Calculation of the Generalized Watson Sums with an Application to the Generalized Heisenberg Ferromagnet. II. Callen Decoupling*

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A new method of calculating the generalized Watson sums is applied to calculate the magnetization of an anisotropic ferromagnet for various Callen-type decoupling schemes. It is shown that although the calculations are somewhat more difficult than for the random-phase approximation, an analytical solution is again obtained.

I. INTRODUCTION

In a previous paper,[1] which we shall refer to as I, a new method of calculating the generalized Watson sums

$$\Phi(\alpha,\eta)=\frac{1}{N}\sum_{k}\left\{\exp\left[\alpha\left(1-\eta\,\frac{J(\vec{k})}{J(0)}\right)\right]-1\right\}^{-1},$$

with $0\le\alpha\le\infty$ and $0\le\eta\le1$, was presented, where the symbols are the same as in Ref. 1. For previous work on these sums the reader is referred to Refs. 1 and 2. Extensive numerical tables have been prepared by Mannari and Kawabata.[3] In I this method was applied to the anisotropic Heisenberg ferromagnet[4] in the random-phase approximation. The purpose of the present paper is to indicate how the methods of I can be extended to treat a more complicated problem, the anisotropic Heisenberg ferromagnet using a Callen decoupling approximation.[5-7]

II. CALLEN DECOUPLING

As defined in I, the nearest-neighbor exchange-interaction model for the anisotropic ferromagnet in the absence of an external field is specified by the Hamiltonian

$$H=-\sum_{i,j}J_{ij}\left[S_i^zS_j^z+\tfrac{1}{2}\eta(S_i^+S_j^-+S_i^-S_j^+)\right], \tag{1}$$

where the sums extend over all lattice sites, $\vec{S}_i$ is the spin operator for a spin on site i, and $J_{ij}=J(\vec{r}_j-\vec{r}_i)$ is the exchange integral. The Ising and Heisenberg models are obtained by setting $\eta=0$ and 1, respectively.

The equation of motion for the Fourier transform of the Green's function $\langle\langle S_g^+;S_m^-\rangle\rangle$ has been derived by Dalton and Wood,[4]

$$E\langle\langle S_g^+;S_m^-\rangle\rangle=\langle S_g^z\rangle\,\frac{\delta_{gm}}{\pi}+2\sum_f J_{gf}\times\left(\langle\langle S_f^zS_g^+;S_m^-\rangle\rangle-\eta\langle\langle S_g^zS_f^+;S_m^-\rangle\rangle\right). \tag{2}$$

It is seen that the equation of motion for $\langle\langle S_g^+;S_m^-\rangle\rangle$ also involves higher-order Green's functions.

Callen has suggested a decoupling scheme for Eq. (2), which enables one to solve for the Green's function $\langle\langle S_g^+;S_m^-\rangle\rangle$ and the corresponding correlation functions.[5] This decoupling approximation is an improvement over the random-phase approximation since it does account for spin correlations. For spin $\frac{1}{2}$, Callen's decoupling is

$$\langle\langle S_g^zS_f^+;S_m^-\rangle\rangle\underset{g\neq f}{\longrightarrow}\langle S^z\rangle\langle\langle S_f^+;S_m^-\rangle\rangle-\alpha\langle S_g^-S_f^+\rangle\langle\langle S_g^+;S_m^-\rangle\rangle, \tag{3}$$

where the decoupling parameter is chosen to have the form

$$\alpha=2\langle S^z\rangle. \tag{4}$$

Using the decoupling (3) and (4), Eq. (2) can be solved for the Green's function $\langle\langle S_g^+;S_m^-\rangle\rangle$. Assuming the lattice to be translationally invariant, one defines the Fourier transforms

$$G(\vec{k})=\sum_{g-m}e^{-i(\vec{g}-\vec{m})\cdot\vec{k}}\langle\langle S_g^+;S_m^-\rangle\rangle, \tag{5}$$

$$J(\vec{k})=\sum_{g-f}e^{-i(\vec{g}-\vec{f})\cdot\vec{k}}J(\vec{g}-\vec{f}), \tag{6}$$

$$\psi(\vec{k})=\sum_{g-f}e^{-i(\vec{g}-\vec{f})\cdot\vec{k}}\langle S_f^-S_g^+\rangle. \tag{7}$$

The resulting equation for $G(\vec{k})$ is

$$G(\vec{k})=\langle S^z\rangle/\pi[E-E(\vec{k})], \tag{8}$$

where

$$E(\vec{k})=2\langle S^z\rangle[J(0)-\eta J(\vec{k})]+\frac{2\gamma}{N}\sum_{k'}[\eta J(\vec{k}')-J(\vec{k}'-\vec{k})\psi(\vec{k}')]. \tag{9}$$

