USING THE ORTHOGONAL OPERATOR EXPANSION METHOD FOR OBTAINING GREEN FUNCTIONS

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The problem of Green functions is discussed in a linear space by making use of the orthogonal operator expansion method. The exact solution of the equation of motion for the two-time Green functions is given and the Roth method generalized.

Next the method of approximate solutions is discussed. The utility of this scheme is testified by applying it to the Heisenberg ferromagnet.

1. *Introduction*

In recent papers [1], [2], [3] the theory of solving the equation of motion for the two-time Green functions (G.F.) was studied. By making use of the orthogonal operator expansion method Shimizu [1] and Morita *et al.* [2] obtained the formal solution of G.F. equations. In [3] Roth also proposed a solution of the G.F. problem, assuming that one can choose a restricted set of n operators $\{A_i\}$ (A_i are operators of aphysical system, n — any natural number) such that the time derivative of any operator A_i can be written as

$$i\frac{dA_i(t)}{dt} = \sum_j K_{ij}A_j(t), \quad i, j = 1, 2, \dots n,$$

where K_{ij} are connected with the Hamiltonian of the physical system. The above methods were applied in [1], [2], [4] to the Heisenberg ferromagnet. Here Shimizu *et al.* truncated the formal exact solution and also used the relation

$$\langle ABC\rangle \approx \langle A\rangle\langle BC\rangle + \langle B\rangle\langle AC\rangle + \langle C\rangle\langle AB\rangle,$$

where A, B, C are spin operators.

To obtain the solution of the G.F. equation of motion we used the orthogonal operator expansion method similiar to that in [1] but with a different definition of the scalar product. Our scalar product is interpreted as a quantum statistical average.

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In Section 2 we give some basic definitions and formulate the problem. In Section 3 a formal, exact solution of the G.F. equation of motion is given and an approximate method proposed. The utility of this model is discussed using as an example the Heisenberg ferromagnet. In Sections 4 and 5 we summarize the results and discuss other possible applications of this method.

2. *The method of orthogonal operators*

Let $\tilde{\tilde{H}}$ be a linear space composed of operators $A, B, C, \ldots$ which act on the elements of a Hilbert space $\tilde{H}$. Let us define in $\tilde{\tilde{H}} \times \tilde{\tilde{H}}$ the symmetric bilinear form $k(A, B)$ where

$$k(A, \alpha B+\beta C) = \alpha^* k(A, B)+\beta^* k(A, C),$$
$$k(\alpha A+\beta B, C) = \alpha k(A, C)+\beta k(B, C), \tag{2.1}$$

and α, β are complex numbers.

If $k(A, A) \geqslant 0$ for every $A \in \tilde{\tilde{H}}$ the bilinear form k is called positive definite. If moreover $k(A, A) = 0 = \rightarrow\rangle A=0$ then k is called a scallar product on $\tilde{\tilde{H}}$ and is denoted by (A, B). We introduce in $\tilde{\tilde{H}}$ the basic orthogonal set $\{O_i\}$ of operators. Orthogonality is defined by means of the scalar product (2.1).

We have thus the equalities

$$(O_i, O_j) = \delta_{ij}, \quad i,j = 1, 2 \ldots \tag{2.2}$$

From the above assumptions it follows that any operator A from $\tilde{\tilde{H}}$ can be written as a linear combination of basic operators

$$A = \sum_i a_i^A O_i. \tag{2.3}$$

On the other hand coefficients a_i^A with a chosen basis completely determine the operator A.

From (2.1) it follows

$$a_i^A = (A, O_i). \tag{2.4}$$

On applying (2.4) to (2.1) one obtains

$$(A, B) = \sum_i a_i^A a_i^{*B}. \tag{2.5}$$

Let us define in $\tilde{\tilde{H}}$ superoperators $\hat{A}, \hat{B}, \hat{C}, \ldots$ by the relations

