

not appear to be at all sensitive to the first-order transition.

Further elucidation of the magnetic structure below 86 °K will have to await a neutron diffraction study in an applied field, preferably with a polarized beam, which is currently being planned.

Note added in proof. A paper by J. B. Goodenough *et al.* [Phys. Rev. B **2**, 4640 (1970)] has recently come to our attention. This deals with the effects of hydrostatic pressure and Jahn-Teller distor-

tions on the magnetic properties of RbFeF_3 , and presents a plausible explanation for many of the puzzling experimental observations previously reported.

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Green's-Function Analysis of the Ising Ferromagnet

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The method of the two-time temperature-dependent Green's function has been used to analyze the Ising model of a ferromagnet in an external magnetic field. The selection of a particular Green's function enables us to write an exact expression for the equation of motion. We are then led to a differential difference equation for the correlation function corresponding to the Green's function. No decoupling assumptions have been made, so the equation is exact for both arbitrary spin and range of interaction. It is shown how various approximate theories may be extracted from our formalism. The exact differential difference equation may be reduced to a partial differential equation. The latter form allows us to generate relations among the magnetization and spin-spin correlation functions. These relations are given in detail for the case of spin $\frac{1}{2}$ and z nearest neighbors.

I. INTRODUCTION

The method of the two-time temperature-dependent Green's function¹ has been used extensively to study magnetic systems based on the Heisen-

berg²⁻⁶ and Ising⁷⁻¹¹ models. To obtain tractable solutions, decoupling procedures have been invoked to terminate the hierarchy of Green's functions generated by the equations of motion. In this paper we consider the Ising model of a ferromagnet with

arbitrary spin and range of interaction. Selection of a particular Green's function enables us to generate those of higher order and thus write the equations of motion in closed form. The correlation function corresponding to the Green's function is then found to satisfy a certain differential difference equation. No approximations have been made, so the result is perfectly general.

Section II presents the formalism of our method and derives the differential difference equation. This is the basis equation used throughout the rest of the paper. In Sec. III we show how the Weiss molecular field,¹² and Bethe-Peierls-Weiss¹³⁻¹⁵ approximations may be obtained from our results; Sec. IV shows how the differential difference equation may be reduced to a partial differential equation. Although it has not been possible to solve the equation, it does permit one to obtain exact relations among the correlation functions in a systematic manner. We consider the case of $S = \frac{1}{2}$ and specifically calculate these relations for one-, two-, and three-dimensional systems. Some of these relations have appeared in the works of Doman and ter Haar,⁷ Callen,⁹ Tahir-Kheli,^{8,10} Oguchi and Ono,¹¹ and Fisher.¹⁶

II. FORMALISM

The Ising model Hamiltonian¹⁷ is given by

$$\mathcal{H} = -\mu H \sum_i S_i^z - \sum_{i,j} J_{ij} S_i^z S_j^z, \quad (2.1)$$

where μS is the magnetic moment per ion, H is the external magnetic field directed along the negative z axis, S_i^z is the z component of the spin operator for the ion at the lattice site i , and J_{ij} is the exchange integral between the ions at the sites i and j . It will be assumed that the exchange integral is a function only of the distance between ions and it is a positive quantity such that the ground state of the system will be ferromagnetically aligned. The method of two-time temperature-dependent Green's functions has been reviewed extensively¹; hence, only the definitions and results of the analysis will be presented here. The Green's function involving the two operators A and B is defined by

$$\langle\langle A(t); B \rangle\rangle \equiv \begin{cases} -i \theta(t) \langle [A(t), B] \rangle & (t > 0) \\ i \theta(-t) \langle [A(t), B] \rangle & (t < 0) \end{cases} \quad (2.2)$$

The function $\theta(t)$ is the unit step (zero for negative argument and unity for positive argument), the single angular brackets denote an average with respect to the density operator $e^{-\beta \mathcal{H}}$ ($\beta = 1/kT$), the square brackets denote the commutator, and $A(t)$ is the operator A in the Heisenberg representation at time t . The time Fourier transform of Eq. (2.2) is a function of $E = \hbar\omega$, and is denoted by $\langle\langle A; B \rangle\rangle_E$. The equation of motion satisfied by

this function is

$$E \langle\langle A; B \rangle\rangle_E = \frac{1}{2} \pi \langle [A, B] \rangle + \langle\langle [A, \mathcal{H}]; B \rangle\rangle_E. \quad (2.3)$$

Knowledge of $\langle\langle A; B \rangle\rangle_E$ suffices to determine the correlation function $\langle BA(t) \rangle$. The relation between the two is given by

$$\begin{aligned} \langle BA(t) \rangle &= \lim_{\epsilon \rightarrow 0} \int_{-\infty}^{+\infty} \frac{\langle\langle A; B \rangle\rangle_{\hbar\omega + i\epsilon} - \langle\langle A; B \rangle\rangle_{\hbar\omega - i\epsilon}}{e^{\beta\hbar\omega} - 1} e^{-i\omega t} d\omega. \end{aligned} \quad (2.4)$$

