

A Study on the Green Function for the Heisenberg Ferro- and Antiferro-magnets*

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〈Abstract〉

The unified Green function theory is developed for the Heisenberg ferro- and antiferro-magnets. The equation of motion for the Green function is decoupled by the Callen decoupling approximation. The Solution of the equation is used to find the transverse correlation functions of spins at, above, and below the Curie temperature for the ferromagnets. The results are found to be consistent with the others.

Heisenberg의 强磁性 및 反强磁性에 關한 Green函數 研究

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〈要 約〉

Heisenberg의 强磁性 및 反强磁性에 대한 統一된 Green 函數理論을 수립하였다.

Green 函數의 運動方程式을 Callen의 decoupling 近似方法으로 分離시켜서 解를 求하고 이 解를 利用하여 强磁性에 대한 Curie 温度 및 그 上下에서 spin의 橫的相關函數를 計算하였다. 이 結果가 다른 研究結果와 一致하였다.

I. Introduction

The properties of ferro- and antiferro-magnetic materials near the transition points has been a subject of many recent theoretical and experimental investigations. One frequently used model for the theoretical interest is the Heisenberg Model, which consists of a regular array of localized spins that are coupled together by the so-called exchange interaction.

The molecular field theory by Weiss¹⁾ is succe-

ssful in predicting the existence of the transition temperature, susceptibility, etc., but it has many weak points such as its failure at low temperature. Bloch²⁾ and later Dyson³⁾ developed the spin wave theory in the Heisenberg model which is applicable for very low temperature regions. However, this theory becomes inaccurate as the temperature increases because of the large density of the spin wave quanta. At a temperature high above the transition point, the $\frac{1}{T}$ expansion of partition function⁴⁾ was

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used to analyze the paramagnetic properties of the Heisenberg model. This method has failed in the temperature regions not so far from the transition point.

Tyablkov⁶⁾ first used the technique of the double-time temperature-dependent Green function⁶⁾ to study the Heisenberg ferromagnets of spin $\frac{1}{2}$. Extension of the Green function theory to higher spin values has also been achieved^{7,8)}. Lee and Liu,⁹ using the Green function theory, have obtained the expressions of many thermodynamical quantities in the vicinity of the transition points. Recently, Yang and Wang¹⁰⁾ have developed the Green function diagrammatic expansion technique and applied to a spin-1 Heisenberg ferromagnet to calculate spin-wave energies and magnetization. The use of the Green function theory has thus grown rapidly because it covers the entire temperature range, including the particularly interesting intermediate region in the neighborhood of the transition point, and agrees satisfactorily with the rigorous results at both very low and very high temperatures.

In this paper, we develop the unified Green function theory for the Heisenberg spin systems of the ferro- and antiferro-magnets. The Hamiltonian for the Heisenberg spin systems are set up. The equation of motion of the Green function are formulated and are decoupled by the Callen decoupling approximation. The solution of the equation of Green function is used to find the static pair correlation function of perpendicular components of spins at, above, and below the Curie temperature of the ferromagnets.

II. Temperature-Dependent Causal Green Functions

The Green functions are the appropriate generalization of the concept of correlation functions. They are intimately connected with

the evaluation of observed quantities and they have well-known advantages when equations are formulated and solved.

For a system of time-independent Hamiltonian H , the temperature-dependent causal Green function $G_{AB}(t)$ involving the two operators A and B is defined by

$$G_{AB}(t) = -i \langle TA(t)B(0) \rangle, \quad (2.1)$$

where $A(t)$ and $B(0)$ are the Heisenberg representations of the operators A and B , expressed in terms of a product of quantized field equations

$$A(t) = \exp(iHt)A \exp(-iHt) \quad (2.2)$$

(a system of units in which $\hbar=1$ is used throughout). The bracket $\langle \dots \rangle$ indicates an average over a grand canonical ensemble of the system at temperature T :

$$\langle \dots \rangle = \text{Tr}(e^{-\beta H} \dots) / \text{Tr}(e^{-\beta H}) \quad (2.3)$$

with $\beta = \frac{1}{kT}$. The symbol T in Eq. (2.1) is the time ordering operator defined for the Boson system by

$$TA(t)B(0) = \theta(t)A(t)B(0) + \theta(-t)B(0)A(t), \quad (2.4)$$

where

$$\theta(t) = \begin{cases} 1 & \text{for } t > 0 \\ 0 & \text{for } t < 0 \end{cases} \quad (2.5)$$

