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Green's-Function Formalism of the One-Dimensional Heisenberg Spin System

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The one-dimensional Heisenberg model with $S=1/2$ is treated with the use of the two-time Green's functions. The hierarchy of the equations of motion of the Green's functions is decoupled at a stage one-step further than Tyablikov's decoupling. The thermal average of the spin component, $\langle S^z\rangle$, is set to zero, because the long-range order does not exist in one dimension. Instead, our Green's functions are expressed in terms of the correlation functions $c_n\equiv 4\langle S_0{}^z S_n{}^z\rangle$. The Green's function is essentially of the form representing undamped spin waves, whose spectrum depends on c_1, c_2 and one more parameter. They are determined by the requirement that c_1 and c_2 should be self-consistent and that c_0 should be unity. The self-consistency equations have been solved analytically at high- and low-temperature limits, and also solved numerically in the whole range of the temperature. Thermodynamic quantities have been calculated using these solutions.

It has turned out that the theory gives the correct high-temperature expansion for the thermodynamic quantities and the correlation functions. The latter is expressed by $c_n=(J/4k_BT)^n$. In the case of ferromagnetic coupling, the correlation function c_n at $T=0$ is equal to 1/3 for all n's. This is what is expected from the correct ground state of the ferromagnetic Heisenberg system. The spin-wave spectrum at $T=0$ also agrees with the correct one. At $T\ll J/k_B$, we find that the specific heat goes as $T^{1/2}$ and the susceptibility goes as T^{-2}. The gross feature of the temperature-dependence of the thermodynamic quantities agrees with Bonner and Fisher. In the case of the antiferromagnetic Heisenberg model, we find $c_1=-0.55407$ and $c_2=0.16100$ at $T=0$, which are fairly close to the exact values. The thermodynamic quantities are also in gross agreement with Bonner and Fisher.

§ 1. Introduction

The one-dimensional Heisenberg system has been the subject of much theoretical and experimental efforts in recent years. It has been proved by Mermin and Wagner[1] that such a system does not possess the long-rang order at any temperature. In some respect, this situation makes the theoretical treatment of this system difficult compared with that of the three-dimensional Heisenberg system. Because of the absence of the long-range order, both the molecular-field theory and the spin-wave theory, which have been so successful in three dimension, become useless. Intuitively, however, one may consider that at low temperatures the correlation between spins decreases only very slowly as the distance between them is increased. In other words, the spins are practically ordered when viewed locally. This would imply that the spin wave is still a practical entity, which may properly describe the excitation of the system.

In this paper, we propose a theory of spin waves which does not require the existence of the long-rang order. The theory is formulated solely in terms of the short-range orders (or the correlation functions). A previous theory of the Heisenberg model which invokes the existence of the long-range order is due to Tyablikov.[2] His decoupling procedure gives a spin-wave spectrum which depends on $\langle S^z\rangle$. Since $\langle S^z\rangle$ vanishes in one dimension, we make a decoupling at a stage one-step further than Tyablikov. Then, the averages such as $\langle S_0^z S_1^z\rangle$ and $\langle S_0^z S_2^z\rangle$ appear. The Green's functions then become of the form of undamped spin waves, whose spectrum depends on these parameters. The latter are determined by the self-consistency requirement, and then the thermodynamic quantities are calculated using the solution. Thus, our procedure is analogous to the Nagaoka decoupling[3] in the problem of the exchange scattering in metals. For the ferromagnetic coupling, the spin-wave spectrum will turn out to be exact at $T=0$. For the antiferromagnetic coupling, it is fairly close to the correct one. It will also turn out that our theory gives the correct high-temperature expansion of the thermodynamic quantities. A numerical solution of the self-consistency equations has been obtained, and with the use of it, the thermodynamic quantities have been calculated in the whole range of the temperature. They are in gross agreement with Bonner and Fisher's numerical calculation on a finite number of spins.[4]

§ 2. Derivation of the basic equations

Our Hamiltonian for the one-dimensional Heisenberg model reads

$$H=-J\sum_{n=-N/2+1}^{N/2} \boldsymbol{S}_n\cdot\boldsymbol{S}_{n+1}\,, \tag{1}$$

where we assume $S=1/2$. We use the formalism of the two-time Green's function, whose time-Fourier transform satisfies the equation

$$\omega\langle\langle A;B\rangle\rangle=(2\pi)^{-1}\langle[A,B]\rangle+\langle\langle[A,H];B\rangle\rangle\,. \tag{2}$$

Here, [ ] denotes the commutator and $\langle\ \rangle$ denotes the thermal average. Let us consider a Green's function $\langle\langle S_0^+;S_n^-\rangle\rangle$, which satisfies

$$\omega\langle\langle S_0^+;S_n^-\rangle\rangle=(\pi)^{-1}\delta_{n0}\langle S_0^z\rangle-J\langle\langle S_0^zS_1^++S_0^zS_{-1}^+-S_0^+S_1^z-S_0^+S_{-1}^z;S_n^-\rangle\rangle\,. \tag{3}$$