We introduce the conventional spin raising and lowering operators $S_i^{\pm} = S_i^x \pm iS_i^y$. The following commutation relations will prove useful:

$$[S_i^+, S_j^-] = 2S_i^z \delta_{ij}, \quad (2.5)$$

$$[S_i^{\pm}, S_j^{\pm}] = \mp S_i^{\pm} \delta_{ij}, \quad (2.6)$$

$$[S_i^{\pm}, e^{aS_j^z}] = (e^{7a} - 1) e^{aS_j^z} S_i^{\pm} \delta_{ij}. \quad (2.7)$$

The last relation follows from Eq. (2.6), where a is a c number. Furthermore, one obtains the operator identity

$$S_i^- S_i^+ = S(S+1) - S_i^z - (S_i^z)^2. \quad (2.8)$$

For reasons which will become evident later, we consider the Green's function

$$\langle\langle \exp(\sum_i a_i S_i^z) S_{\mathbf{r}}^+; S_{\mathbf{r}}^- \rangle\rangle_E. \quad (2.9)$$

The summation in the exponential runs over the N lattice sites and the a_i 's are a set of N c -number parameters, eventually to be set equal to zero. Using Eq. (2.3), the equation of motion satisfied by the Green's function Eq. (2.9) is

$$\begin{aligned} (E - \mu H) \langle\langle \exp(\sum_i a_i S_i^z) S_{\mathbf{r}}^+; S_{\mathbf{r}}^- \rangle\rangle_E - 2 \sum_j J_{\mathbf{r}\mathbf{j}} & \\ \times \langle\langle \exp(\sum_i a_i S_i^z) S_{\mathbf{j}}^z S_{\mathbf{r}}^+; S_{\mathbf{r}}^- \rangle\rangle_E = \phi_{\mathbf{r}}, & \quad (2.10) \end{aligned}$$

where

$$\phi_{\mathbf{r}, i} = \langle [\exp(\sum_i a_i S_i^z) S_{\mathbf{r}}^+; S_{\mathbf{r}}^-] \rangle. \quad (2.11)$$

The second term on the left-hand side of Eq. (2.10) is a Green's function of higher order than the original one, Eq. (2.9), owing to the presence of the operator $S_{\mathbf{j}}^z$. In previous works this higher-order Green's function was determined by either finding its equation of motion or by making some kind of approximation. The approximation invoked by Tyablikov,² for example, consisted of replacing the operator $S_{\mathbf{j}}^z$ by its average value $\langle S_{\mathbf{j}}^z \rangle$. This procedure leads to the Weiss¹² molecular-field result. Owing to our choice of the Green's function, it is unnecessary to resort to any approximation. We point out that the higher-order Green's function $\langle\langle \exp(\sum_i a_i S_i^z) S_{\mathbf{r}}^z S_{\mathbf{r}}^+; S_{\mathbf{r}}^- \rangle\rangle_E$ may be generated by taking the partial derivative of the original Green's function Eq. (2.9), with respect to the parameter $a_{\mathbf{j}}$. Thus Eq. (2.10) may be rewritten as

$$\left(E - \mu H - 2 \sum_j J_{gj} \frac{\partial}{\partial a_j}\right) \langle \langle \exp(\sum_i a_i S_i^z) S_g^+ S_i^- \rangle \rangle_E = \frac{\phi_{g,i}}{2\pi}. \quad (2.12)$$

The correlation function $\langle S_i^- \exp(\sum_i a_i S_i^z) S_i^+ \rangle$ may be found by using Eqs. (2.4) and (2.12); taking $t=0$,

$$\langle S_i^- \exp(\sum_i a_i S_i^z) S_i^+ \rangle = \left[\exp\left(\beta\mu H + 2\beta \sum_j J_{gj} \frac{\partial}{\partial a_j}\right) - 1 \right]^{-1} \phi_{g,i}. \quad (2.13)$$

The commutation relations Eqs. (2.5)–(2.7) enable us to evaluate the function $\phi_{g,i}$. The result is

$$\phi_{g,i} = 2 \langle \exp(\sum_i a_i S_i^z) S_g^z \rangle \delta_{gi} + (1 - e^{a_i}) \langle \exp(\sum_i a_i S_i^z) S_i^- S_i^+ \rangle. \quad (2.14)$$

It is convenient to introduce the function

$$\Omega(\{a_i\}) \equiv \langle \exp(\sum_i a_i S_i^z) \rangle, \quad (2.15)$$

where $\{a_i\}$ means the set of the N parameters a_i . Letting $g=l$ and again using the commutation relations, all of the correlation functions may be expressed in terms of Ω and its partial derivatives as follows:

$$\begin{aligned} e^{a_g} \left[S(S+1) - \frac{\partial}{\partial a_g} - \frac{\partial^2}{\partial a_g^2} \right] \Omega \\ = \left[\exp\left(\beta\mu H + 2\beta \sum_i J_{gi} \frac{\partial}{\partial a_i}\right) - 1 \right]^{-1} \\ \times \left\{ 2 \frac{\partial}{\partial a_g} + (1 - e^{a_g}) \left[S(S+1) - \frac{\partial}{\partial a_g} - \frac{\partial^2}{\partial a_g^2} \right] \right\} \Omega. \end{aligned} \quad (2.16)$$