The equations of motion for the Green functions (2.1) are derived as follows: Differentiating the Green functions with respect to time we first get the equation

$$\begin{aligned} i \frac{d}{dt} G_{AB}(t) &= \frac{d\theta(t)}{dt} \langle A(t)B(0) \rangle \\ &+ \frac{d\theta(-t)}{dt} \langle B(0)A(t) \rangle \\ &- i \langle Tt \frac{dA(t)}{dt} B(0) \rangle. \end{aligned} \quad (2.6)$$

Using the equation of motion for the operator $A(t)$

$$i \frac{dA}{dt} = [A, H] \quad (2.7)$$

and the relation between the discontinuous function $\theta(t)$ and the Dirac δ function of t

$$\theta(t) = \int_{-\infty}^t \delta(t') dt'. \quad (2.8)$$

Eq. (2.6) becomes

$$i \frac{d}{dt} G_{AB}(t) = \delta(t) \langle [A(t), B(0)] \rangle + i \langle T[H(t), A(t)] B(0) \rangle. \quad (2.9)$$

Because $G_{AB}(t > 0)$ and $G_{AB}(t < 0)$ are analytic functions for the complex values of the time arguments in the region $0 < (Im t) < -\beta$ and $0 < (Im t) < \beta$, respectively, and if one extends the definition of T -operator to mean " $i \times t$ " ordering operator, the Green functions are well defined in the region $-\beta < \tau < 0$ and $0 < \tau < \beta$ for imaginary time argument with $\tau = it$. The equation of motion for $G_{AB}(\tau)$ can be written in the form

$$\frac{d}{d\tau} G_{AB}(\tau) = \delta(\tau) \langle [A(\tau), B(0)] \rangle + \langle T[H(\tau), A(\tau)] B(0) \rangle. \quad (2.10)$$

The Green functions on the right hand side of Eq. (2.10) are of a higher order than the initial one. One can construct for them also equations of the kind Eq. (2.10) and one can obtain a chain of coupled equations of the Green functions.

There exists an important property of these Green functions. The Green function is a periodic function of τ with period β . It can be shown easily from its definition that

$$\begin{aligned} G_{AB}(\tau - \beta) &= G_{AB}(\tau) \quad \text{for } \beta > \tau > 0 \\ G_{AB}(\tau + \beta) &= G_{AB}(\tau) \quad \text{for } -\beta < \tau < 0 \end{aligned} \quad (2.11)$$

Because of its periodic property the causal Green function $G_{AB}(\tau)$ can be expanded as

$$\begin{aligned} G_{AB}(\tau) &= \frac{1}{\beta} \sum_n G_{AB}(n) \exp(-i w_n \tau) \\ G_{AB}(n) &= \int_{-\frac{\beta}{2}}^{\frac{\beta}{2}} d\tau G_{AB}(\tau) \exp(i w_n \tau) \end{aligned} \quad (2.12)$$

with $w_n = \frac{2\pi n}{\beta}$, where n is integer. This periodicity allows one to extend the definition of the Green function outside the range $(-\beta, \beta)$.

III. Green Function Equations of the Heisenberg Spin Systems

If one confines one's considerations to a cubic crystal and divides the lattice points into two sub-lattices, denoted by l and m , the Hamiltonian for the two sub-lattices Heisenberg spin

systems may be written as

$$\begin{aligned} H = & - \sum_{l,m,j} J_{l,m,j} \vec{S}_{l,i} \cdot \vec{S}_{m,j} - h \sum_i S_{l,i}^z (1 + \delta_{lm}) \\ & + h \sum_m S_{m,j}^z (1 - \delta_{lm}) \end{aligned} \quad (3.1)$$

where the indices i, j denote the lattice sites, S_{li} is the spin operator for the ion site i of sub-lattice l , h is the effective magnetic field in energy units, and $J_{l,m,j}$ are the exchange coupling constants. It must be such that the spins on sub-lattice l are preferentially orientated in the $+z$ direction and those on sub-lattice m in the $-z$ direction, z being the direction of the spontaneous magnetization. Thus, for $l=m$, Eq. (3.1) reduces to the ferromagnetic Hamiltonian, whereas, for $l \neq m$ this is the antiferro-magnetic Hamiltonian.