$$\hat{A}O_i = \sum_j [\hat{A}]_{ij} O_j. \tag{2.6}$$

$$[\hat{A}]_{ij} = (\hat{A}O_i, O_j). \tag{2.7}$$

The product $\hat{A}$ and $\hat{B}$ denoted $\hat{A} \cdot \hat{B}$ $[\hat{A}\hat{B}O_i \equiv \hat{A}(\hat{B}O_i)]$ is also a superoperator $\hat{C}$. Matrix elements of $\hat{C}$ can be written in the form

$$[\hat{C}]_{ij} = \sum_k [\hat{A}]_{ik} [\hat{B}]_{kj}. \tag{2.8}$$

Let us distinguish a special set of superoperators in $\tilde{\tilde{H}}$ denoted by $\hat{A}^{\times}, \hat{B}^{\times}, \hat{C}^{\times}, \ldots$ They are defined by relations

$$\hat{A}^{\times}C = AC - CA, \quad A, C \in \tilde{\tilde{H}}. \tag{2.9}$$

The matrix elements of (2.9) are also determined by (2.7).

Next we consider a quantum mechanical system described by the Hamiltonian $H = H^{\dagger}$ independent of time and defined in $\tilde{\tilde{H}}$ space.

Let A be an operator defined for this system. Using the Heisenberg picture $A(t)$ is described by

$$A(t) = e^{iHt}A(0)e^{-iHt}. \tag{2.10}$$

It is a formal solution of the Heisenberg equation of motion

$$-i\frac{dA(t)}{dt} = \hat{H}^{\times}A(t). \tag{2.11}$$

The solution (2.10) can be written in a superoperator form

$$A(t) = \hat{U}(t)\,A(0), \tag{2.12}$$

where $\hat{U}(t)$ is a superoperator which is determined by the equation

$$\frac{d\hat{U}(t)}{dt} = i(\hat{U}t)\cdot\hat{H}^{\times}, \tag{2.13}$$

with the boundary condition $\hat{U}(0) = \hat{I}$ ($\hat{I}$ is identity superoperator) and in the stationary case has the form

$$\hat{U}(t) = e^{i\hat{H}^{\times}t}. \tag{2.14}$$

Now we specify a scalar product (2.5)

$$(A, B) = \mathrm{Tr}\,(\varrho[A, B^{+}]_{\alpha}), \tag{2.15}$$

where

$$[A, B^{+}]_{\alpha} = AB^{+} + \alpha B^{+}A, \tag{2.16}$$

and $\alpha = \pm 1, 0$, ϱ is a special hermitian operator with non negative eigenvalues and $\mathrm{Tr}\,\varrho < \infty$. (The case with $\alpha = -1$ should be treated carefully because (A, A) need not be a definite form.) If the operator ϱ has the form

$$\varrho = \frac{e^{-\beta H}}{\mathrm{Tr}\,e^{-\beta H}}, \quad \beta = \frac{1}{kT}, \tag{2.17}$$

(2.15) has the simple physical interpretation of a quantum statistical average

$$(A, B) = \langle [A, B^{+}]_{\alpha} \rangle, \tag{2.18}$$

where $\langle \ldots \rangle$ denote $\mathrm{Tr}\,(\varrho \ldots)$.

Next ϱ is assumed to have the form (2.17). It is easy to see that the superoperator $\hat{H}^{\times}$ is hermitian. It follows from $\hat{H}^{\times}\varrho = 0$. In general $\hat{B}^{\times}$ need not be a hermitian superoperator. We can easily see that

$$(A, \hat{B}^{\times}C) = (\hat{B}^{\times}A, C) + \langle \varrho^{-1}[B, \varrho]_{-}[A, C^{+}]_{\alpha}\rangle, B = B^{+}. \tag{2.19}$$

From the hermicity of $\hat{H}^{\times}$ we can prove that $\hat{U}(t)$ is a unitary superoperator.