Tyablikov[2] proposed a decoupling such as $\langle\langle S_0^zS_1^+;S_n^-\rangle\rangle\to\langle S_0^z\rangle\cdot\langle\langle S_1^+;S_n^-\rangle\rangle$. This is not a good approximation in one dimension, because it was proved by Mermin and Wagner[1] that the spontaneous magnetization $\langle S^z\rangle$ vanishes in one dimension. So, we write the equation of motion for Green's functions on the right-hand side of Eq. (3). Thus, for example, we have

$$\begin{aligned}\omega\langle\langle S_0^zS_1^+;S_n^-\rangle\rangle&=(2\pi)^{-1}\{2\delta_{n1}\langle S_0^zS_1^z\rangle-\delta_{n0}\langle S_0^-S_1^+\rangle\}\\&\quad+J\langle\langle S_0^zS_2^zS_1^+-S_0^zS_1^zS_2^++\tfrac{1}{2}S_1^+S_0^-S_{-1}^+-\tfrac{1}{2}S_1^+S_0^+S_{-1}^-+\tfrac{1}{4}S_1^+-\tfrac{1}{4}S_0^+;S_n^-\rangle\rangle\,.\end{aligned} \tag{4}$$

Now, we decouple the Green's functions on the right-hand side of this equation. The simplest way to do this would be to set, for example, $\langle\langle S_0^z S_2^z S_1^+; S_n^-\rangle\rangle \to \langle S_0^z S_2^z\rangle\langle\langle S_1^+; S_n^-\rangle\rangle$. It will turn out to be important to introduce a parameter α and set

$$\langle\langle S_0^z S_2^z S_1^+; S_n^-\rangle\rangle \to \alpha\langle S_0^z S_2^z\rangle\langle\langle S_1^+; S_n^-\rangle\rangle\,,$$
$$\langle\langle S_1^+ S_0^- S_{-1}^+; S_n^-\rangle\rangle \to \alpha\langle S_1^+ S_0^-\rangle\langle\langle S_{-1}^+; S_n^-\rangle\rangle + \alpha\langle S_0^- S_{-1}^+\rangle\langle\langle S_1^+; S_n^-\rangle\rangle,\ \text{etc.} \tag{5}$$

The reason for the occurrence of α will be seen as

$$\begin{aligned}\langle\langle S_0^z S_2^z S_1^+; S_n^-\rangle\rangle &\equiv \langle\langle S_0^z S_2^z\{\alpha+2(1-\alpha)S_1^z\}S_1^+; S_n^-\rangle\rangle\\ &\to \langle S_0^z S_2^z\{\alpha+2(1-\alpha)S_1^z\}\rangle\langle\langle S_1^+; S_n^-\rangle\rangle\\ &= \alpha\langle S_0^z S_2^z\rangle\langle\langle S_1^+; S_n^-\rangle\rangle\,.\end{aligned} \tag{6}$$

The first line of Eq. (6) is valid for an arbitrary α. For simplicity, we use the same α, wherever decoupling like Eq. (6) is introduced.

We introduce the correlation function (or short-range order) c_n, which is defined by

$$c_n = 4\langle S_0^z S_n^z\rangle = 2\langle S_0^- S_n^+\rangle = 2\langle S_0^+ S_n^-\rangle\,. \qquad (n=0, 1, 2, \cdots) \tag{7}$$

We also define $\tilde{c}_n$ by

$$\tilde{c}_n = \alpha c_n\,. \tag{8}$$

Then, we find after the decoupling like Eq. (6)

$$\begin{aligned}&\omega\langle\langle S_0^z S_1^+ + S_0^z S_{-1}^+ - S_0^+ S_1^z - S_0^+ S_{-1}^z; S_n^-\rangle\rangle\\ &\quad = (A_n/2\pi) + J\{\tfrac{1}{2}(1+\tilde{c}_1+\tilde{c}_2)\langle\langle S_1^+ + S_{-1}^+; S_n^-\rangle\rangle\\ &\qquad - \tfrac{1}{2}\tilde{c}_1\langle\langle S_2^+ + S_{-2}^+; S_n^-\rangle\rangle - (1+\tilde{c}_2)\langle\langle S_0^+; S_n^-\rangle\rangle\},\end{aligned} \tag{9}$$

where

$$A_n = \begin{cases} c_1\,, & n=1,\ -1\,,\\ -2c_1\,, & n=0\,,\\ 0, & \text{otherwise}\,.\end{cases} \tag{10}$$

Equations (3) and (9) are easily solved by defining the Fourier transform of $\langle\langle S_0^+; S_n^-\rangle\rangle$, i.e.,

$$G_k(\omega) \equiv \sum_n e^{inka}\langle\langle S_0^+; S_n^-\rangle\rangle\,, \tag{11}$$

where a is the lattice spacing. We find

$$G_k(\omega) = (c_1 J/\pi)\,(1-\cos ka)\,/\,(\omega^2-\omega_k^2), \tag{12}$$

where

$$\omega_k \equiv |J|\,\{(1-\cos ka)\,(1-\tilde{c}_1+\tilde{c}_2-2\tilde{c}_1\cos ka)\}^{1/2}. \tag{13}$$

We also find

$$\Gamma_k(\omega)\equiv\sum_n e^{inka}\langle\langle S_0^z S_1^+; S_n^-\rangle\rangle=(c_1/4\pi)(e^{ika}-1)\omega/(\omega^2-\omega_k^2). \tag{14}$$