Upon rearrangement we obtain the major result of this section

$$\left\{ \exp\left(a_g + \beta\mu H + 2\beta \sum_i J_{gi} \frac{\partial}{\partial a_i}\right) \left[\frac{\partial^2}{\partial a_g^2} + \frac{\partial}{\partial a_g} - S(S+1) \right] - \left[\frac{\partial^2}{\partial a_g^2} - \frac{\partial}{\partial a_g} - S(S+1) \right] \right\} \Omega = 0. \quad (2.17)$$

Equation (2.17) is a differential difference equation for the function Ω of the N -independent variables a_i . No approximations have been used in deriving Eq. (2.17), so it is an exact equation for arbitrary spin S , and range of interaction J_{gi} . The differential operator in the exponential has the effect of translating the arguments of Ω from a_i to $a_i + 2\beta J_{gi}$. Notice that when the lattice index $i=g$, then $J_{gg}=0$, so that the operator $\sum_i J_{gi} \partial/\partial a_i$ commutes with a_g , $\partial/\partial a_g$, and $\partial^2/\partial a_g^2$. In order to completely specify the solution to Eq. (2.17), further conditions are needed. One of these is immediately obtained from the definition of Ω in Eq. (2.15),

$$\Omega(\{a_i\}=0) = 1. \quad (2.18)$$

In addition, a set of N conditions is obtained from the operator identity

$$\prod_{p=-S}^S (S_i^z - p) = 0. \quad (2.19)$$

In terms of the differential operator $\partial/\partial a_i$ and the function Ω , Eq. (2.19) may be expressed as

$$\prod_{p=-S}^S \left(\frac{\partial}{\partial a_i} - p \right) \Omega = 0. \quad (2.20)$$

Taking the average value of Eq. (2.19), one obtains Eq. (2.20), but with the function Ω and its derivatives evaluated for $\{a_i\}=0$. This is the analog of Eq. (47) in Callen's⁴ paper, and represents an initial condition. However, we emphasize that Eq. (2.20) is valid for the entire range of the independent variables a_i . Hence Eq. (2.20) may be regarded as a set of N subsidiary partial differential equations that Ω must satisfy; Eq. (2.17) explicitly shows the independent variable a_g , but since the index g ranges over the N lattice sites there are actually N differential difference equations. Further initial conditions may be obtained by physical reasoning. For example, translational invariance requires that the magnetization

$$\langle S_i^z \rangle = \frac{\partial \Omega}{\partial a_i} \Big|_{\{a_k\}=0}$$

be independent of the lattice site i , and thus

$$\frac{\partial \Omega}{\partial a_i} \Big|_{\{a_k\}=0} = \frac{\partial \Omega}{\partial a_j} \Big|_{\{a_k\}=0} \quad (2.21)$$

for all i and j .

Once the function Ω has been determined, all of the higher-order correlation functions may be obtained by repeated partial differentiation.

III. APPROXIMATE THEORIES

We shall show how the Weiss¹² molecular field and Bethe-Peierls-Weiss¹³⁻¹⁵ (BPW) theories may be extracted from our formalism Eq. (2.17). However, let us first derive some general results which do not depend on any approximations. Introducing the notation

$$\begin{aligned} D_i &\equiv \frac{\partial}{\partial a_i}, \quad D^n \equiv i_1 i_2 \cdots i_n \equiv \frac{\partial^n}{\partial a_{i_1} \partial a_{i_2} \cdots \partial a_{i_n}}, \\ h &= \beta\mu H, \end{aligned} \quad (3.1)$$

the differential equations which Ω must satisfy, Eqs. (2.17) and (2.20), are written as

$$\left\{ \exp(a_g + h + 2\beta \sum_i J_{gi} D_i) [D_g^2 + D_g - S(S+1)] \right.$$

$$-[D_g^2 - D_g - S(S+1)]\Omega = 0, \quad (3.2)$$

$$\prod_{p=-S}^S (D_i - p)\Omega = 0. \quad (3.3)$$

The most general solution may be put in the form

$$\Omega = \sum_{\{n_i\}=0}^{\infty} A_{\{n_i\}} \exp[\sum_i a_i (n_i + \lambda_i)], \quad (3.4)$$

where the first sum means the sum over all positive integers n_i , the sum in the exponential runs over the N lattice sites, the expansion coefficients $A_{\{n_i\}}$ are functions only of the integers n_i , and finally the λ_i are as yet undetermined constants. Inserting Eq. (3.4) into Eq. (3.3), we obtain

$$\sum_{\{n_i\}=0}^{\infty} A_{\{n_i\}} \exp[\sum_i a_i (n_i + \lambda_i)] \prod_{p=-S}^S (n_i + \lambda_i - p) = 0. \quad (3.5)$$

