

A Study on the Temperature Dependence of the Specific Heat near the Curie Temperature of the Heisenberg Ferromagnets

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〈Abstract〉

The temperature dependence of the specific heat above the Curie temperature of the Heisenberg ferromagnets has been studied by use of thermal Green function theory developed in previous work. The spin correlation functions have been calculated from the solutions of the equation of motion of the perturbed Green function of the Heisenberg ferromagnet spin system, after linearizing by the Callen decoupling approximation. And then the specific heat of the Heisenberg ferromagnets was calculated from the spin correlation functions. The temperature dependence of the specific heat was found to be consistent with the other works.

Curie溫度 附近에서 強磁性體의 比熱溫度 依存性 研究

羅 商 均
材 料 工 學 科

〈要 約〉

Heisenberg 強磁性體의 Curie溫度 附近에서 比熱의 溫度 依存성을 지난 研究에서 얻은 Green函數 理論에 의하여 研究하였다. Heisenberg 強磁性體 Spin系에 關한 攝動 Green函數의 運動方程式의 解를 Callen Decoupling 近似方法으로 線型化시켜 求하였고 이 解를 利用하여 Spin의 相關函數를 計算하였다. Spin 相關函數를 利用하여 얻은 Heisenberg 強磁性體의 比熱 溫度依存성이 다른 研究結果와 一致함을 얻었다.

I. Introduction

It has been one of the most important subjects to study the temperature-dependence of the specific heat of the ferromagnets near the transition points between the ferromagnetic and paramagnetic phases. The model used for the theoretical study was the Heisenberg model, which consists of a regular array of localized spins that are coupled together by exchange

interaction. The thermal properties of the Heisenberg spin systems have been frequently explained by the thermal Green function theory during the last several years. The most important feature of the Green's function theory is that it treats the entire temperature range, and that it agrees with the spin-wave theory¹⁻³⁾ at very low temperatures as well as statistical theory⁴⁻⁵⁾ at very high temperatures. This theory also makes it possible to understand a number of physical phenomena that occur above and at the transition temperature point.

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Although much progress⁸⁻¹⁰⁾ has been made to explain the thermal properties of Heisenberg spin systems in the direction of Green's function theory, it has not been entirely successful because of the mathematical difficulties in solving the model. In a previous study,¹¹⁾ the unified Green's function theory for the Heisenberg spin systems has been developed and the Callen decoupling approximation was introduced to get rid of mathematical difficulties in solving the exact equation of motion for the Green's function.

The present work was conducted by use of this unified thermal Green's function theory to explain the temperature-dependence of the specific heat near the transition temperature point of the Heisenberg ferromagnets. In the process of the calculation for the specific heat, the transverse and longitudinal correlation functions between the spins of the Heisenberg ferromagnets have to be mentioned because these correlation functions play a fundamental role not only for calculation of the specific heat but also for the study of the other thermodynamical properties.

II. The Unperturbed and Perturbed Thermal Green Functions

For a system of time-independent Hamiltonian H , the unperturbed temperature-dependent Green function $G_{AB}(t)$ involving 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 Schrödinger operators A and B , expressed in terms of a product of quantized field equations

$$A(t) = e^{iHt} A e^{-iHt} \quad (2-2)$$

with $\hbar=1$ and the bracket $\langle \dots \rangle$ indicates an average over a grand canonical ensemble of the system at temperature T such as

$$\langle \dots \rangle = \text{Tr} \left(e^{-\frac{\beta H}{kT}} \dots \right) / \text{Tr} \left(e^{-\frac{\beta H}{kT}} \right). \quad (2-3)$$

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 $\theta(t)$ is the unit step function defined by

$$\theta(t) = \begin{cases} 1 & \text{for } t > 0 \\ 0 & \text{for } t < 0 \end{cases} \quad (2-5)$$

and has the relation with the Dirac delta function

$$\theta(t) = \int_{-\infty}^t \delta(t') dt'. \quad (2-6)$$

The Green function $G_{AB}(t > 0)$ and $G_{AB}(t < 0)$ are analytic function for the complex values of the time arguments in the region $0 > \text{Im } t > -\beta$ and $0 < \text{Im } t < \beta$, respectively. Therefore, 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 $\tau = it$.