G_k and Γ_k as obtained in Eqs. (12) and (14) involve three parameters, c_1, c_2 and α. These are determined by requiring that c_1 and c_2 should be self-consistent and that c_0 should be identically equal to unity (from definition (7)). From the relation

$$\langle S_n^- S_0^+\rangle=i\int_{-\infty}^{\infty}\{\langle\langle S_0^+; S_n^-\rangle\rangle_{\omega+i\delta}-\langle\langle S_0^+; S_n^-\rangle\rangle_{\omega-i\delta}\}n(\omega/k_BT)d\omega, \tag{15}$$

we find

$$c_n=(2c_1J/N)\sum_k e^{-inka}\{(1-\cos ka)/\omega_k\}\{2n(\omega_k/k_BT)+1\}, \tag{16}$$

where $n(x)=1/(e^x-1)$. We have set $\hbar=1$. Three equations for $n=0, 1, 2$ are used to determine c_1, c_2 and α. Before describing how to determine these parameters, we note that the averages such as $\langle S_0^z S_1^+ S_n^-\rangle$ $(n\neq 0, 1)$ vanish in our formalism as they naturally should. This is seen by using Eq. (14) in the equation similar to Eq. (15), where $\langle\langle S_0^+; S_n^-\rangle\rangle$ is replaced by $\langle\langle S_0^z S_1^+; S_n^-\rangle\rangle$.

§ 3. High-temperature limit

It is convenient to introduce a dimensionless parameter θ by

$$\theta=k_BT/J. \tag{17}$$

It may be positive or negative, depending on the sign of J. At high temperature ($|\theta|\gg 1$), Eq. (16) may be solved iteratively by expansion in terms of θ^{-1}. We may set $n(\omega/k_BT)\sim k_BT/\omega$. We note that $\tilde{c}_1\sim\theta^{-1}$ and $\tilde{c}_2\sim\theta^{-2}$, so ω_k may be expanded in terms of $\tilde{c}_1$ and $\tilde{c}_2$. Then, Eq. (16) for $n=1$ reads

$$c_1=4c_1\theta N^{-1}\sum_k e^{-ika}(1-\tilde{c}_1+\tilde{c}_2-2\tilde{c}_1\cos ka)^{-1}\simeq 4c_1\theta\tilde{c}_1.$$

Similarly, Eq. (16) for $n=2$ reads

$$c_2=4c_1\theta N^{-1}\sum_k e^{-2ika}(1-\tilde{c}_1+\tilde{c}_2-2\tilde{c}_1\cos ka)^{-1}\simeq 4c_1\theta\tilde{c}_1^2.$$

Equation (16) for $n=0$ reads $1\equiv c_0=4c_1\theta$. From these results, we find

$$c_1=1/4\theta, \qquad c_2=1/(4\theta)^2, \qquad \alpha=1. \tag{18}$$

These values are identical to the direct high-temperature expansion of the correlation functions, which does not involve any approximation. Furthermore, one can show in the leading term in θ^{-1} that

$$c_n=1/(4\theta)^n. \tag{19}$$

This also agrees with the direct expansion of c_n.

§ 4. Low-temperature limit ($J>0$)

In the low-temperature limit, Eq. (16) may be solved by expansion in terms of θ (or $\theta^{1/2}$). The solution for $J>0$ is quite different from that for $J<0$. In this section, we consider the case of $J>0$.

We first note that, even at $T=0$, it is not allowed to neglect $n(\omega_k/k_BT)$ in Eq. (16). As we shall see later, $1-3\tilde{c}_1+\tilde{c}_2$ tends to zero as T goes to zero. Then, $\omega_k \propto k^2$ for small k. The first term of Eq. (16) (the part involving $n(\omega_k/k_BT)$) then becomes, for small k,

$$(2c_1J/N)\sum_k e^{-inka}(1-\cos ka)\,(k_BT/\omega_k^2) \propto T\sum_k k^{-2},$$

which is divergent for finite T. We shall see that $1-3\tilde{c}_1+\tilde{c}_2$ tends to zero in such a way that the above sum remains finite as T goes to zero.

We define δ and ω_k by

$$\delta=(1-3\tilde{c}_1+\tilde{c}_2)/4\tilde{c}_1\,, \tag{20}$$

$$\omega_x=2(2\tilde{c}_1)^{1/2}J\sin x(\sin^2 x+\delta)^{1/2}. \qquad (x=ka/2) \tag{21}$$

Equation (16) is expressed by

$$\tilde{c}_n=(2/\pi)\,(2\tilde{c}_1)^{1/2}\left\{2\int_0^{\pi/2}\sin x\cos 2nx(\sin^2 x+\delta)^{-1/2}n(\omega_x/k_BT)\,dx+K_n\right\}, \tag{22}$$

where

$$K_n\equiv\int_0^{\pi/2}\sin x\cos 2nx(\sin^2 x+\delta)^{-1/2}dx$$

$$=\begin{cases}\sin^{-1}(1+\delta)^{-1/2}, & n=0\,,\\ -\delta^{1/2}+\delta\sin^{-1}(1+\delta)^{-1/2}, & n=1\,,\\ -\delta^{1/2}(1+3\delta)+\delta(2+3\delta)\sin^{-1}(1+\delta)^{-1/2}, & n=2\,.\end{cases} \tag{23}$$