The Hamiltonian H given in Eq. (3.1) is now used to develop the Green function for the Heisenberg ferro- and antiferro-magnets. The temperature-dependent causal Green function for the two sub-lattice spin systems is defined as

$$G_{l,m,j}(a, \tau) = \langle T S_{l,i}^+(\tau) \exp(a S_{m,j}^z) S_{m,j}^- \rangle \quad (3.2)$$

with

$$S_{li}^+(\tau) = \exp(\tau H) S_{li}^+ \exp(-\tau H) \quad (3.3)$$

$$S_{li}^\pm = S_{li}^x \pm i S_{li}^y, \quad (3.4)$$

where a in the exponent is a parameter.

As shown in Eq. (2.10), the equation of motion for the Green functions is

$$\begin{aligned} \frac{d}{d\tau} G_{l,m,j}(a, \tau) &= \delta(\tau) \delta_{lm} \delta_{ij} \theta_{li}(a) \\ &+ \langle T[H(\tau), S_{li}^+(\tau)] \exp(a S_{m,j}^z) S_{m,j}^- \rangle, \end{aligned} \quad (3.5)$$

where

$$\theta_{li}(a) = \langle [S_{li}^-, \exp(a S_{li}^z) S_{li}^-] \rangle. \quad (3.6)$$

Using the transformation between the two different representations

$$[H(\tau), S_{li}^+(\tau)] = \exp(\tau H) [H, S_{li}^+] \exp(-\tau H) \quad (3.7)$$

and the commutation rules of

$$\begin{aligned} [S_{mj}^+, S_{li}^+] &= 0 \\ [S_{mj}^-, S_{li}^+] &= -2\delta_{lm} \delta_{ij} S_{li}^z \\ [S_{mj}^z, S_{li}^+] &= \delta_{lm} \delta_{ij} S_{li}^z \end{aligned} \quad (3.8)$$

the equation of motion for the Green function,

Eq. (3.5), becomes

$$\begin{aligned} -\frac{d}{d\tau} G_{li,mj}(a, \tau) &= \delta(\tau) \delta_{lm} \delta_{ij} \theta_{li}(a) \\ &\quad -h(1+\delta_{ln}) \langle T\{S_{li}^+(\tau)\} \exp(aS_{nk}^z) S_{nk}^- \rangle \\ &\quad +h(1-\delta_{mn}) \langle T\{S_{mj}^+(\tau)\} \exp(aS_{nk}^z) S_{nk}^- \rangle \\ &\quad +2 \sum_{n,k} J_{li,nk} \langle T\{S_{li}^+(\tau)\} S_{nk}^z(\tau) \\ &\quad -S_{li}^z(\tau) S_{nk}^+(\tau) \rangle \exp(aS_{mj}^z) S_{mj}^- \rangle. \end{aligned} \quad (3.9)$$

The right side of Eq. (3.9) contains Green functions of a higher order than that on the left. The equation of motion for them bring Green functions of an even higher order, resulting in an infinite chain of coupled equations for Green functions of all orders.

Equations (3.9) are exact, however, the solution of this chain of equations is extremely complicated in the general statement of the problem. One can sometimes by approximation method uncouple the chains of Eq. (3.9), i.e. reduce it to a finite set of equations, which can then be solved.

The method frequently used in the past to linearize the coupled equation is the random phase approximation (RPA)^{1,2} in which the operator S^z is replaced by its average value $\langle S^z \rangle$ and the fluctuations of S^z are ignored. Results of this approximation disagree when compare with those of the low-temperature theory.