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

$$i \frac{dA(t)}{dt} = [A, H], \quad (2-7)$$

the equation of motion for the unperturbed thermal Green function $G_{AB}(\tau)$ can be written in the form as follows.

$$\begin{aligned} \frac{d}{d\tau} G_{AB}(\tau) &= \delta(\tau) \langle [A(\tau), B(0)] \rangle \\ &+ \langle T [H(\tau), A(\tau)] B(0) \rangle. \end{aligned} \quad (2-8)$$

If one considers a perturbed system represented by a time-dependent perturbed Hamiltonian H' , the perturbed Green function is defined as

$$G'_{AB}(t) = -i \langle A(t)B(0) \rangle', \quad (2-9)$$

and the Heisenberg operator $A(t)$ is formulated as

$$A(t) = U(-\infty, t) A U(t, -\infty) \quad (2-10)$$

for a perturbation turned on adiabatically at $t = -\infty$. The time development operator $U(t, t')$ is determined by

$$i \frac{\partial U(t, t')}{\partial t} = H' U(t, t') \quad (2-11)$$

$$U(t, t') = 1. \quad (2-12)$$

The equation of motion for the perturbed Green function with imaginary time argument can also be found as

$$\begin{aligned} \frac{d}{d\tau} G'_{AB}(\tau) = & \delta(\tau) \langle [A, B] \rangle' \\ & + \langle T[H'(\tau), A(\tau)]B(0) \rangle \end{aligned} \quad (2-13)$$

where

$$\langle [A, B] \rangle' = \text{Tr}\{\rho'(0)[A, B]\} \quad (2-14)$$

being ρ' is the density operator for the perturbed system, and one can write for ρ'

$$i \frac{d\rho'}{dt} = [H', \rho']. \quad (2-15)$$

There exists an important property of the Green functions. The unperturbed and perturbed Green functions are both the periodic functions of τ with period β . For example, the unperturbed Green function has the periodic property such as

$$\begin{aligned} G_{AB}(\tau - \beta) &= G_{AB}(\tau) \text{ for } \beta > \tau > 0 \\ G_{AB}(\tau + \beta) &= G_{AB}(\tau) \text{ for } -\beta < \tau < 0. \end{aligned} \quad (2-16)$$

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

$$G_{AB}(\tau) = \frac{1}{\beta} \sum_n G_{AB}(n) \exp(-i w_n \tau) \quad (2-17)$$

$$G_{AB}(\tau) = \int_{-\beta/2}^{\beta/2} d\tau' G_{AB}(\tau') \exp(i w_n \tau)$$

with $w_n = \frac{2\pi n}{\beta}$, where n is integer. The periodicity allows one to extend the definition of the unperturbed and perturbed Green function outside the domain $-\beta < \tau < 0$ and $0 < \tau < \beta$.

III. The Equation of Motion for the Heisenberg Ferromagnet Spin Systems.

The time-independent Hamiltonian for the Heisenberg spin systems of the ferro- and antiferromagnet spin systems was found to be

$$\begin{aligned} H = & - \sum_{l, m_j} J_{l, m_j} \bar{S}_{li} \cdot \bar{S}_{m_j} - \frac{\hbar}{2} \sum_{li} S_{li}^z (1 + \delta_{lm}) \\ & + \frac{\hbar}{2} \sum_{m_j} S_{m_j}^z (1 - \delta_{lm}), \end{aligned} \quad (3-1)$$

where the spin lattice points are divided into two sublattices denoted by l and m . The indices i, j represent the sublattice sites, S_{li} the spin operator for the ion site i of sublattice l , and J_{l, m_j} the exchange coupling constants. It must be such that the spins on sublattice l are

preferentially oriented in the $+z$ direction and those on sublattice m in the $-z$ direction, z being the direction of the spontaneous magnetization.

