\rangle\rangle_E$ can be related back to the time-dependent correlation function $\langle BA(t)\rangle$ *via* the spectral theorem

$$\langle BA(t)\rangle = C_{AB} + i\int_{-\infty}^{\infty} \frac{\langle\langle A|B\rangle\rangle_{E+i0^+} - \langle\langle A|B\rangle\rangle_{E-i0^+}}{e^{\beta E}-1} e^{-iEt} dE, \tag{2.22}$$

where

$$C_{AB} = (\sum_k e^{\beta\varepsilon_k})^{-1} \sum_{\substack{m,n \\ \varepsilon_m=\varepsilon_n}} e^{-\beta\varepsilon_n}\langle n|A|m\rangle \langle m|B|n\rangle, \tag{2.23}$$

for details see references [3] and [6].

By taking into account the relations (2.11), (2.12) and (2.13) and the definition of the scalar product, the formula (2.23) can be written in the form

$$C_{AB} = \sum_{\{P'_i\}\{P''_i\}} (A, O_{0,P'_1,\ldots,P'_s})(O_{0,P''_1,\ldots,P''_s}, B^+)\langle O_{0,P'_1,\ldots,P'_s}O^+_{0,P''_1,\ldots,P''_s}\rangle. \tag{2.24}$$

The scalar product (..., ...) may be defined in various ways. We shall use a definition which has the simple physical interpretation as the quantum statistical average in the equilibrium state. We have

$$(A, B)_\alpha = \mathrm{Tr}\,(\varrho[A, B^+]_\alpha), \qquad \alpha = 0 \text{ or } 1. \tag{2.25}$$

With this scalar product the superoperator $\hat{H}^x$ is Hermitian in $\tilde{\tilde{H}}$. Next we use (2.25) with $\alpha = 0$. Then, from (2.24) one obtains

$$C_{AB} = \sum_{\{P'_i\}} \langle AO^+_{0,P'_1,\ldots,P'_s}\rangle \langle O_{0,P'_1,\ldots,P'_s}B\rangle, \tag{2.26}$$

or, in the particular case when $A = B^+$,

$$C_{AA^+} = \sum_{\{P'_i\}} |\langle AO^+_{0,P'_1,\ldots P'_s}\rangle|^2. \tag{2.27}$$

The equation (2.26) can be written in another form. We can always include in the basis set the identity operator which will belong to $\omega = 0$. Taking this into account we have

$$C_{AB} = \langle A\rangle \langle B\rangle + \sum_{\{P'_i\}}{}' \langle AO^+_{0,P'_1,\ldots,P'_s}\rangle \langle O_{0,P'_1,\ldots,P'_s}B\rangle, \tag{2.28}$$

where the sum extends over all operators $O_{0,P_1',\ldots,P'_s}$ except the identity operator. A similar result was obtained by Suzuki in [6].

3. *The zero-frequency anomaly for the spin pair correlation functions of the Heisenberg ferromagnet*

As we considered above, the retarded commutator Green function does not contain complete information about the correlation functions. In general C_{AB} is not equal to zero, and we have to use the formula (2.22). The problem of this anomaly was discussed in more details in [3] and [6]. Next we shall discuss this anomaly for the spin pair correlation functions of the Heisenberg ferromagnet.

The Hamiltonian of the system is given by

$$H = -\omega_0 S_0^3 - \frac{1}{N}\sum_q J_q(S_q^+ S_{-q}^- + S_q^3 S_{-q}^3) \tag{3.1}$$

where $S_q^{\pm 3}$, J_q are the spatial Fourier components of the spin operators $S_f^{\pm 3}$ and the exchange integral J_{fg}, and ω_0 represents the external magnetic field. The exact calculation of C_{AB} according to (2.26) is more complicated because we do not know the eigen-operators of $\hat{H}^x$ for $\omega = 0$. We can only calculate C_{AB} in the same approximation as we have used in the Green function problem.