3. Formal solution of the equation of motion for the two time retarded G. F. and the approximation method

Using the notation introduced in Section 2 the two time thermal retarded G. F. can be written for $\alpha = 0$

$$G_B^A(t) = -i\Theta(t)\,(1, \hat{B}^{\times}\hat{U}(t)\,A(0)) \equiv \langle\!\langle A^{+}(t)|B^{+}(0)\rangle\!\rangle, \tag{3.1}$$

and for $\alpha = \pm 1$

$$G_B^A(t) = -i\alpha\Theta(t)\,(B^{+}, \hat{U}(t)\,A(0)) = \langle\!\langle A^{+}(t)\,B^{+}\rangle\!\rangle, \tag{3.2}$$

where $\Theta(t)$ is a unit step function ($= 1$ for $t > 0$ and $= 0$ for $t < 0$). A and B are operators involving dynamical variables of the system.

For all these functions the Fourier transform is defined as follows

$$G(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\omega t}G(\omega)d\omega. \tag{3.3}$$

Let A be a physical quantity which is also an element of the basic set ($A = O_j$) the corresponding G. F. being labelled by $G_B^j(t)$. The equation of motion for $G_B^j(t)$ has the form

$$i\frac{dG_B^j(t)}{dt} = P_B^j\delta(t) + \sum_i K_{ij}G_B^i(t). \tag{3.4}$$

It is easy to see that the Fourier transform of $G_B^j(t)$ satisfies

$$\sum_i (\omega\delta_{ij} - K_{ij})G_B^i(\omega) = P_B^j, \tag{3.5}$$

where for $\alpha = 0$

$$K_{ij} = [\hat{H}^{\times}]_{ij} = \langle O_i[O_j^{+}, H]_{-}\rangle, \tag{3.6}$$

$$P_B^j = \langle [O_j^{+}, B^{+}]_{-}\rangle, \tag{3.7}$$

and for $\alpha = \pm 1$

$$K_{ij} = \langle [O_i, [O_j^{+}, H]_{-}]_{\alpha}\rangle, \tag{3.8}$$

$$P_B^j = \alpha\,\langle [B^{+}, O_j^{+}]_{\alpha}\rangle. \tag{3.9}$$

In deriving (3.6)–(3.9) the relations (2.1)–(2.6) were used. We call the function $G_B^j(t)$ basic G. Fs. Any G. F. can be expressed by $G_B^j(t)$.

For instance

$$G_F^{ABC}(t) = -i\Theta(t)\,(1, \hat{F}^\times \hat{U}(t)ABC) = \sum_i a_i^{*ABC} G_F^i(t), \tag{3.10}$$

where

$$G_F^i(t) = -i\Theta(t)\,(1, \hat{F}^\times \hat{U}(t)\,O_i), \tag{3.11}$$

and

$$a_i^{ABC} = (ABC, O_i). \tag{3.12}$$

We should take into account that $G_F^i(t)$ are G. Fs. of different orders. In (3.10) there is a linear combination of G. Fs. of various possible orders.

Next we introduce the projection superoperators $\hat{P}_i$ defined by the relations

$$\hat{P}_i B = a_i^B O_i, \; a_i^B = (B, O_i). \tag{3.13}$$

The superoperator $\sum_i \hat{P}_i$ is the identity superoperator in $\tilde{\tilde{H}}$

$$\sum_i \hat{P}_i = \hat{I}. \tag{3.14}$$

Using (3.14) the term (3.12) can be expressed

$$(O_i, ABC) = \sum_i (O_i, O_j C)\,(O_j, AB). \tag{3.15}$$

This procedure can be applied also to the second term in (3.15). From the above considerations we see that the application of the projection superoperators can simplify the procedure of obtaining G. Fs. of higher orders. The simple approximated solutions of (3.15) can be obtained by taking instead of $\{O_i\}$ the uncompletely restricted orthogonal set of operators $\{O_i\}_{AP}$ (this set is not a basis in the $\tilde{\tilde{H}}$ space). We shall call $\{O_i\}_{AP}$ an approximating basic set.

Adding more operators to the set $\{O_i\}_{AP}$ we can obtain as a result a better approximation. We can also obtain results with a better approximation by changing the scalar product and choosing one that gives more rapidly converging solutions. It is interesting to notice that the identity superoperator may often be chosen as the element of $\sum_i \hat{P}_i$. We shall apply the above procedures to the Heisenberg ferromagnet.