As δ tends to zero, $K_n(n\geqq 1)$ vanishes. The leading term of $\tilde{c}_n(n\geqq 1)$ is, then, obtained from the first term of Eq. (22) by setting $n(\omega_x/k_BT)$ to k_BT/ω_x:

$$\tilde{c}_n=(2/\pi)\theta\int_0^{\pi/2}\cos 2nx/(\sin^2 x+\delta)\,dx$$

$$=\theta\{\delta(1+\delta)\}^{-1/2}[1+2\delta-2\{\delta(1+\delta)\}^{1/2}]^n. \tag{24}$$

This is correct up to the leading term in θ, which is independent of n. So, we have $\tilde{c}_1=\tilde{c}_2$ at $T=0$. From this result and $\delta=0$, we have $\tilde{c}_1=\tilde{c}_2=1/2$ at $T=0$. Then, from Eq. (24), we find

$$\delta=4\theta^2. \qquad (\theta\ll 1) \tag{25}$$

We need another relation between $\tilde{c}_1$ and $\tilde{c}_2$, which is obtained by making their difference. From Eq. (22), we have, in the leading term,

$$\tilde{c}_1-\tilde{c}_2\cong(4/\pi)\,(2\tilde{c}_1)^{1/2}\int_0^{\pi/2}\sin x(\cos 2x-\cos 4x)\,(\sin^2 x+\delta)^{-1/2}n(\omega_x/k_BT)\,dx$$

$$\cong (24/\pi)\,(2\tilde{c}_1)^{1/2}\int_0^{\pi/2} x^3 (x^2+\delta)^{-1/2} n(\omega_x/k_B T)\,dx$$
$$\cong (24/\pi)\,(2\tilde{c}_1)^{1/2}\theta^{3/2}(2\tilde{c}_1)^{-3/4}(\pi/8) I$$
$$\cong 3I\theta^{3/2} \tag{26}$$

with $I=(2\pi)^{-1/2}\zeta(3/2)=1.042$, where ζ is Riemann's zeta function. Equations (25) and (26) may be solved for $\tilde{c}_1$ and $\tilde{c}_2$, and we find

$$\tilde{c}_1=\tfrac{1}{2}-\tfrac{3}{2}I\theta^{3/2}+O(\theta^2), \tag{27}$$
$$\tilde{c}_2=\tfrac{1}{2}-\tfrac{9}{2}I\theta^{3/2}+O(\theta^2). \tag{28}$$

Our next task is to determine α. From Eq. (22) for $n=0$ and $n=1$, we have

$$\alpha-\tilde{c}_1 \cong (2/\pi)\,(2\tilde{c}_1)^{1/2}\left\{\frac{\pi}{2}I\theta^{3/2}+K_0-K_1\right\}.$$

From Eq. (23), we have

$$K_0-K_1=\pi/2+O(\theta^2).$$

Then, we find, within the terms of $\theta^{3/2}$,

$$\alpha=\tilde{c}_1+(2\tilde{c}_1)^{1/2}\{1+I\theta^{3/2}\}$$
$$=\tfrac{3}{2}-2I\theta^{3/2}. \tag{29}$$

We arrive at our final results:

$$c_1=\tilde{c}_1/\alpha=\tfrac{1}{3}-\tfrac{5}{9}I\theta^{3/2}, \tag{30}$$
$$c_2=\tilde{c}_2/\alpha=\tfrac{1}{3}-\tfrac{23}{9}I\theta^{3/2}. \tag{31}$$

This procedure has been put forward two-step further, resulting in

$$c_1=\frac{1}{3}-\frac{5}{9}I\theta^{3/2}+\frac{28}{9}\theta^2+\left\{\frac{\zeta(5/2)}{2^{7/2}\pi^{1/2}}+\frac{34\sqrt{2}}{3\pi}I'\right\}\theta^{5/2}, \tag{32}$$
$$c_2=\frac{1}{3}-\frac{23}{9}I\theta^{3/2}+\frac{148}{9}\theta^2+\left\{\frac{11\zeta(5/2)}{2^{7/2}\pi^{1/2}}+\frac{182\sqrt{2}}{3\pi}I'\right\}\theta^{5/2}, \tag{33}$$

where

$$I'=\int_0^\infty dx\,x^{-1/2}\{1/(e^x-1)-1/x\}$$
$$=-2.593\,.$$

§ 5. Low-temperature limit ($J<0$)

In this case, $\tilde{c}_1$ is negative. It is covenient to define δ and ω_x as follows:

$$\delta=\frac{1-3\tilde{c}_1+\tilde{c}_2}{4|\tilde{c}_1|}, \tag{34}$$

$$\omega_x = 2|J|(2|\tilde{c}_1|)^{1/2} \sin x (\cos^2 x + \delta - 1)^{1/2}. \tag{35}$$