The familiar methods often applied to the Heisenberg ferromagnet are actually equivalent to seeking the solutions of the equation

$$\hat{H}^x S_k^+ = \omega_k S_k^+, \tag{3.2}$$

where

$$\omega_k = \frac{(\hat{H}^x S_k^+, S_k^+)_\alpha}{(S_k^+, S_k^+)_\alpha} = \frac{\langle [[H, S_k^+]_-, S_{-k}^-]_\alpha \rangle}{\langle [S_k^+, S_{-k}^-]_\alpha \rangle}. \tag{3.3}$$

In the simplest approximation ω_k can be written using the scalar product with $\alpha = 0$. Then the equation (3.3) becomes

$$\omega_k = \omega_0 + \frac{2}{N} \sum_q (J_q - J_{k-q}) \frac{\langle S_{k-q}^+ S_q^3 S_{-k}^- \rangle}{\langle S_k^+ S_{-k}^- \rangle}. \tag{3.4}$$

If we apply to the above formula the Tiablikov decoupling [11] procedure we obtain

$$\omega_k = \omega_0 + 2\sigma(J_0 - J_k), \qquad \sigma = \langle S^3 \rangle. \tag{3.5}$$

If we use the Callen, [10], [4] procedure we have

$$\omega_k = \omega_0 + 2\sigma(J_0 - J_k) + \frac{2\bar{\alpha}}{N} \sum_q (J_q - J_{k-q}) \langle S_q^+ S_{-q}^- \rangle. \tag{3.6}$$

Detailed considerations are given in [1], [4] and [12]. All simple approximations commonly used to the Heisenberg ferromagnet espacially in the low temperature region can be obtained in the form of approximate solutions of Eq. (3.2). In this approximation S_k^+ are the eigen-operators of $\hat{H}^x$ with $\omega_k \neq 0$. It was emphasized in Section 2 that the eigen-operators with $\omega \neq 0$ are orthogonal to the eigen-operators $O_{0,P_1', \dots, P_s'}$. Hence,

$$\langle S_k^+ O_{0,P'_1,\dots,P'_s}^+ \rangle = (S_k^+, O_{0,P'_1,\dots,P'_s}) = 0. \tag{3.7}$$

Then from (2.27) we see that $C_{S_k^+ S_{-k}^-}$ is approximately equal to zero. Let us consider the posibilities of calculating these anomaly constants C_{AB} exactly. If the Heisenberg ferromagnet has translational symmetry we can probably assume that the operators $O_{0,P_1', \dots, P_s'}$ do not prefer any lattice site, which implies

$$(S_k^+, O_{0,P'_1,\dots,P'_s}) = \langle S_k^+ O_{0,P'_1,\dots,P'_s}^+ \rangle \sim \delta_{k,0}. \tag{3.8}$$

The longitudinal spin pair correlation function can be discussed in much the same way, *i. e.*

$$(S_k^3, O_{0,P'_1,\dots,P'_s}) = \langle S_k^3 O_{0,P'_1,\dots,P'_s}^+ \rangle \sim \delta_{k,0}. \tag{3.9}$$

Then, from (3.8) and (3.9) it follows that $C_{S_k^+S_{-k}^-}$ and $C_{S_k^3S_{-k}^3}$ should be exactly equal to zero (for $k \neq 0$). More complicated spin correlation functions can also be treated by the above method. The formula (2.27) should prove an efficient tool in examining the zero-frequency anomaly of correlation functions.

4. Summary

Let us briefly summarize our result. In Section 2 we have presented a method for calculating the zero-frequency anomaly constants C_{AB} of correlation functions. This method is a simple generalization of that given by Suzuki [6]. In our formula various scalar product can be used. In Section 3 we have calculated the constant C_{AB} for the transverse pair correlation functions of the Heisenberg ferromagnet. By performing the calculations in the same approximations as the ones used in the Green functions we have shown that $C_{S_k^+S_{-k}^-} \approx 0$. The same result seems to hold rigorously for $C_{S_k^+S_{-k}^-}$ and $C_{S_k^3S_{-k}^3}$. The method can be also used for more complicated cases.

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