To take into account the fluctuations of S^z around its statistical average, Callen decoupling approximation (CDA)³ is used in this work. Decoupling scheme of the form of the Green function is given by

$$\begin{aligned} \langle T\{S_{li}^z(\tau) S_{mj}^+(\tau)\} B \rangle &= \langle S_{li}^z(\tau) \rangle \\ &\quad \times \langle T S_{mj}^+(\tau) B \rangle \\ -\alpha \langle S_{li}^-(\tau) S_{mj}^+(\tau) \rangle &\langle T S_{li}^+(\tau) B \rangle \end{aligned} \quad (3.10)$$

with $\alpha = \frac{\langle S_{mj}^z \rangle}{2S^2}$ for general spin S .

Inserting the decoupling approximation Eq. (3.10) into the Eq. (3.9) and using the periodic property of the Green function given in Eq. (3.12) one obtains a finite set of equations.

$$\begin{aligned} -i\omega_n G_{li,mj}(a, n) &= \delta_{lm} \delta_{ij} \theta_{li}(a) \\ &\quad -h(1+\delta_{ln}) G_{li,nk}(a, n) + h(1-\delta_{mn}) G_{mj,nk}(a, n) \\ &\quad -2 \sum_{n,k} J_{li,nk} \left\{ \langle S_{li}^z \rangle \left[1 + \frac{\phi_{nk,li}^{(0)}}{2S^2} \right] G_{nk,mj}(a, n) \right. \\ &\quad \left. - \langle S_{nk}^z \rangle \left[1 + \frac{\phi_{li,nk}^{(0)}}{2S^2} \right] G_{li,mj}(a, n) \right\}. \end{aligned} \quad (3.11)$$

Here,

$$\phi_{li,nk}(\tau, a) = \langle \exp(aS_{li}^z(\tau)) S_{li}^-(\tau) S_{nk}^+(\tau) \rangle$$

and

$$\begin{aligned} \phi_{li,nk}(\tau, a) &= \phi_{li,nk}(a) \text{ because } \langle S_{li}^z(\tau) \rangle \\ &= \langle S_{li}^z \rangle. \end{aligned} \quad (3.12)$$

The linearized equation, Eq. (3.11), can readily be solved if one introduces the following Fourier transformations:

$$\begin{aligned} G_{li,mj}(a, n) &= \frac{2}{N} \sum_q G_{lm,q}(a, n) \exp(i\vec{q} \cdot (\vec{r}_{li} - \vec{r}_{mj})) \\ G_{lm,q}(a, n) &= \sum_{l,j} G_{li,mj}(a, n) \exp(-i\vec{q} \cdot (\vec{r}_{li} - \vec{r}_{mj})) \end{aligned} \quad (3.13)$$

$$\begin{aligned} J_{li,mj} &= \frac{2}{N} \sum_q J_{lm}(q) \exp(-i\vec{q} \cdot (\vec{r}_{li} - \vec{r}_{mj})) \\ J_{lm}(q) &= \sum_{l,j} J_{li,mj} \exp(i\vec{q} \cdot (\vec{r}_{li} - \vec{r}_{mj})) \end{aligned} \quad (3.14)$$

$$\begin{aligned} \phi_{li,mj}(a) &= \frac{2}{N} \sum_q \phi_{lm,q}(a) \exp(-i\vec{q} \cdot (\vec{r}_{li} - \vec{r}_{mj})) \\ \phi_{lm,q}(a) &= \sum_{l,j} \phi_{li,mj}(a) \exp(i\vec{q} \cdot (\vec{r}_{li} - \vec{r}_{mj})) \end{aligned} \quad (3.15)$$

where $\frac{N}{2}$ is the number of spin sites in each sub-lattice, \vec{r}_{li} is the position vector of the site i in sub-lattice l and the q -sum is over the allowed wave vectors.

The translational invariance implies that $\theta_{li}(a)$ and $\langle S_{li}^z \rangle$ are independent of l :

$$\begin{aligned} \theta_{li}(a) &= \langle [S_{li}^+, \exp(aS_{li}^z) S_{li}^-] \rangle = \theta_l(a) \\ \theta_l(0) &= 2m_l \\ \langle S_{li}^z \rangle &= \langle S_l^z \rangle = m_l, \end{aligned} \quad (3.16)$$

m_l being the sub-lattice magnetization per spin in the sub-lattice.