Equation (16) reads

$$\tilde{c}_n = (2/\pi)(2|\tilde{c}_1|)^{1/2} \left\{ 2 \int_0^{\pi/2} \sin x \cos 2nx (\cos^2 x + \delta - 1)^{-1/2} n(\omega_x / k_B T) dx + L_n \right\}, \tag{36}$$

where

$$L_n = \int_0^{\pi/2} \sin x \cos 2nx (\cos^2 x + \delta - 1)^{-1/2} dx \tag{37}$$

$$= \begin{cases} \log\{(1+\delta^{1/2})/(\delta-1)^{1/2}\}, & n=0, \\ \delta^{1/2} - \delta \log\{(1+\delta^{1/2})/(\delta-1)^{1/2}\}, & n=1, \\ -(3\delta-2)L_1 - \delta^{1/2}, & n=2. \end{cases} \tag{38}$$

Contrary to the ferromagnetic case, δ remains greater than unity at all the temperatures, and so the integral in Eq. (36) vanishes as T goes to zero. The leading term of the integral at low temperatures is in T^2 and is expressed by $(\pi^2/48)\theta^2/|\tilde{c}_1|\delta^{3/2}$. This result and Eq. (38) may be put into Eq. (36) for $n=1$ and 2, and they may be solved for $\tilde{c}_1$ and $\tilde{c}_2$. We find

$$|\tilde{c}_1| = 0.97206 + 2.14\theta^2, \qquad \tilde{c}_2 = 0.28246 + 1.59\theta^2. \tag{39}$$

These results are put into Eq. (36) for $n=0$, and we find

$$\alpha = 1.75441 + 3.9\theta^2.$$

So, we obtain finally

$$|c_1| = 0.55407 - 0.02799\theta^2, \qquad c_2 = 0.16100 + 0.91\theta^2. \tag{40}$$

§ 6. Numerical solution at arbitrary temperatures

At arbitrary temperatures, we have solved Eq. (22) and Eq. (36) numerically. The results for c_1 and c_2 in the ferromagnetic case are shown in Fig. 1. The points represent the direct high-temperature expansion which does not involve any approximation such as our decoupling. B-F means the result obtained by Bonner and Fisher numerically for a chain of 11 spins. The results for $J<0$ are shown in Fig. 2. The points again represent the direct high-temperature expansion. B-F means the estimated limit for infinite number of spins as obtained by Bonner and Fisher.

§ 7. Discussion of the results ($J>0$)

From Eq. (22), one sees that, at a finite temperature, c_n tends to zero as $n \to \infty$. On the other hand, one sees from Eq. (24) that, for a fixed n, c_n tends to 1/3, irrespective of n, as T tends to zero. This is the value which is ex-

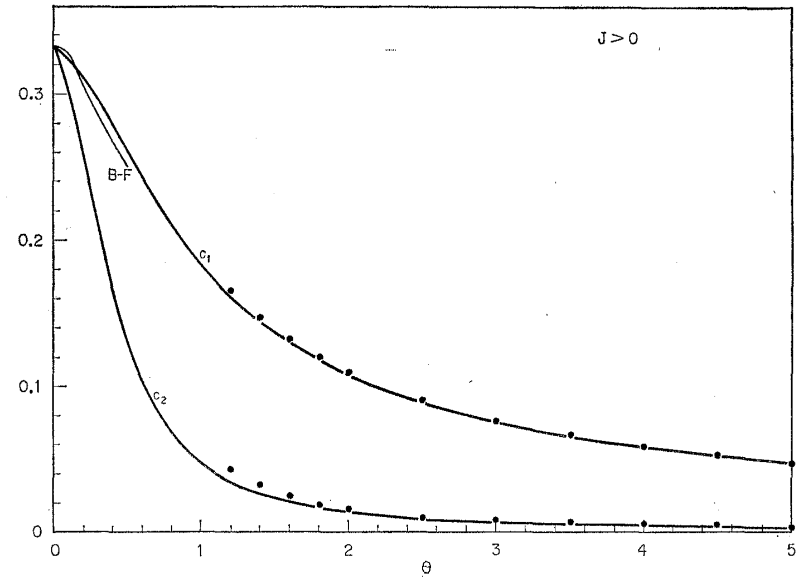

Fig. 1. Correlation functions vs $\theta=k_BT/J$ for the one-dimensional ferromagnetic Heisenberg system. The lines are the results of numerical solution of Eq. (22). The points represent direct high-temperature expansion. B-F represents Bonner and Fisher's numerical calculation on a chain of 11 spins.

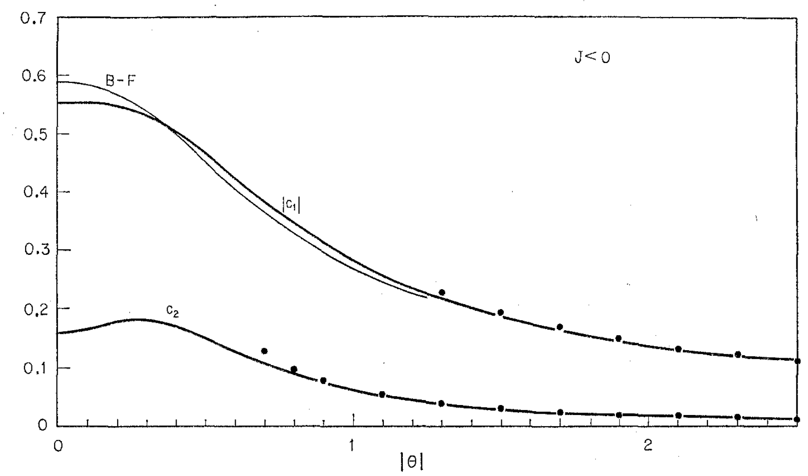

Fig. 2. Correlation functions vs $|\theta|=k_BT/|J|$ for the one-dimensional antiferromagnetic Heisenberg system. The lines are the results of numerical solution of Eq. (36). The points represent direct high-temperature expansion. B-F represents the estimated limit for infinite number of spins as obtained by Bonner and Fisher.