The above must be true for all values of i , and furthermore $A_{\{n_i\}} = 0$ for $n_i > S - \lambda_i$ or $n_i < -S - \lambda_i$. Hence the n_i 's are restricted, and Eq. (3.4) becomes

$$\Omega = \sum_{\{n_i\}=\{-S-\lambda_i\}}^{\{S-\lambda_i\}} A_{\{n_i\}} \exp[\sum_i a_i (n_i + \lambda_i)]. \quad (3.6)$$

In addition $\lambda_i \leq -S$, since $n_i \geq 0$. The constants λ_i are found from the indicial equation, obtained by putting Eq. (3.6) into Eq. (3.2), thus,

$$\lambda_i^2 - \lambda_i - S(S+1) = 0; \quad (3.7)$$

Eq. (3.7) yields $\lambda_i = -S, S+1$, but only $\lambda_i = -S$ will satisfy the requirement $\lambda_i \leq -S$, so that the solution takes the form

$$\Omega = \prod_{i=1}^N \frac{\sinh(S + \frac{1}{2})(a_i + h + 2\beta Jz \langle S_i^z \rangle) / \sinh(\frac{1}{2})(a_i + h + 2\beta Jz \langle S_i^z \rangle)}{\sinh(S + \frac{1}{2})(h + 2\beta Jz \langle S_i^z \rangle) / \sinh(\frac{1}{2})(h + 2\beta Jz \langle S_i^z \rangle)}. \quad (3.12)$$

Notice that the solution is a product of individual functions, which is consistent with the original assumption. The magnetization is obtained by differentiating Eq. (3.12) with respect to a_i and subsequently setting $\{a_i\} = 0$. The result is

$$\langle S_i^z \rangle = S B_S [S(h + 2\beta Jz \langle S_i^z \rangle)], \quad (3.13)$$

where $B_S(x)$ is the familiar Brillouin function defined by

$$B_S(x) = \frac{S + \frac{1}{2}}{S} \coth \frac{S + \frac{1}{2}}{S} x - \frac{1}{2S} \coth \frac{x}{2S}. \quad (3.14)$$

The expression for $\langle S_i^z \rangle$ is, of course, the result given by molecular-field theory.

The BPW method considers a cluster of spins, where the interaction between the central spin and its z nearest neighbors within the cluster is treated

$$\Omega = \sum_{\{n_i\}=0}^{2S} A_{\{n_i\}} \exp[\sum_i a_i (n_i - S)], \quad (3.8)$$

which is a perfectly general result.

The physics of the cooperative phenomena is contained in the operator $\exp(2\beta \sum_i J_{gi} D_i)$. Expanding the exponential and operating on Ω , Eq. (2.15), it is seen that all of the higher-order spin-spin correlation functions are generated. Molecular-field theory ignores these correlations in the sense that it replaces the average of spin products by the product of the averages. Hence, the operator $2\beta \sum_i J_{gi} D_i$ in the exponential may be replaced by $2\beta \sum_i J_{gi} \langle S_i^z \rangle$ and Eq. (3.2) becomes an ordinary second-order differential equation. Putting Eq. (3.8) into Eq. (3.2) and letting J be the exchange integral for z nearest neighbors, we find a recursion relation among the coefficients $A_{\{n_i\}}$, namely,

$$A_{n_1 \dots n_g + 1, \dots, n_N} = e^{h + 2\beta Jz \langle S_i^z \rangle} A_{n_1 \dots n_g, \dots, n_N}, \quad (3.9)$$

whose solution is

$$A_{n_1 \dots n_g, \dots, n_N} = e^{n_g (h + 2\beta Jz \langle S_i^z \rangle)} A_{n_1, \dots, 0, \dots, n_N}. \quad (3.10)$$

The summation over n_g may now be performed, and the functional dependence on the variable a_g is given by

$$\frac{\sinh(a_g + h + 2\beta Jz \langle S_i^z \rangle)(S + \frac{1}{2})}{\sinh(\frac{1}{2}(a_g + h + 2\beta Jz \langle S_i^z \rangle))}. \quad (3.11)$$