The system of $l=m$ in Eq(3-1) represents the ordered spin state which behaves as if magnetic moment of the constituent particles were aligned parallel ($+z$ direction) and is called the ferromagnetic. Thus, the Hamiltonian for the Heisenberg ferromagnets becomes, from Eq. (3-1), as follows;

$$H = \sum_{ij} J_{ij} \bar{S}_i \cdot \bar{S}_j - \hbar \sum_i S_i^z. \quad (3-2)$$

If one considers a perturbed system turned on adiabatically at $t = -\infty$, then the perturbed Hamiltonian for such a system can be expressed as

$$H' = H + H_t, \quad (3-3)$$

where the first term H is the time-independent Hamiltonian of Eq(3-1) (or Eq. 3-2). The second term H_t in Eq. (3-3) is a space- and time-dependent perturbation and can be represented by

$$H_t = -f \sum_i S_i^z \exp(i\vec{q} \cdot \vec{R}_{ij} + (\epsilon - i w) t), \quad \epsilon = 0^+ \quad (3-4)$$

f being a small parameter proportional to the amplitude of an external *a. c.* field.

Using the perturbed Hamiltonian, the thermal Green function for the Heisenberg ferromagnet spin system with a time dependent perturbation (hereafter called the perturbed Green function) is defined, like Eq. (2-9), as

$$G_{ij}'(a, \tau) = \langle T S_i^+(a, \tau) \exp(a S_j^z) S_j^-(0) \rangle' \quad (3-5)$$

with

$$S_i^+(\tau) = e^{\tau H'} S_i^+ e^{-\tau H'} \quad (3-6)$$

$$S_i^\pm = S_i^\pm \pm i S_i^y, \quad (3-7)$$

where T is the τ ordering operator and a in the exponent is a parameter.

The equation of motion for time perturbed Green function, $G_{ij}'(a, \tau)$, can be written, with help of Eq. (2-13) and variable changes ω by $i(w_n - \epsilon)$ and t by $-\tau$ in Eq. (3-4), as

$$\begin{aligned} \frac{d}{d\tau} G_{ij}'(a, \tau) = & \delta(\tau) \delta_{ij} \theta_i'(a) - \hbar G_{ij}'(a, \tau) \\ & - f \exp(i\vec{q} \cdot \vec{R}_{ij} - i w_n \tau) G_{ij}'(a, \tau) \end{aligned}$$

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$$-2\sum_k J_{ik} \{ \langle [TS_i^z(\tau)S_i^+(\tau) - TS_i^+(\tau)S_i^z(\tau)] \cdot \exp(\mathbf{a}S_i^+) S_i^- \rangle \}, \quad (3-8)$$

where

$$\theta_i' = \langle [S_i^+, \exp(\mathbf{a}S_i^+) S_i^-] \rangle. \quad (3-9)$$

In deriving Eq. (3-8), the following commutation rules

$$\begin{aligned} [S_j^+, S_i^+] &= 0 \\ [S_j^-, S_i^+] &= -2\delta_{ij} S_i^+ \\ [S_j^+, S_i^-] &= \delta_{ij} S_i^+ \end{aligned} \quad (3-10)$$

and the transformation between two different representations

$$[H'(\tau) S_i^+(\tau)] = e^{-H'} [H', S_i^+] e^{-\tau H'} \quad (3-11)$$

$$[H', S_i^+] = -2\sum_k J_{ik} (S_i^+ S_k^+ - S_k^+ S_i^+) - h S_i^+ \quad (3-12)$$

are used.

The right side of Eq. (3-8) contains the perturbed Green functions of a higher order than that on the left. The equation of motion for them brings the perturbed Green functions of an even higher order, resulting in an infinite chain of completed equations for the perturbed Green functions of all orders. Even though Eq. (3-8) are exact, it is extremely complicated to find the solution of this chain equation of the perturbed Green functions.