4. Applications

Let us consider a simple two-spin Heisenberg ferromagnet in external magnetic field. The Hamiltonian of this system has the form

$$H = -\mu h(S_1^3 + S_2^3) - 2J[S_1^3 S_2^3 + \tfrac{1}{2}(S_1^+ S_2^- + S_1^- S_2^+)], \tag{4.1}$$

where S^3 and $S^{\pm}$ are the spin operators, h is an external magnetic field and J the exchange coupling constant. The approximating set of basic operators is chosen to be

$$O_1 = 1, \quad O_2 = \frac{S_1^-}{C_2}, \quad O_3 = \frac{S_2^+}{C_3}. \tag{4.2}$$

These operators are orthogonal in the sense (2.15) whereas $\alpha = 0$, ϱ has the form (2.17) with the Hamiltonian (4.1), C_2, C_3 are the normalization constants. We find the G. F. $\langle\langle S_1^+(t)|S_1^-(0)\rangle\rangle$ by using the formulas (3.1), (3.5), (3.6), (3.7). The explicit form of (3.5) in matrix notation is

$$\begin{bmatrix} \omega & 0 & 0 \\ 0 & \omega - K_{22} & -K_{23} \\ 0 & -K_{32} & \omega - K_{33} \end{bmatrix} \begin{bmatrix} G_B^1(\omega) \\ G_B^2(\omega) \\ G_B^3(\omega) \end{bmatrix} = \begin{bmatrix} O \\ P_B^2 \\ O \end{bmatrix}, \tag{4.3}$$

where $K_{j1} = K_{1j} = 0$ for $j = 1, 2, 3$ and

$$K_{23} = -2J\sigma \frac{C_3}{C_2}, \quad K_{32} = -2J\sigma \frac{C_2}{C_3},$$

$$K_{22} = -K_{33} = \mu h + 2J\sigma, \ \sigma = \langle S^3 \rangle. \tag{4.4}$$

To obtain relations (4.4) we use (3.6), (3.7) with the Hamiltonian (4.1) and approximating set (4.2). We shall consider in detail the scalar product $(S_1^-, S_2^3 S_1^-)$ which should be evaluated.

For the Hamiltonian (4.1) we have

$$(S_{1,2}^{\pm}, S_{1,2}^3) = 0. \tag{4.5}$$

Using the projection superoperators (3.14) and (4.5) one obtains

$$(S_1^-, S_2^3 S_1^-) = \sum_{i=1}^{3} (S_1^- S_1^+, \hat{P}_i S_2^3) = (1, S_2^3)(S_1^-, S_1^-). \tag{4.6}$$

If $B = C_2 S_1^-$ is substituted into equation (4.3) one obtains the following forms for the G. F.

$$G_B^2(\omega) = \frac{2\sigma(\omega - \mu h - 2\sigma J)}{(\omega - \mu h - 2\sigma J)^2 - 4J^2\sigma^2}. \tag{4.7}$$

These G. F. have the same form as the G. F. evaluated by using the Tyablikov decoupling approximation. This example was also considered by using the decoupling procedure of Roth [3] which corresponds to the above method with scalar product for $\alpha = \pm 1$. These solutions are fully discussed in [3].

Example 2

We consider the isotropic Heisenberg ferromagnet. The Hamiltonian of this system is of the form

$$H = -\mu h \sum_f S_f^3 - \sum_{f,g} J_{fg}(S_f^- S_g^+ + S_f^3 S_g^3), \tag{4.8}$$

where S^+, S^3 are spin operators, J_{fg} is the exchange coupling constant for the sites f and g. We assume that $J_{ff} = 0$ and also that h is the z-component of the external magnetic field. The spatial Fourier transformation is defined as follows

$$S_k^\beta = \frac{1}{\sqrt{N}} \sum_f e^{ikf} S_f^\beta, \quad \beta = \pm, 3,$$

$$J_{fg} = \frac{1}{N} \sum_k e^{-ik(f-g)} J_k, \tag{4.9}$$

where the subscripts f, g ($\boldsymbol{k}$, $\boldsymbol{q}$) denote the sites of the simple (reciprocal) lattice and N is the number of the sites in crystal. Thus the Hamiltonian takes the form

$$H = -\mu h \sqrt{N} S_0^3 - \sum_q J_q (S_q^- S_{-q}^+ + S_q^3 S_{-q}^3). \tag{4.10}$$