pected for the correct ground state of the ferromagnetic Heisenberg system, which does not possess spontaneous magnetization. Furthermore, we note that, at $T=0$, the spin-wave spectrum becomes $\omega_k=J(1-\cos ka)$, because $\tilde{c}_1=\tilde{c}_2=1/2$ at $T=0$. This is also the correct spin wave spectrum of the ground state. At finite temperatures, Eq. (13) implies $\omega_k \propto k$ for small k.

Let us now discuss thermodynamic properties. The internal energy is the average of the Hamiltonian (1), and is expressed by $E=-(3/4)c_1JN$. In Fig. 3, $(E-E(0))/JN$ is plotted vs θ. Curve (a) represents the result of numerical computation. Curve (b) is obtained from the low-temperature expansion (30). It is to be noted that the numerical result (a) approaches the low-temperature asymptote (b) only very slowly. However, if one uses Eq. (32), one finds a good agreement with Curve (a) up to $\theta\simeq0.01$. The specific heat is obtained by differentiating E with respect to T. Curve (a) of Fig. 4 represents the numerical result. Lines (b) and (c) represent high- and low-temperature asymptote, respectively. The low-temperature asymptote is obtained from Eq. (30) as

$$C=Nk_B(5/8)I\theta^{1/2}. \tag{41}$$

This is 5/6 times what the simple spin-wave theory predicts, and is close to what Bonner and Fisher suggested from their numerical calculation on finite number of spins. The points (d) represent Bonner and Fisher's result for a chain of 11 spins. The calculated value of entropy per spin at T=infinite

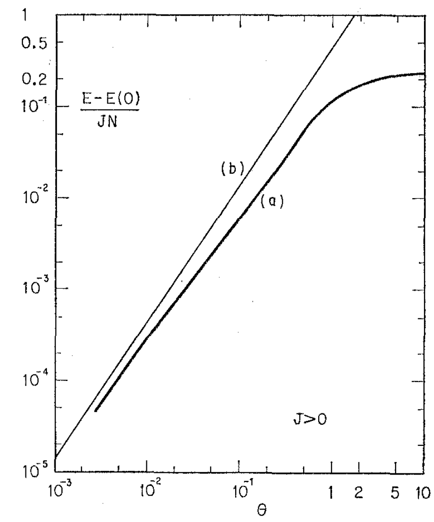

Fig. 3. The internal energy vs $\theta=k_BT/J$ for the one-dimensional ferromagnetic Heisenberg system. Curve (a) is obtained from numerical solution of Eq. (22). Curve (b) represents the low-temperature asymptote obtained from Eq. (30).

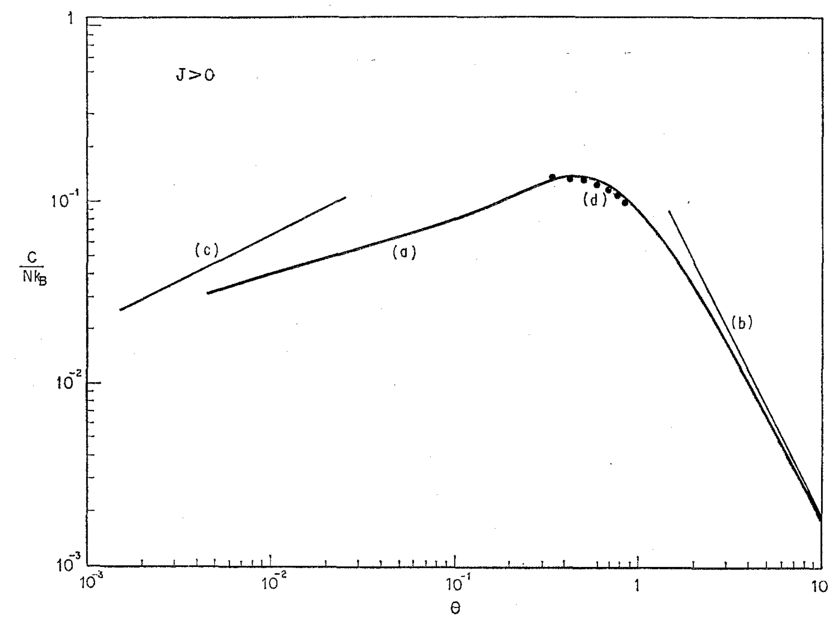

Fig. 4. The specific heat of the one-dimensional ferromagnetic Heisenberg system vs $\theta=k_BT/J$. Curve (a) is obtained from numerical solution of Eq. (22). Curves (b) and (c) represent the high- and low-temperature asymptote, respectively. The points (d) represent Bonner and Fisher's result for a chain of 11 spins.