The procedure may be repeated for all values of g , and is identical to Eq. (3.11), except for the label index on a . The constants $A_{0,0,\dots,0}$ can be evaluated from the initial condition Eq. (2.18), and the total solution for Ω is

exactly. The remaining interactions are then approximated by an effective internal field which is determined self-consistently. Let us designate the variable associated with the central spin as a_0 and those of the z nearest neighbors as a_i , where $i = 1, 2, \dots, z$. The operator $2\beta \sum_i J_{gi} D_i$ will have the following forms for the values of g and i :

$$2\beta \sum_i J_{gi} D_i = \begin{cases} 2\beta J(D_1 + D_2 + \dots + D_z) \\ \text{for } g=0, i=1, 2, \dots, z \end{cases} \quad (3.15)$$

$$2\beta \sum_i J_{gi} D_i = \begin{cases} 2\beta J D_0 + h_1(z-1) \\ \text{for } g=1, 2, \dots, z, i \neq g \end{cases} \quad (3.16)$$

$$2\beta \sum_i J_{gi} D_i = \begin{cases} h_1 z \\ \text{for } g, i \neq 0, 1, 2, \dots, z. \end{cases} \quad (3.17)$$

The exact value of the operator has been used when g is the central spin with z nearest neighbors. When g is within the cluster, but not the central spin, we use the exact expression for the interaction between the cluster and central spin ($2\beta J D_0$), but approximate the remaining $z - 1$ interactions by an effective field per nearest pair h_1 , hence the term $h_1(z - 1)$. Finally, for any spin g outside the cluster having z nearest neighbors the effective field per nearest-neighbor pair is again used, yielding the term $h_1 z$. The detailed solution to Ω is given in the Appendix. The magnetization is found by differentiating the solution for Ω with respect to a_i , and then setting $\{a_i\} = 0$. The resulting equations are the BPW expressions for spin S , and nearest-neighbor interactions.

IV. EXACT RESULTS

It is possible to make further simplifications in our theory by examining the operator $e^{2\beta J \sum_i D_i}$ more carefully; Eq. (2.20) is a polynomial equation of order $2S + 1$ in the operator D_i . Hence D_i^{2S+1} may be written in terms of $D_i^{2S-1}, D_i^{2S-3}, \dots$ where the coefficients of the operators depend on S . Using this expression in the formal expansion for $e^{2\beta J \sum_i D_i}$, one would obtain a series in D_i , whose highest power would be $2S$. Rather than explicitly calculate the polynomial for D_i^{2S+1} , let us set

$$e^{2\beta J \sum_i D_i} = \sum_{i=0}^{2S} F_i(\beta J_{gi}, S) D_i^i, \tag{4.1}$$

where the coefficients F_i depend only on βJ_{gi} and S . To evaluate the F_i , use Eq. (3.8) for Ω , and let Eq. (4.1) operate on Ω , such that

$$\begin{aligned} \sum_{\{n_i\}=0}^{2S} A_{\{n_i\}} \exp \left(\sum_{i=1}^N a_i (n_i - S) + 2\beta \sum_k J_{gk} (n_k - S) \right) \\ = \sum_{i=0}^{2S} F_i(\beta J_{gk}, S) \sum_{\{n_i\}=0}^{2S} A_{\{n_i\}} \\ \times \exp \left(\sum_{i=1}^N a_i (n_i - S) \right) (n_k - S)^i. \end{aligned} \tag{4.2}$$

Equating like powers of e^{a_i} , the following equations are found for the F_i :

$$\begin{aligned} F_0 + (-S)F_1 + (-S)^2 F_2 + \dots + (-S)^{2S} F_{2S} &= e^{-2\beta J_{gk} S}, \\ F_0 + (-S+1)F_1 + (-S+1)^2 F_2 + \dots + (-S+1)^{2S} F_{2S} \\ &= e^{-2\beta J_{gk} (S-1)}, \\ \vdots \\ F_0 + (S-1)F_1 + (S-1)^2 F_2 + \dots + (S-1)^{2S} F_{2S} \\ &= e^{2\beta J_{gk} (S-1)}, \\ F_0 + SF_1 + S^2 F_2 + \dots + S^{2S} F_{2S} &= e^{2\beta J_{gk} S}. \end{aligned} \tag{4.3}$$

There are $2S + 1$ equations and this is just the number of unknowns $F_i(\beta J, S)$. The set of simultaneous equations has been solved for the values $S = \frac{1}{2}, 1, \frac{3}{2}, 2$, and the coefficients $F_i(\beta J, S)$ are listed in Table I. The differential difference equation, Eq. (3.2), has thus been reduced to a partial differential equation. Assuming nearest-neighbor interactions only (J is the value of the exchange integral for z nearest neighbors), Eq. (3.2) with the aid of Eq. (4.1) becomes

$$\left\{ e^{(a_g+h)} \prod_{i=1}^z \left[\sum_{l=0}^{2S} F_l(\beta J, S) D_i^l \right] [D_g^2 + D_g - S(S+1)] - [D_g^2 - D_g - S(S+1)] \right\} \Omega = 0. \tag{4.4}$$