The sum in Eq. (9) is taken over all wave-lattice vectors in the first Brillouin zone. By the usual methods,[5] one finds that the correlation function (7) is given by

$$\psi(\vec{k})=2\langle S^z\rangle\varphi(\vec{k}), \tag{10}$$

where

$$\varphi(\vec{k})=(e^{\beta E(\vec{k})}-1)^{-1}. \tag{11}$$

For simple lattices with nearest-neighbor interac-

tions the exchange integral is

$$J(\vec{k}) = J\sum_{\delta} e^{i\vec{k}\cdot\vec{\delta}} , \tag{12}$$

where δ is the nearest-neighbor vector and J is a nearest-neighbor exchange integral. Equation (9) then has the form

$$E(\vec{k}) = 2\langle S^z\rangle J(0)\left(1 + 2\alpha\eta f - \frac{J(\kappa)}{J(0)}(\eta + 2\alpha f)\right) , \tag{13}$$

where

$$f = [NJ(0)]^{-1}\sum_k J(\vec{k})\varphi(\vec{k}) . \tag{14}$$

To obtain the magnetization, one calculates $\langle S^z\rangle$ from the relation

$$\langle S^z\rangle = \tfrac{1}{2}(1 + 2\Phi)^{-1} , \tag{15}$$

where

$$\Phi = \frac{1}{N}\sum_k \varphi(\vec{k}) , \tag{16}$$

with $\varphi(k)$, $E(k)$, and f defined by Eqs. (11), (13), and (14), respectively. Equations (13)–(15) are the set of equations which are to be solved self-consistently for $\langle S^z\rangle$.

III. FORMAL SOLUTION

As in I, we consider only cubic crystals. It was shown in I that for the cubic lattices, the Brillouin-zone sums can be written in the form

$$\frac{1}{N}\sum_k \to \frac{1}{\pi^3}\int_0^{\pi}\int_0^{\pi}\int_0^{\pi} dx\,dy\,dz , \tag{17}$$

where

$$\text{sc}: \quad x = k_x a, \quad y = k_y a, \quad z = k_z a , \tag{18}$$

$$\text{bcc, fcc}: \quad x = \tfrac{1}{2}k_x a, \quad y = \tfrac{1}{2}k_y a, \quad z = \tfrac{1}{2}k_z a . \tag{19}$$

Using the techniques outlined in I, one obtains, in a similar fashion as Eq. (7) of I,

$$\Phi = I_1 + I_2 - \tfrac{1}{2} , \tag{20}$$

with the additional equation

$$f = J_1 + J_2 , \tag{21}$$

where

$$I_1 = (2\pi^3 Q\xi)^{-1}\int_0^{\pi}\int_0^{\pi}\int_0^{\pi} dx\,dy\,dz\left(1 - g\frac{J(x_1y_1z)}{J(0)}\right)^{-1} , \tag{22}$$

$$I_2 = (2\pi^3 Q\xi)^{-1}\sum_{R=1}^{\infty}\int_0^{\pi}\int_0^{\pi}\int_0^{\pi} dx\,dy\,dz \times\left[\left(1 - g\frac{J(x_1y_1z)}{J(0)} + i\Gamma(R)\right)^{-1} + \text{c.c.}\right] , \tag{23}$$

$$J_1 = (2\pi^3 Q\xi)^{-1}\int_0^{\pi}\int_0^{\pi}\int_0^{\pi} dx\,dy\,dz\,\frac{J(x_1y_1z)}{J(0)} \times\left(1 - g\frac{J(x_1y_1z)}{J(0)}\right)^{-1} , \tag{24}$$

$$J_2 = (2\pi^3 Q\xi)^{-1}\sum_{R=1}^{\infty}\int_0^{\pi}\int_0^{\pi}\int_0^{\pi} dx\,dy\,dz\,\frac{J(x_1y_1z)}{J(0)} \times\left[\left(1 - g\frac{J(x_1y_1z)}{J(0)} + i\Gamma(R)\right) + \text{c.c.}\right] , \tag{25}$$

where

$$\xi = 1 + 2\alpha\eta f , \tag{26}$$

$$g = (\eta + 2\alpha f)/\xi , \tag{27}$$

$$Q = \langle S^z\rangle J(0)/\kappa T , \tag{28}$$

$$\Gamma(R) = \pi R/Q . \tag{29}$$

Let us consider the special case of the bcc lattice. Then, using the techniques described in I, one obtains

$$I_1 = (2Q\xi)^{-1}(2K(\kappa)/\pi)^2 , \tag{30}$$

$$I_2 = (2Q\xi)^{-1}[Q\xi\coth Q\xi - 1 + \tfrac{1}{8}g^2Q\xi^3(\operatorname{csch}^2 Q\xi)\coth Q\xi - \tfrac{1}{8}g^2] , \tag{31}$$

$$J_1 = (2Q\xi g)^{-1}\{[2K(\kappa)/\pi]^2 - 1\} , \tag{32}$$

$$J_2 = g(16Q\xi)^{-1}(Q^2\operatorname{csch}^2 Q\xi - 1) . \tag{33}$$

Here $K(\kappa)$ is a complete elliptic integral of the first kind and

$$\kappa^2 = \tfrac{1}{2}[1 - (1 - g^2)^{1/2}] . \tag{34}$$

The magnetization is then found by solving Eqs. (15) and (16) together with Eqs. (20), (21), and (30)–(34).