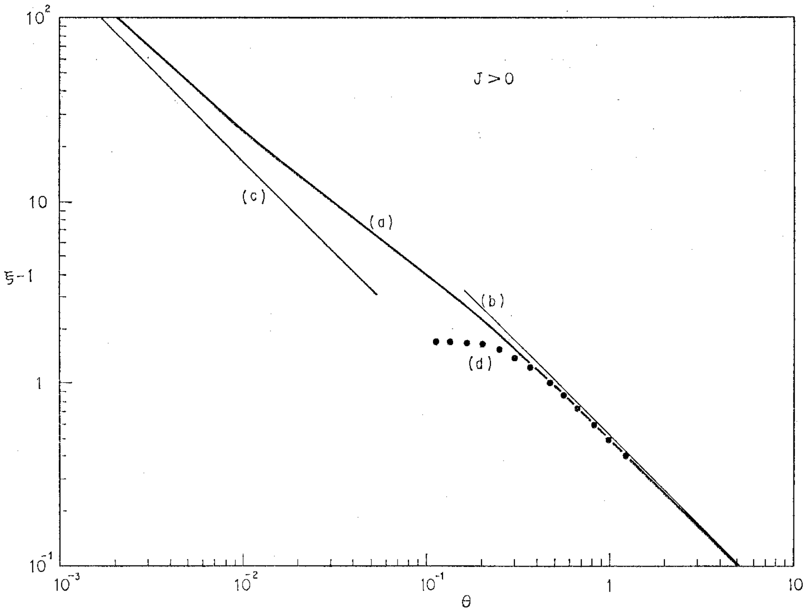

Fig. 5. $\xi-1$ vs $\theta=k_BT/J$ for the one-dimensional ferromagnetic Heisenberg system. ξ is proportional to the Curie constant and approaches unity at high temperatures. Curve (a) represents the numerical calculation based on Eq. (22). Curves (b) and (c) represent high- and low-temperature asymptote, respectively. Both of them have the slope of -1. The points (d) represent Bonner and Fisher's numerical calculation for a chain of 11 spins.

is 0.56, which is rather close to the exact value log 2.

Let us next consider the magnetic susceptibility, which is expressed by

$$\chi=(Ng^2\mu_B{}^2/4k_BT)\sum_n c_n$$
$$\equiv(Ng^2\mu_B{}^2/4k_BT)\xi\,. \tag{42}$$

From Eq. (16), we have

$$\xi=2c_1J\lim_{k\to 0}\{(1-\cos ka)/\omega_k\}\{2n(\omega_k/k_BT)+1\}$$
$$=4c_1\theta/(1-3\tilde{c}_1+\tilde{c}_2)\,. \tag{43}$$

At high temperatures, one finds from Eq. (16) $c_1=(1/4\theta)(1-1/4\theta)$ and hence $\xi=1+1/2\theta$. At low temperatures, one finds $\xi=(4/3)\theta/4\tilde{c}_1\delta=1/6\theta$. Thus $\xi-1$ is proportional to θ^{-1} in both limits with different numerical factors. In Fig. 5, $\xi-1$ is plotted vs θ together with two asymptotes. Between the two asymptotes, the slope is approximately $-4/5$. This is what was suggested by Bonner and Fisher. They also suggested that the true low-temperature asymptote may set in below $\theta=0.1$. Our result indicates that it may actually set in at θ as small as 10^{-3}.

§ 8. Discussion of the results ($J<0$)

In the antiferromagnetic linear chain, the exact value of c_1 at $T=0$ is -0.59086.[5)] Bonner and Fisher found $c_2=0.25407$ for a chain of 10 spins.

This is expected to be close to correct limit of infinite number of spins. Our results, Eq. (40), compare with these values fairly well. The spin-wave spectrum, Eq. (13), is linear in k, for small k, and at $T=0$, we have $\omega_k=1.44|J|ka$. This is also close to the exact value at $T=0$ obtained by des Cloizeaux and Pearson,[6] i.e., $\omega_k=(\pi/2)|J| \times|\sin ka|$. At larger k values, however, Eq. (13) deviates from the exact value. Especially, Eq. (13) does not possess double periodicity of $|\sin ka|$.

The internal energy is plotted vs $|\theta|$ in Fig. 6, where the low-temperature asymptote as obtained from Eq. (40) is also shown. Contrary to the ferromagnetic case, the numerical result approaches the asymptote very rapidly. The specific heat is shown in Fig. 7 together with Bonner and Fisher's estimate based on their numerical calculation on finite number of spins. They agree fairly well except at the lowest temperatures, where

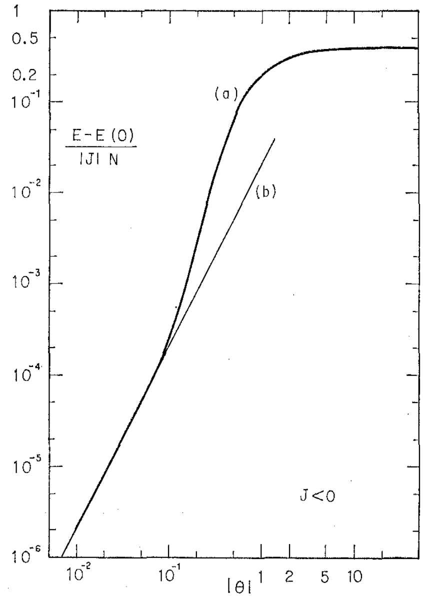

Fig. 6. The internal energy of the one-dimensional antiferromagnetic Heisenberg system vs $|\theta|=k_BT/|J|$. Curve (a) is obtained from numerical solution of Eq. (36). Curve (b) represents the low-temperature asymptote obtained from Eq. (40).