Notice that the two highest-order derivatives in Eq. (4.4) are D_{g, i_1, i_2}^{2S+2} and $D_{g, i_1, \dots, i_z}^{2S+1}$. Now for the case of $S = \frac{1}{2}$, the highest-order derivative is $D_{g, i_1, \dots, i_z}^{2S+1}$, since $D_i^2 \Omega = \frac{1}{4} \Omega$. However, by writing Eq. (3.2) in a slightly different form, we may reduce the order from $D_{g, i_1, \dots, i_z}^{2S+1}$ to D_{i_1, \dots, i_z} , as follows:

$$\begin{aligned} [D_g - \frac{1}{2} [\exp(a_g + h + 2\beta \sum J_{gi} D_i) - 1] \\ \times [\exp(a_g + h + 2\beta \sum J_{gi} D_i) + 1]^{-1}] \Omega = 0, \end{aligned} \tag{4.5}$$

where we have explicitly used $D_g^2 \Omega = \frac{1}{4} \Omega$ for $S = \frac{1}{2}$. Equation (4.5) is identical to Eq. (4) of Callen's paper when it is evaluated for $\{a_i\} = 0$. Thus $[D_g \Omega]_{\{a_i\}=0} = \langle S_g^z \rangle$, so that

$$\langle S_g^z \rangle = \frac{1}{2} \langle \tanh \frac{1}{2} (h + 2\beta \sum J_{gi} S_i^z) \rangle. \tag{4.6}$$

Using the results of Table I for $S = \frac{1}{2}$, we have

$$e^{2\beta J D_i} = \cosh \beta J + 2(\sinh \beta J) D_i. \tag{4.7}$$

The inverse operator $[\exp(a_g + h + 2\beta \sum J_{gi} D_i) + 1]^{-1}$ could now be formally expanded and it is easily seen that the highest-order derivative is D_{i_1, \dots, i_z}^z , so we have reduced the order of the derivatives by using the form Eq. (4.5). Rather than expand the inverse operator, let us set

$$\begin{aligned} \sum_{i=0}^z G_i(a_g)_{i_1, i_2, \dots, i_i} D_{i_1, i_2, \dots, i_i}^i \\ = \frac{1}{2} [\exp(a_g + h + 2\beta J \sum D_i) - 1] \\ \times [\exp(a_g + h + 2\beta J \sum D_i) + 1]^{-1}, \end{aligned} \tag{4.8}$$

where the coefficients $G_i(a_g)$ are functions of the independent variables $a_g, \beta J$, and z . The second summation is over all l -tuples i_1, i_2, \dots, i_l having g as the nearest neighbor. For example, $l = 2$ is the sum over the pairs (i, j) which are nearest neighbors of g and contains, then, $\frac{1}{2} z(z - 1)$ terms. Using Eq. (3.8) for Ω with $S = \frac{1}{2}$, and letting Eq. (4.7) operate on Ω , one has

TABLE I. Coefficients $F_i(\beta J)$ in Eq. (4.1). $\sinh l\beta J = S_l$ and $\cosh l\beta J = C_l$.

S	F_0	F_1	F_2	F_3	F_4
$\frac{1}{2}$	C_1	$2S_1$	0	0	0
1	1	$C_2 - 1$	S_2	0	0
$\frac{3}{2}$	$\frac{1}{8}(9C_1 - C_3)$	$\frac{1}{12}(27S_1 - S_3)$	$\frac{1}{2}(C_3 - C_1)$	$\frac{1}{8}(S_3 - 3S_1)$	0
2	1	$\frac{1}{6}(8S_2 - S_4)$	$\frac{1}{12}(16C_2 - C_4 - 15)$	$\frac{1}{6}(S_4 - 2S_2)$	$\frac{1}{12}(3 + C_4 - 4C_2)$

$$\sum_{\{n_i\}=0}^1 A_{\{n_i\}} \left[\sum a_i (n_i - \frac{1}{2}) \right] \left(G_0(a_g) + G_1(a_g) \sum_i (n_i - \frac{1}{2}) + G_2(a_g) \sum_{(i,j)} (n_i - \frac{1}{2})(n_j - \frac{1}{2}) + \dots + G_z(a_g) (n_{i_1} - \frac{1}{2}) \dots (n_{i_z} - \frac{1}{2}) \right) \\ = \sum_{\{n_i\}=0}^1 A_{\{n_i\}} \exp \left[\sum a_i (n_i - \frac{1}{2}) \right] \frac{1}{2} \frac{\exp[a_g + h + 2\beta J \sum (n_i - 1/2)] - 1}{\exp[a_g + h + 2\beta J \sum (n_i - 1/2)] + 1} \quad (4.9)$$