After the spatial Fourier transformation of Eq. (3.13) to Eq. (3.15), the equation of motion of the Green function, Eq. (3.11), leads to

$$\begin{aligned} -i\omega_n G_{lm,q}(a, n) &= \delta_{lm} \theta_l(a) - h(1+\delta_{ln}) G_{lm,q}(a, n) \\ &\quad + h(1-\delta_{mn}) G_{mn,q}(a, n) \\ &\quad + 2m_l \left[J(0) - \frac{1}{N S^2} \sum_{q'} J(q') \phi_{ln,q'}^{(0)} \right] G_{lm,q}(a, n) \end{aligned}$$

$$-2m_i \left[J(q) + \frac{1}{NS^2} \sum_{q'} J(q' - q) \phi_{n_i, q'}(0) \right] G_{nm, q}(a, n). \quad (3.17)$$

It is now ready to find the solution of the equation of motion for the Green function. This solution will be useful for the study of the properties of the thermodynamics of the Heisenberg spin systems. From now on we consider only the ferromagnetic spin system of $l=m$. The solution of Eq. (3.17) is then given by

$$G_q(a, n) = \frac{\theta(a)}{w_q - iw_n} \quad (3.18)$$

where

$$w_q = 2h + 2mJ(0, q) + \frac{2m}{NS^2} \sum_{q'} J(q', q - q) \phi_{q'}(0) \quad (3.19)$$

with

$$J(q, q') = J(q) - J(q'). \quad (3.20)$$

Using the transformation in Eq. (2.12) along with Eq. (3.18) one finds the Green function of the ferromagnetic spin system in the τ -representation

$$\begin{aligned} G_q(a, \tau) &= \theta(a) \frac{1}{\beta} \sum_n \frac{\exp(-iw_n \tau)}{w_q - iw_n} \\ &= \theta(a) \frac{\exp(w_q \tau)}{1 - \exp(-\beta w_q)} \end{aligned} \quad (3.21)$$

It can also be written in the form that

$$\begin{aligned} G_q(a, \tau=0^-) &= G_q(a, \tau=\beta^-) \\ &= \theta(a) \frac{1}{\exp(\beta w_q) - 1}. \end{aligned} \quad (3.22)$$

The Eq. (3.6) defining $\theta(a)$, Eq. (3.19) defining w_q and Eq. (3.22) are the basic equations of the theory.

IV. Transverse Spin Correlation Functions of the Heisenberg Ferromagnets

The spin correlation functions play a fundamental role in thermodynamical studies of the Heisenberg magnets. The Green function in the τ -representation will be used here to find the transverse spin correlation function of the ferromagnets.

Introducing the Fourier transforms of spin operators by

$$\begin{aligned} \hat{S}_q &= \sum_i \hat{S}_i \exp(-i\vec{q} \cdot \vec{r}_i) \\ \hat{S}_i &= \frac{1}{N} \sum_q \hat{S}_q \exp(i\vec{q} \cdot \vec{r}_i) \end{aligned} \quad (4.1)$$

one can write the spin correlation function

$$\begin{aligned} \langle S_{-q}^- S_q^+ \rangle &= \sum_{i,j} \langle S_i^- S_j^+ \rangle \exp(i\vec{q} \cdot \vec{r}_{ij}) \\ \langle S_{-q}^+ S_q^- \rangle &= \sum_{i,j} \langle S_i^+ S_j^- \rangle \exp(i\vec{q} \cdot \vec{r}_{ij}) \end{aligned} \quad (4.2)$$

From the equations (3.2), (3.13), (3.21), (3.22) and (4.2), it follows that

$$\begin{aligned} \langle S_{-q}^- S_q^+ \rangle &= NG_q(a=0, \tau=0^-) \\ N\theta(0) &= \frac{1}{\exp(\beta w_q) - 1} \\ \langle S_{-q}^+ S_q^- \rangle &= NG_{-q}(a=0, \tau=0^+) \\ &= N\theta(0) \frac{\exp(\beta w_{-q})}{\exp(\beta w_{-q}) - 1} \end{aligned} \quad (4.3)$$

The transverse spin correlation functions in the configuration space are given by

$$\begin{aligned} \langle S_i^- S_j^+ \rangle &= G_{i,j}(a=0, \tau=0^-) \\ &= \frac{2m}{N} \sum_q \frac{1}{\exp(\beta w_q) - 1} \exp(-i\vec{q} \cdot \vec{r}_{ij}) \\ \langle S_i^+ S_j^- \rangle &= G_{i,j}(a=0, \tau=0^+) \\ &= \frac{2m}{N} \sum_q \frac{\exp(\beta w_{-q})}{\exp(\beta w_{-q}) - 1} \exp(-i\vec{q} \cdot \vec{r}_{ij}) \end{aligned} \quad (4.4)$$

with $\theta(0) = 2m$.