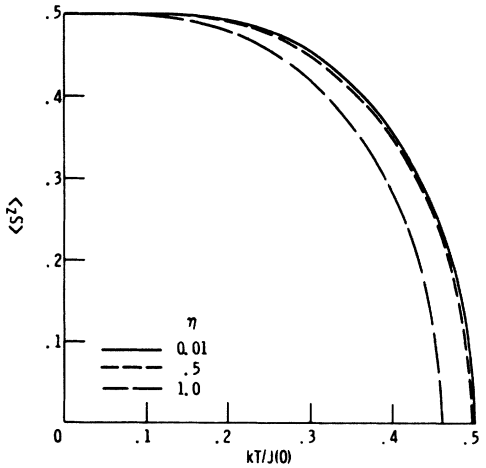

FIG. 1. Magnetization as a function of the reduced temperature for the bcc lattice with spin $\frac{1}{2}$ and Callen decoupling parameter $\alpha = 2\langle S^z\rangle$.

TABLE I. Curie temperatures $T_c/J(0)$ for the spin $\frac{1}{2}$ anisotropic ferromagnet on a bcc lattice using the Callen decoupling with $\alpha = 2\langle S^z\rangle$.

	$\kappa T_c/J(0)$			
η	RPA[a]	Callen[b]	Present calculation	Padé approx.[c]
0.01	0.5000	...	0.5000	0.3970[d]
0.50	0.4830	...	0.4970	0.3821
1.00	0.3589	0.4625[e]	0.4601	0.3194[f]

[a]See Ref. 1.
[b]See Ref. 5.
[c]See Ref. 4.
[d]For $\eta = 0$.
[e]Disagreement with the present calculation is probably a result of the numerical methods used in Ref. 5.
[f]Baker *et al.* (Ref. 10) give 0.3154.

IV. RESULTS

The results for $\langle S^z\rangle$ vs temperature for spin $\frac{1}{2}$ and several values of the anisotropy parameter η are shown in Fig. 1 for the bcc lattice. Here the Callen decoupling parameter is $\alpha = 2\langle S^z\rangle$. For $\eta = 0$ the Callen decoupling approximation must give no solutions for $\alpha \neq 0$. For $\eta = 0$ the only solution is $\alpha = 0$, which corresponds to the random-phase approximation of I. It is seen that the Callen approximation for the anisotropic ferromagnet leads to second-order transitions with higher transition temperatures than those obtained in I. As in I, the effect of the anisotropy parameter η is to shift the transition downward for increasing η. Similar results are obtained for the other cubic lattices and for higher spin. Using the results of Sec. III, the low-temperature behavior of the anisotropic model can be examined following Callen's treatment,[5] with similar results for $\eta = 1$.

The values of the Curie temperatures $\kappa T_c/J(0)$ are shown in Table I for spin $\frac{1}{2}$. A comparison with the random-phase approximation[1] and Padé-approximant[4, 8–10] results is given. As in Callen's work for $\eta = 1$, we have found that the Callen decoupling scheme is much more reliable for large spin. It is particularly bad for spin $\frac{1}{2}$. In the large-spin limit, the results of Callen's approximation are found to agree within a few percent with those of the Padé results.[8, 9] The advantage of Callen's method is that it provides a theory for general spin which is approximately valid through the entire temperature range with low-temperature results in agreement with the Dyson result for $\eta = 1$. The Callen decoupling scheme is reliable for spins greater than $\frac{1}{2}$, which is the case for most problems of practical interest.

We have also examined the anisotropic ferromagnet with $0 \leq \eta \leq 1$ using a form for the decoupling parameter proposed by Copeland and Gersch,[6]

$$\alpha = \langle 2S^z\rangle^p , \tag{35}$$

where p is a positive integer.[7] For $p = 1$ this form reduces to Eq. (4). It is found that for $p \geq 3$ a second-order transition is obtained with the same Curie point for all p. For the bcc lattice the values of $\kappa T_c/J(0)$ for $\eta = 0.01$, 0.5, 1.0 and 0.500, 0.4831, 0.3589, respectively. For $1 < p < 3$ a first-order transition is obtained for $\eta = 1$, while second-order transitions can be found for smaller values of η.

We have thus seen that although the Callen decoupling leads to a more complex system of consistent equations than the random-phase approximation, again an analytical solution can be obtained. This solution again does not require series expansions or extensive computer calculations. We have therefore illustrated the utility of the methods developed in I in a variety of problems in magnetism. We hope that these methods will be found useful in the solution of other similar problems.

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