Equating like powers of e^{a_g} yields

$$G_0(a_g) + G_1(a_g) \sum_i (n_i - \frac{1}{2}) + G_2(a_g) \\ \times \sum_{(i,j)} (n_i - \frac{1}{2})(n_j - \frac{1}{2}) + \dots \\ = \frac{1}{2} \tanh \frac{1}{2} [a_g + h + 2\beta J \sum (n_i - \frac{1}{2})], \quad (4.10)$$

where the n_i can take the values 0 and 1. It would appear that there are 2^z equations; however, many of these are redundant. The nonredundant equations are obtained by letting all the $n_i = 1$, then all $n_i = 1$ except one, $n_j = 0$, and so on until all the $n_i = 0$. In this manner we obtain $z+1$ equations which is just the correct number to determine the coefficients $G_i(a_g)$. These are

$$G_0 \pm z \frac{1}{2} G_1 + \frac{z(z-1)}{2} \left(\frac{1}{2} \right)^2 G_2 \pm \frac{z(z-1)(z-2)}{3!} \left(\frac{1}{2} \right)^3 G_3 + \dots \\ + (\pm \frac{1}{2})^z G_z = \frac{1}{2} \tanh \frac{1}{2} (a_g + h \pm z\beta J),$$

$$G_0 \pm (z-2) \frac{1}{2} G_1 + \frac{(z-1)(z-4)}{2} \left(\frac{1}{2} \right)^2 G_2 \\ \pm \frac{(z-1)(z-2)(z-6)}{3!} \left(\frac{1}{2} \right)^3 G_3 + \dots \\ - (\pm \frac{1}{2})^z G_z = \frac{1}{2} \tanh \frac{1}{2} [a_g + h \pm (z-2)\beta J],$$

$$G_0 \pm (z-4) \frac{1}{2} G_1 + \frac{z^2 - 9z + 16}{2} \left(\frac{1}{2} \right)^2 G_2 \\ \pm \frac{(z-2)(z-4)(z-9)}{3!} \left(\frac{1}{2} \right)^3 G_3 + \dots \\ + (\pm \frac{1}{2})^z G_z = \frac{1}{2} \tanh \frac{1}{2} [a_g + h \pm (z-4)\beta J], \quad (4.11)$$

⋮

The $G_i(a_g)$ are listed in Table II for the values $z = 2, 3, 4$, and 6. Let us write out the differential equation, Eq. (4.5), using Eq. (4.8):

$$D_g \Omega = \left(G_0 + G_1 \sum_i D_i + G_2 \sum_{(i,j)} D_{i,j}^2 + G_3 \sum_{(i,j,k)} D_{i,j,k}^3 + \dots + G_z D_{i_1 i_2 \dots i_z}^z \right) \Omega \quad (4.12)$$

It has not been possible to solve the differential equation but the above form proves very useful for generating relations among the spin-spin correlation functions. If we perform the indicated differentiations, and then set $\{a_i\} = 0$, Eq. (4.12) yields a relation among the magnetization, two-spin, three-spin, etc., correlation functions. Furthermore, if we agree not to differentiate with respect to a_g , letting $a_g = 0$, and the external field $h = 0$, a great simplification results. Table II shows that for $a_g = h = 0$, all of the even coefficients G_0 , G_2 , and G_4 , vanish for all values of z . Equation (4.12) then predicts that for zero external field, the odd-number spin correlation functions vanish for $T \geq T_c$, as was shown by Tahir-Kheli.¹⁰

The three cases for $z = 2, 4, 6$ will now be considered in more detail.

The one-dimensional linear chain corresponds to $z = 2$, and labeling the spin indices by $1, 2, \dots, n, \dots, N$, Eq. (4.12) becomes

$$D_n \Omega = G_1 (D_{n-1} + D_{n+1}) \Omega \quad (a_n = h = 0) \quad (4.13)$$

Equation (4.13) immediately shows that the spontaneous magnetization vanishes for zero external field, since translational invariance requires

$$\langle S_n^z \rangle = \langle S_{n-1}^z \rangle = \langle S_{n+1}^z \rangle \equiv \langle S^z \rangle,$$

and thus

$$\langle S^z \rangle (1 - 2G_1) = 0 \quad (4.14)$$

Differentiating Eq. (4.13) with respect to a_{n+m} yields

$$D_{n,n+m}^2 \Omega = G_1 (D_{n-1,n+m}^2 + D_{n+1,n+m}^2) \Omega \quad (4.15)$$

Designating the two-spin correlation function $\langle S_n^z S_{n+m}^z \rangle$ by M_m , where the spins are separated by m lattice spacings, and setting $\{a_i\} = 0$, we have

$$M_m = G_1 (M_{m+1} + M_{m-1}) \quad (4.16)$$

Using Table II for G_1 , the above recursion relation is easily solved for M_m and the result is

$$M_m = \frac{1}{4} (\tanh \frac{1}{2} \beta J)^m \quad (4.17)$$

It is also possible to obtain the magnetization and correlation functions for $\hbar \neq 0$. By further differentiations one may obtain recursion relations among the quantities $\langle S_n^z S_1^z \rangle$, $\langle S_1^z S_2^z S_n^z \rangle$, and $\langle S_1^z S_3^z S_n^z \rangle$, and these again may be solved to yield the standard results.