It is very difficult to find the basic set of operators $\{O_i\}$. For the first order approximation the set $\{O_i\}_{AP}$ is taken

$$O_1 = 1, \quad O_{-k,2} = \frac{S_{-k}^-}{C_{-k}}, \quad O_{k,3} = \frac{S_k^+}{C_k}, \tag{4.11}$$

where C_k, C_{-k} are normalization constants and $O_1 = 1$ is the identity operator. These operators (4.11) are orthogonal in the sense (2.15) with $\alpha = 0$. The density matrix operator ϱ is taken with the Hamiltonian (4.8). The $\boldsymbol{k}$ vector is not established and the set $\{O_i\}_{AP}$ consists of $(2N+1)$ operators. By letting $B = C_k S_k^+$ in equations (3.5) with the approximating set (4.11) the G. F. $G_B^2(\omega)$ is obtained. It has the form

$$G_B^2(\omega) = \frac{2\langle S_0^3 \rangle}{\omega - K_{22}}. \tag{4.12}$$

To obtain (4.12) we must notice that

$$K_{1j} = K_{j1} = 0 \text{ for } j = 1, 2, 3,$$

and $K_{22} = K_{32} = 0$ which follows from the symmetry of the Hamiltonian. The coefficients K_{22} are given by

$$K_{22} = \mu h + \frac{2}{\sqrt{N}} \sum_q (J_q - J_{k-q}) \frac{(S_{-k}^- S_{k-q}^+, S_{-q}^3)}{(S_{-k}^-, S_{-k}^-)}. \tag{4.13}$$

The scalar product in the second term can be decoupled by using the projection operator (3.14). We obtain

$$(S_{-k}^- S_{k-q}^+, S_{-q}^3) = (1, S_q^3)(S_{-k}^-, S_{q-k}^-). \tag{4.14}$$

From (4.14) we obtain

$$K_{22} = \mu h + 2\sigma(J^0 - J_k),$$
$$\sigma = \langle S_0^3 \rangle. \tag{4.15}$$

The term (4.15) is the same as the result obtained by using the Tyablikov decoupling scheme. The second example is clearly a generalization of the first one.

5. *Conclusions*

We have use the orthogonal operator expansion method to obtain the solution of the G. F. equation of motion. By taking the definite set of orthogonal operators $\{O_i\}$ and operator B, the problem of G. F. is determined exactly. This is easy to see from (3.1), (3.2), (3.5) where the G. F. is defined by a scalar product. A simple formal solution is given and the approximating procedures are proposed.

In Section 4 the scalar product (2.15) with $\alpha = 0$ was used and the results are in agreement with papers [1] and [4]. The coefficients K_{ij} following from (3.8) correspond to the cofficients E_{ij} which are used in [3] and [4]. Taking $\{A_j\}$ in [4] which are orthogonal in the sense (2.15) with $\alpha = \pm 1$ we obtain K_{ij} linear with E_{ij}. In [4] the simple two spin Heisenberg ferromagnet was studied by using the familiar method. Better results can be obtained by applying in the Roth method the operators

$$A_1 = S_1^+, A_2 = S_2^+.$$

It is easy to see that operators A_1, A_2 are orthogonal in the sense (2.15) with $\alpha = \pm 1$. The authors have also investigated the isotropic Heisenberg ferromagnet using the method of Roth. In this case the orthogonal approximating set $\{A_j\}_{AP}$ consists of $2N$ operators in the form

$$A_{k,1} = S_k^+, A_{k,2} = S_{-k}^-.$$

However, in order to obtain the familiar results the decoupling procedure

$$\langle S_{k-q}^3 S_{q-k}^3 \rangle \cong \langle S_{k-q}^3 \rangle \langle S_{q-k}^3 \rangle$$

had to be used. This is a kind of the Tyablikov decoupling.

In this paper the decoupling problem is eliminated automatically by using the orthogonal relations and the projection superoperators.

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