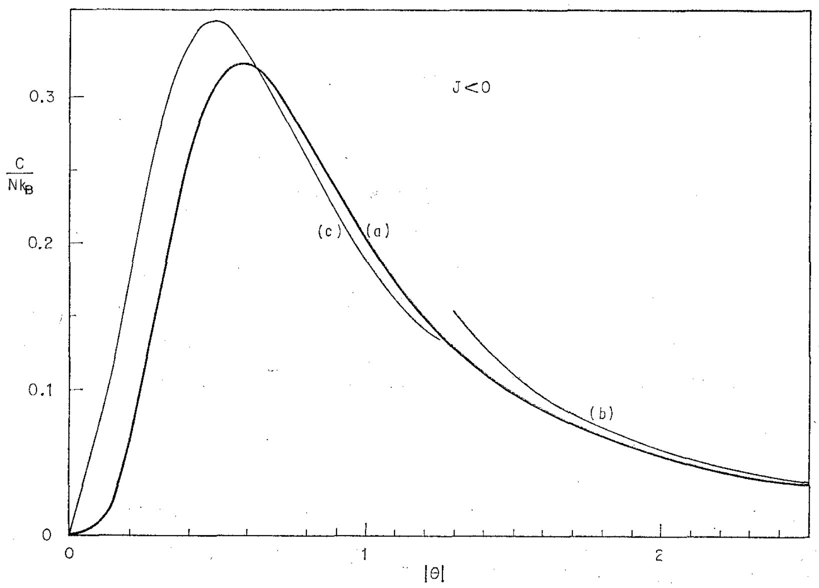

Fig. 7. The specific heat of the one-dimensional antiferromagnetic Heisenberg system vs $|\theta|=k_BT/|J|$. Curve (a) is obtained from numerical solution of Eq. (36). Curve (b) represents the high-temperature expansion $C=(3/16)Nk_B(\theta^{-2}-\theta^{-3}/2)$.Curve (c) is Bonner and Fisher's estimate based on their numerical calculation on finite number of spins.

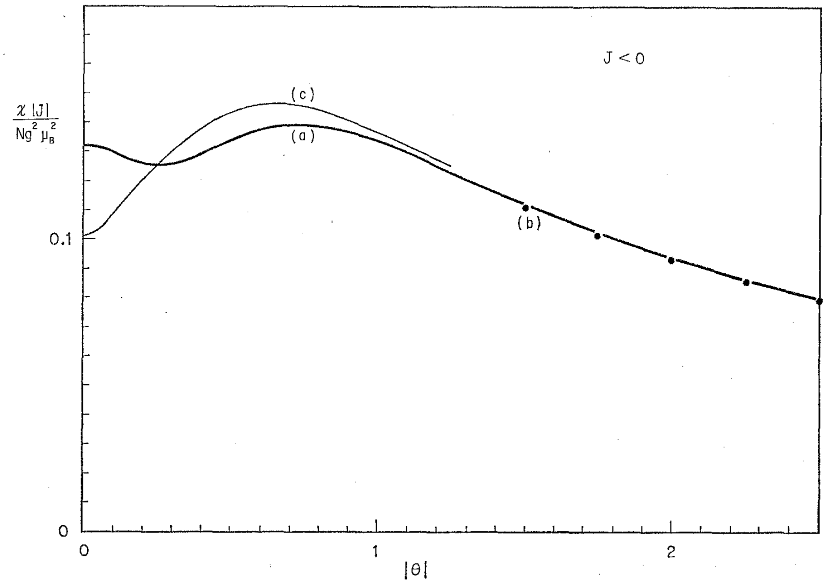

Fig. 8. The magnetic susceptibility of the one-dimensional antiferromagnetic Heisenberg system vs $|\theta|=k_BT/|J|$. Curve (a) is the result obtained from numerical solution of Eq. (36). The points (b) represent the high-temperature expansion $\chi=(Ng^2\mu_B{}^2/4k_BT)\times(1+1/2\theta)$. Curve (c) represents Bonner and Fisher's estimate based on their calculation on finite number of spins.

our theory predicts the linear dependence on T with a coefficient much smaller than Bonner and Fisher's. This may be related to the approximate nature of our spin-wave spectrum at low temperatures. The calculated value of entropy per spin at T=infinite is 0.50.

Our result of the susceptibility is shown in Fig. 8 together with Bonner and Fisher. They agree fairly well except at the lowest temperatures, where our curve shows an upward turnover.

§ 9. Conclusion

We have proposed a theory of spin waves which involves solely the short-range order and does not require the existence of the long-range order. We have seen that the theory gives reasonable gross features of the thermodynamic properties at all the temperatures for both signs of the exchange.

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