The Callen decoupling approximation¹²⁾ (CDA) is applied in this work to reduce Eq. (3-8) to a finite set of equation, which can be solved. The Eq. (3-3) becomes, after linearizing by CDA, as follows;

$$\begin{aligned} \frac{d}{d\tau} G_{ij}'(\mathbf{a}, \tau) &= \delta(\tau) \delta_{ij} \theta_i'(\mathbf{a}) - h G_{ij}'(\mathbf{a}, \tau) \\ &- f \exp(i\hat{\mathbf{q}} \cdot \bar{\mathbf{R}}_{ij} - i w_n \tau) G_{ij}'(\mathbf{a}, \tau) \\ &- 2\sum_k J_{ik} \{ \langle S_i^+ \rangle' [1 + \phi_{ik}'(0)/2S^2] G_{ij}'(\mathbf{a}, \tau) \\ &- \langle S_i^+ \rangle' [1 + \phi_{ki}'(0)/2S^2] G_{ij}'(\mathbf{a}, \tau) \}, \end{aligned} \quad (3-13)$$

where

$$\begin{aligned} \phi_{ik}'(\mathbf{a}, \tau) &= \langle \exp(\mathbf{a}S_i^+(\tau)) S_i^-(\tau) S_k^+(\tau) \rangle' \\ &= \phi_{ik}'(\mathbf{a}) \end{aligned} \quad (3-14)$$

$$\begin{aligned} \langle S_i^z(\tau) \rangle' &= \text{Tr} \{ e^{-\beta H'} e^{\tau H'} S_i^z e^{-\tau H'} \} / \text{Tr} (e^{-\beta H'}) \\ &= \langle S_i^z \rangle'. \end{aligned} \quad (3-15)$$

The perturbed quantities in Eq. (3-13), $G_{ij}'(\mathbf{a}, \tau)$,

$\theta_i'(\mathbf{a})$, $\langle S_i^z \rangle'$, and $\phi_{ik}'(\mathbf{a})$, can be expanded in power of a small parameter f with little physical consequence in the higher power of f . They are developed as follows;

$$G_{ij}'(\mathbf{a}, \tau) = G_{ij}(\mathbf{a}, \tau) + f G_{ij}^{(1)}(\mathbf{a}, \tau) + f^2(\dots) + \dots \quad (3-16)$$

$$\begin{aligned} \theta_i'(\mathbf{a}) &= \theta(\mathbf{a}) + f \exp(-i w_n \tau) \theta_i^{(1)}(\mathbf{a}, w_n) \\ &+ f^2(\dots) + \dots \end{aligned} \quad (3-17)$$

$$\begin{aligned} \langle S_i^z \rangle' &= \langle S_i^z \rangle + f \exp(-i w_n \tau) S_i^{(1)}(w_n) \\ &+ f^2(\dots) + \dots \end{aligned} \quad (3-18)$$

$$\begin{aligned} \phi_{ik}'(\mathbf{a}) &= \phi_{ik}(\mathbf{a}) + f \exp(-i w_n \tau) \phi_{ik}^{(1)}(\mathbf{a}, w_n) \\ &+ f^2(\dots) + \dots. \end{aligned} \quad (3-19)$$

Expanding Eq. (3-13) in power of f using Eqs. (3-16)–(3-19) and collecting the zeroth order terms and the first order terms, respectively, one obtains two different equations of motion for the thermal Green functions. The equation of motion for the zeroth order terms of f in Eq. (3-13) becomes

$$\begin{aligned} \frac{d}{d\tau} G_{ij}(\mathbf{a}, \tau) &= \delta(\tau) \delta_{ij} \theta_i(\mathbf{a}) - h G_{ij}(\mathbf{a}, \tau) \\ &- 2\sum_k J_{ik} \{ \langle S_i^z \rangle [1 + \phi_{ik}(0)/2S^2] G_{ij}(\mathbf{a}, \tau) \\ &- \langle S_i^z \rangle [1 + \phi_{ki}(0)/2S^2] G_{kj}(\mathbf{a}, \tau) \}, \end{aligned} \quad (3-20)$$

and the equation of motion for the first order terms of f in Eq. (3-13) is given by