We can thus write the static pair correlation function of perpendicular components of spins:

$$\begin{aligned} \langle S_i^x S_j^x \rangle &= \frac{1}{N} \sum_q \phi^{xx}(q) \exp(-i\vec{q} \cdot \vec{r}_{ij}) \\ \langle S_i^y S_j^y \rangle &= \frac{1}{N} \sum_q \phi^{yy}(q) \exp(-i\vec{q} \cdot \vec{r}_{ij}) \end{aligned} \quad (4.5)$$

where $\phi^{xx}(q)$, etc., can be expressed by making use of Eq. (4.4) as

$$\phi^{xx}(q) = \phi^{yy}(q) = \frac{m}{2} \frac{\exp(\beta w_q) + 1}{\exp(\beta w_q) - 1} \quad (4.6)$$

These results agree with the calculations of Kawasaki and Mori⁽¹⁾ and Liu⁽²⁾. However, the expression of w_q given by Kawasaki and Mori disagree with our results in the third term of Eq. (3.19).

If one considers the nearest neighbor interactions only, the exchange constant J_{l, m_j} can be written as

$$J_{l, q} = \sum_{i, (\pm\delta)} J, \quad (4.7)$$

where δ is any nearest neighbor vector and J is the nearest neighbor interaction constant. In this case, one can write w_q in Eq. (3.19) in

the form of

$$w_q = 2h + 2mRJ(0, q) \quad (4.8)$$

with

$$R = 1 + \frac{1}{2NS^2} \sum_q J(q) \phi_s(0). \quad (4.9)$$

As mentioned before, Kawasaki and Mori¹¹⁾ ignored partly the w_q effect in resulting that $R=1$, which is quite different from Eq. (4.9).

Using Eq. (4.8) and expanding the exponential functions in Eq. (4.6), one finds the transverse correlation functions at, above, and below the Curie temperature T_c :

$$\langle S^x S^x \rangle = \frac{1}{N} \sum_q \phi^{xx}(q) \exp(-i\vec{q} \cdot \vec{r}_{i,1,2\bar{x}}),$$

where

$$\phi^{xx}(q) = \frac{kT}{-2 + \chi + 2RJ(0, q)} \quad (4.10)$$

for $T > T_c$ and $h \neq 0$. Here the susceptibility χ for a single spin is defined by

$$\chi = \lim_{h \rightarrow 0} \frac{m}{h}. \quad (4.11)$$

Below the Curie temperature T_c , ϕ^{xx} in Eq. (4.6) are obtained as

$$\phi^{xx}(q) = \frac{kT}{2RJ(0, q)} \quad (4.12)$$

We have thus shown the transverse spin correlation function in the entire temperature range, including the particularly interesting intermediate region in the vicinity of the Curie temperature for the Heisenberg ferromagnets.

V. Conclusion

The unified Green function theory was developed for the Heisenberg spin systems of the ferro- and antiferro-magnets. The exact equation of motion for the Green function, which involves higher-order Green function, was decoupled by the Callen decoupling approximation for its solution.

It was found that for arbitrary spin quantum number S , temperature T , and exchange constant J_{ij} , Eq. (3.6) defining $\theta(a)$, Eq. (3.19) defining w_q , and Eq. (3.22) for $G_q(a, \tau)$ constitute the basic equations for the theory. The pair correlation function of perpendicular components of spins at, above, and below the Curie temperature for the ferromagnet was calculated and found to agree with the other results.

Further work will be concerned with the longitudinal correlation function of the ferromagnet and the application of those correlation functions for the study of the thermodynamics and transport properties. The same technique will also be used for the Heisenberg antiferromagnet.

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