$$\begin{aligned} \frac{d}{d\tau} G_{ij}^{(1)}(\mathbf{a}, \tau) &= \delta(\tau) \delta_{ij} \exp(-i w_n \tau) \theta_i^{(1)}(\mathbf{a}, \tau) \\ &- \exp(i\hat{\mathbf{q}} \cdot \bar{\mathbf{R}}_{ij} - i w_n \tau) G_{ij}(\mathbf{a}, \tau) - h G_{ij}^{(1)}(\mathbf{a}, \tau) \\ &- 2 \langle S_i^z \rangle \sum_k J_{ik} \{ [1 + \phi_{ik}(0)/2S^2] G_{ij}^{(1)}(\mathbf{a}, \tau) \\ &- [1 + \phi_{ki}(0)/2S^2] G_{ij}^{(1)}(\mathbf{a}, \tau) \} \\ &+ 2 \exp(-i w_n \tau) \sum_k J_{ik} \{ S_i(w_n) [1 + \phi_{ki}(0)/2S^2] \\ &G_{kj}(\mathbf{a}, \tau) \\ &- S_k(w_n) [1 + \phi_{ik}(0)/2S^2] G_{ij}(\mathbf{a}, \tau) \}. \end{aligned} \quad (3-21)$$

These equations of motion, Eq. (3-20) and Eq. (3-21), are very important because their solutions open the direct path to the spin correlation functions which play the fundamental role in thermodynamical studies of the Heisenberg ferromagnet. The zeroth order $\theta_i(\mathbf{a})$ and $\langle S_i^z \rangle$ are assumed to be independent of the

spin sites because of the translational invariance. Then, we have

$$\theta_i(\mathbf{a}) = \langle [S_i^+, \exp(\mathbf{a}S_i^z)S_i^-] \rangle = \theta(\mathbf{a}) \quad (3-22)$$

$$\langle S_i^z \rangle = \langle S^z \rangle = m \quad (3-23)$$

$$\theta(0) = 2m, \quad (3-24)$$

m being the magnetization per spin site.

By applying space and time transforms of the zeroth and first order terms of the physical quantities to Eqs. (3-20) and (3-21), respectively, each solution of the equations of motion of the zeroth order and the first order Green functions can be written as follows;

$$G_q(\mathbf{a}, \tau^- = 0) = \phi_q(\mathbf{a}) = \Phi\theta(\mathbf{a}) \quad (3-25)$$

$$\begin{aligned} G_{ij}^{(1)}(\mathbf{a}, \tau^- = 0) &= \phi_i^{(1)}(\mathbf{a}, w_n) \\ &= \Phi^{(1)}\theta_i^{(1)}(\mathbf{a}, w_n) + \theta(\mathbf{a})U_i(\mathbf{q}, w_n), \end{aligned} \quad (3-26)$$

where

$$\Phi = \frac{1}{\exp(\beta w_q) - 1} \quad (3-27)$$

$$\Phi^{(1)} = \frac{1}{N} \sum_q \Phi \quad (3-28)$$

$$\begin{aligned} U_i(\mathbf{q}_1, w_n) &= \frac{1}{N} \sum_{q_1} \frac{N(w_{q_1-q}) - N(w_{q_1})}{w_{q_1-q} - w_{q_1} + iw_n} \\ &\quad \cdot \exp(i\vec{q}_1 \cdot \vec{R}_i) \\ &+ \frac{1}{N^2} \frac{1}{m} \sum_{q_1, q_2} \frac{N(w_{q_1}) - N(w_{q_2})}{w_{q_1} - w_{q_2} + iw_n} (w_{q_1-q_2} - w_{q_2}) \\ &\quad S_{q_1-q_2}(w_n) \exp(i(\vec{q}_1 - \vec{q}_2) \cdot \vec{R}_i) \end{aligned} \quad (3-29)$$

$$w_q = h + 2mJ(0, q) + \frac{m}{NS^2} \sum_{q'} J(q', q' - q) \phi_{q'}(0) \quad (3-30)$$

$$J(q, q') = J(q) - J(q'). \quad (3-31)$$

Both of the solutions given in Eqs. (3-25) and (3-26) can be used to develop the spin correlation functions of the Heisenberg ferromagnets.

IV. The Spin Correlation Functions of the Heisenberg Ferromagnet Spin Systems.

It was noted that the spin correlation functions play a fundamental role for the study of the thermal properties of the Heisenberg spin systems. In this work the correlation functions will be used to calculate the temperature

dependence of the specific heat of the Heisenberg ferromagnets.

Form the solution of Eq. (3-25), the equation of motion of the zeroth order Green function, the transverse spin correlation functions can be expressed as follows;

$$\begin{aligned} \langle S_{-q}^- S_q^+ \rangle &= NG_q(\mathbf{a}=0, \tau=0^-) \\ &= 2Nm \frac{1}{\exp(\beta w_q) - 1} \end{aligned} \quad (4-1)$$

$$\begin{aligned} \langle S_{-q}^+ S_q^- \rangle &= NG_{-q}(\mathbf{a}=0, \tau=0^+) \\ &= 2Nm \frac{\exp(\beta w_{-q})}{\exp(\beta w_q) - 1} \end{aligned}$$

or they can be written in the configuration space after the Fourier transforms;

$$\begin{aligned} \langle S_i^- S_j^+ \rangle &= G_{ij}(\mathbf{a}=0, \tau=0^-) \\ &= \frac{2m}{N} \sum_q \frac{1}{\exp(\beta w_q) - 1} \exp(-i\vec{q} \cdot \vec{r}_{ij}), \\ \langle S_i^+ S_j^- \rangle &= G_{ij}(\mathbf{a}=0, \tau=0^+) \\ &= \frac{2m}{N} \sum_q \frac{\exp(\beta w_{-q})}{\exp(\beta w_q) - 1} \exp(-i\vec{q} \cdot \vec{r}_{ij}). \end{aligned} \quad (4-2)$$

One can, thus, write the spin correlation of perpendicular components of spins as follows:

$$\begin{aligned} \langle S_i^x S_j^y \rangle &= \frac{1}{N} \sum_q \phi^{xx}(q) \exp(-i\vec{q} \cdot \vec{r}_{ij}) \\ \langle S_i^y S_j^x \rangle &= \frac{1}{N} \sum_q \phi^{yy}(q) \exp(-i\vec{q} \cdot \vec{r}_{ij}), \end{aligned} \quad (4-3)$$

where $\phi^{xx}(q)$ etc, can be expressed by making use of Eq. (4-2) as

$$\phi^{xx}(q) = \phi^{yy}(q) = \frac{m}{2} \frac{\exp(\beta w_q) + 1}{\exp(\beta w_q) - 1}. \quad (4-4)$$

The longitudinal spin correlation function can also be found as follows: It one defines the perturbed expectation value of the operator S_i^z ,

$$\langle S_i^z \rangle' = \text{Tr}(\rho' S_i^z) \quad (4-5)$$

where ρ' is the density operator for the perturbed system such as;

$$i \frac{d\rho'}{dt} = [H', \rho'] \quad (4-6)$$

$$\rho'(t = -\infty) = \rho. \quad (4-7)$$

Then, the expansion of the expectation value of $\langle S_i^z \rangle$ into a power series of f can be given by

$$\langle S_i^z \rangle' = \langle S_i^z \rangle + f S_i^{(1)}(w) \exp(\epsilon t - i w t) \quad (4-8)$$

and

$$\langle S_i^z \rangle = T_r(\rho S_i^z) = m,$$

where m is the spontaneous magnetization per spin in absence of the *a. c.* field and

$$S_i^{(1)}(w) = -i \int_{-\infty}^0 \langle [S_{-q}^z(t'), S_i^z(0)] \rangle \exp(\epsilon t' - i w t') dt'. \quad (4-9)$$

In Eq. (4-9), $S_i^{(1)}(w)$ was expressed in terms of the longitudinal spin correlation function, $\langle S_{-q}^z(t'), S_i^z(0) \rangle$.

This function can be written in a spectral representation as follows;

$$\langle S_{-q}^z(t), S_i^z(0) \rangle = \int_{-\infty}^{\infty} \frac{dw}{2\pi} J_z(q, w) \exp(-i w t) \quad (4-10)$$

with reference to

$$J_z(q, w) = 2\pi \sum \rho_m \langle m | S_{-q}^z | n \rangle \langle n | S_i^z | m \rangle \delta(E_m - E_n + w) \quad (4-11)$$

$$\rho_m = \exp(-\beta E_m) / T_r(\exp(-\beta H)), \quad (4-12)$$

and $|n\rangle$ and E_n are the complete set of eigenfunction and eigenvalues of the time independent Hamiltonian such that

$$H|n\rangle = E_n|n\rangle \text{ and } \sum_n |n\rangle \langle n| = 1. \quad (4-13)$$

After some mathematical calculations, the $J_z(q, w)$ of Eq. (4-11) becomes

$$J_z(q, w) = \frac{i}{\exp(-\beta w) - 1} [S_q^{(1)}(-i w + \epsilon) - S_q^{(1)}(-i w - \epsilon)], \quad (4-14)$$

where $S_q^{(1)}(w_n)$ are the Fourier components of $S_i^{(1)}(w_n)$ in Eq. (4-9) such as

$$S_q^{(1)}(w_n) = \sum_i S_i^{(1)}(w_n) \exp(-i \vec{q} \cdot \vec{r}_{ij}) \quad (4-15)$$

and it can be expressed as

$$S_q^{(1)}(w_n) = G_q^z(w_n) = i w - \epsilon \quad (4-16)$$

if we define the *zz* Green function in the imaginary formalism

$$G_q^z = \langle T S_{-q}^z(\tau) S_q^z(0) \rangle, \quad -\beta \leq \tau \leq \beta. \quad (4-17)$$

Using Eq. (4-8) and the solution of the first order perturbed Green function, $G_{ij}^{(1)}(a, \tau = 0^-)$, Eq. (3-26), we have for $S_i^{(1)}(w_n)$

$$S_i^{(1)}(w_n) = \xi U_i(q, w_n), \quad (4-18)$$

where

$$\xi = \left[\frac{\Phi^s(1+\Phi)^s}{(1+\Phi)^{2s+1} - \Phi^{2s+1}} (2s+1) \right]^2 - 1. \quad (4-19)$$

The inverse space transform of Eq. (4-19) becomes

$$S^{(1)} = \frac{\xi \sum_{q_1} \frac{N(w_{q_1-q}) - N(w_{q_1})}{w_{q_1-q} - w_{q_1} + i w_n}}{1 + \frac{\xi}{m} \sum_{q_1} \frac{N(w_{q_1}) - N(w_{q_1-q})}{w_{q_1-q} - w_{q_1} + i w_n} [w_{q_1-q} - w_q]}.$$

From Eq. (4-10) together with Eqs. (4-14) and (4-20) the longitudinal spin correlation function can be found. Because of mathematical complexities we consider the nearest neighbor (*nn*) interactions from this point. In this case, one can write the exchange constant J_{ij}

$$J_{ij} = \delta_{ij}, \quad i, j \quad (4-21)$$

with $\vec{\delta}$ being any *nn* vector and J the exchange constant. The Fourier transforms of the exchange constant become

$$J(q) = J \sum \exp(i \vec{q} \cdot \vec{\delta})$$

$$J = \frac{1}{N} \sum_q J(q) \exp(-i \vec{q} \cdot \vec{\delta}). \quad (4-22)$$

For the case of *nn* interaction it can be shown that

$$\sum_{q'} J(q', q' - q) \phi_{q'}(0) = \frac{1}{J(0)} J(0, q) \sum_{q'} J(q') \phi_{q'}(0) \quad (4-23)$$

and hence, one can write

$$w_q = w_{-q} = h + 2mRJ(0, q) \quad (4-24)$$

with reference to

$$R = 1 + \frac{1}{2NS^2J(0)} \sum_{q'} J(q') \phi_{q'}(0). \quad (4-25)$$

The transverse and longitudinal spin correlation functions above the Curie temperature are found as follows: Above the Curie temperature T_c , the magnetization vanishes as the external magnetic field $h \rightarrow 0$. In this case, one can define the paramagnetic susceptibility χ by

$$\chi = \lim_{h \rightarrow 0} \frac{m}{h}. \quad (4-26)$$

Expanding the exponential function in Eq. (4-2) and keeping only dominant terms, one finds the transverse spin correlation function for $T > T_c$ and $h \rightarrow 0$

$$\begin{aligned} \langle S_i^- S_j^+ \rangle &= \langle S_i^+ S_j^- \rangle \\ &= \frac{1}{N\beta} \sum_q \frac{2\chi}{1 + 2\chi RJ(0, q)} \exp(-i \vec{q} \cdot \vec{r}_{ij}) \end{aligned} \quad (4-27)$$

with reference to

$$R = 1 + \frac{1}{2NS^2J(0)} \sum_q \frac{J(q')}{\beta RJ(0, q)}. \quad (4-28)$$

The longitudinal spin correlation function above T_c becomes, from Eq. (4-10),

$$\langle S_i^z S_i^z \rangle = \frac{N}{\beta} \frac{\chi}{1 + 2\chi RJ(0, q)} \quad (4-29)$$

or

$$\langle S_i^z S_j^z \rangle = \frac{1}{N\beta} \sum_q \frac{\chi}{1 + 2\chi RJ(0, q)} \exp(-i\mathbf{q} \cdot \mathbf{r}_{ij}). \quad (4-30)$$

V. Energy and Specific Heat

The internal energy of the Heisenberg ferromagnet spin system can be found from the Hamiltonian described in Eq. (3-1). It is

$$E = \langle H \rangle = -Nhm - \frac{1}{N} \sum_q J(q) \langle \hat{S}_q \cdot \hat{S}_q \rangle. \quad (5-1)$$

Here, the internal energy is expressed in terms of the correlation functions of the spins. The specific heat, then, can be obtained by differentiating the internal energy with respect to temperature. The specific heat is a fundamental quantity of the thermodynamics, because specific heat is necessary quantity for evaluation of the entropy and all the other thermodynamic functions can be calculated from the entropy.

In Chapter IV, the spin correlation functions have already been obtained in Eqs. (4-27) and (4-30) to observe the nearest neighbor interactions. Because of mathematical complexities, one can consider the paramagnetic temperature region when the external magnetic field $h \rightarrow 0$. In this case, from Eqs. (5-1), (4-27), and (4-30), it follows that

$$E = -\frac{3}{\beta} \sum_q \frac{J(q)}{\frac{1}{\chi} + 2RJ(0, q)} \quad (5-2)$$

Differentiating Eq. (5-2) with respect to temperature, one finds the specific heat approximately,

$$C \cong \frac{3}{2} \frac{N}{R} \left[1 - \frac{\langle [+2\chi RJ(0, q)]^{-1} \rangle^2}{\langle [1 + 2\chi RJ(0, q)]^{-2} \rangle} \right] \cdot \left\{ 1 + \frac{T\chi^2}{NS^2J(0)} \sum_q \frac{J(q)}{1 + 2\chi RJ(0, q)} \right\}^{-1} \quad (5-3)$$

One needs the high temperature expansion of χ to obtain the explicit temperature dependence of C . The specific heat for the nearest neighbor interactions for temperature above the Curie point is thus obtained for its final expression as follows;

$$C = 6N \frac{J^2(0)}{z} \left(\frac{S(S+1)}{3} \right)^2 \frac{1}{T^2} + \dots \quad (5-4)$$

with the number of the nearest neighbor,

$$z = \frac{1}{\frac{1}{N} \sum_q \left(\frac{J(q)}{J(0)} \right)^2}. \quad (5-5)$$

VI. Conclusion

The temperature dependence of the specific heat in the paramagnetic temperature region has been studied by use of the thermal Green function theory. A Green function of two operators at two spin sites was defined and the equation of this Green function for the Heisenberg ferromagnet spin system was found. The equations of motion of the zeroth and first order Green functions were linearized by Callen decoupling approximation and the linearized equations of motion were solved under the light of a perturbed Hamiltonian to find the spin correlation functions which play the fundamental role in calculating the specific heat.

The specific heat of the Heisenberg ferromagnet in the paramagnetic temperature region was found to be Eq. (5-4). If one compare the result of this work with that of Liu's one⁷⁾, one can write the specific heat as follows;

$$C = C_{\text{Liu}}^{\text{present}} \cdot \frac{1}{R \left\{ 1 + \frac{T\chi^2}{NS^2J(0)} \sum_q \frac{J(q)}{1 + 2\chi RJ(0, q)} \right\}}$$

Since $R > 1$ for $T > T_c$ and monotonically decreases to $R_\infty = 1$, the present result is an improvement over the other result.

On the basis of this investigation, one can conclude that it seems worth-while to use thermal Green function theory to obtain better

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quantitative results in studies of realistic magnetic systems.

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