The two-dimensional lattices with $z=4$ could be either, say, the quadratic net or the Kagomé lattices. For this case Eq. (4.12) becomes

$$D_0 \Omega = [G_1 (D_1 + D_2 + D_3 + D_4) + G_3 (D_{1,2,3}^3 + D_{1,2,4}^3 + D_{1,3,4}^3 + D_{2,3,4}^3)] \Omega = 0, \\ a_0 = \hbar = 0 \quad (4.18)$$

The index zero refers to an arbitrary lattice point, while the indices 1, 2, 3, and 4, correspond to the four nearest neighbors of zero. Let us designate the correlation functions by

$$\langle S_i^z S_j^z \rangle \equiv M_{i,j} \langle S_i^z S_j^z S_k^z \rangle \\ \equiv M_{i,j,k} \langle S_i^z S_j^z S_k^z S_l^z \rangle \equiv M_{i,j,k,l} \quad (4.19)$$

The magnetization and three-spin correlation functions are related by

$$\langle S^z \rangle (1 - 4G_1) = 4G_3 M_{1,2,3},$$

since

$$M_{1,2,3} = M_{1,2,4} = M_{1,3,4} = M_{2,3,4} \quad (4.20)$$

Differentiating Eq. (4.18) with respect to a_n , where n refers to an arbitrary lattice point (not equal to 0, 1, 2, 3, and 4), yields

$$M_{0,n} = G_1 (M_{1,n} + M_{2,n} + M_{3,n} + M_{4,n}) \\ + G_3 (M_{1,2,3,n} + M_{1,2,4,n} + M_{1,3,4,n} + M_{2,3,4,n}) \quad (4.21)$$

The explicit dependence of the three-spin correlation function may be found by using Onsager's¹⁸ result for $\langle S^z \rangle$ in Eq. (4.20). Similar considerations can be applied to Eq. (4.21) to determine the four-spin correlation function by using the calculations of Kaufman and Onsager¹⁹ for the two-spin correlation function. Another relation is given by differentiating with respect to a_1 , and then a_n ,

$$M_{0,1,n} = G_1 \langle \frac{1}{4} S^z \rangle + (M_{1,2,n} + M_{1,3,n} + M_{1,4,n}) \\ + G_3 [(\frac{1}{4} M_{2,3,n} + M_{2,4,n} + M_{3,4,n}) \\ + M_{1,2,3,4,n}] \quad (4.22)$$

The above procedure can obviously be extended to relate the correlation functions for an arbitrary number of spin operators. It is interesting to note that the functional forms for the correlations depend only on the coordination number z . Thus, the magnetization and three-spin correlation function are related in exactly the same way for the quadratic net and Kagomé lattices. This is not to say that the magnetizations are given by the same functional dependence on βJ in the two cases. In principle, one could establish recursion relations among the correlation functions as in the one-dimensional case and by also invoking the symmetry of the lattice. As shown in Fig. 1, the four three-spin correlations are identical in the quadratic lattice but not in the Kagome. Hence the recursion relations would differ in the two cases.

The simplest three-dimensional case is given by $z=6$. Proceeding as above and using the same notation, we have

$$\langle S^z \rangle (1 - 6G_1) = G_3 \sum_{(i,j,k)} M_{i,j,k} \\ + G_5 \sum_{(i,j,k,l,m)} M_{i,j,k,l,m} \quad (4.23)$$

$$M_{0,n} = G_1 \sum_{i=1}^6 M_{i,n} + G_3 \sum_{(i,j,k)} M_{i,j,k,n} \\ + G_5 \sum_{(i,j,k,l,m)} M_{i,j,k,l,m,n} \quad (4.24)$$

Equation (4.23) relates the magnetization to the three- and five-spin correlations, whereas Eq. (4.24) relates the two-spin with the four- and six-spin correlations.

The specific relations we have derived for $z=2, 4$, and 6 have previously been found by Oguchi and Ono.¹¹ For example, our Eqs. (4.16) and (4.17) are equivalent to their Eqs. (2.25) and (2.26). They consider each lattice separately and calculate the necessary number of Green's functions to determine relations among the correlation functions. However, in our method one does not have to find the various Green's functions for each lattice. Thus Eq. (4.12) may be used directly to find relations among the correlation functions for any lattice. Fisher¹⁶ has derived general expressions for the two-spin correlations in terms of higher-order correlations and explicitly works out the case for $z=3$. Our results agree with his, and we have specifically given the relations for $z=4, 6$ by Eqs.

TABLE II. Coefficients $G_l(a_g)$ in Eq. (4.8). $\tanh \frac{1}{2}(a_g + h \pm l\beta J) = T_{\pm l}$ and $\tanh \frac{1}{2}(a_g + h) = T$.

G_l	2	3	z	4	6
G_0	$\frac{1}{8}[T_{+2} + T_{-2} + 2T]$	$\frac{1}{16}[T_{+3} + T_{-3} + 3(T_{+1} + T_{-1})]$	$\frac{1}{8}[\frac{1}{2}(T_{+4} + T_{-4}) + T_{+2} + T_{-2} + \frac{3}{2}T]$	$\frac{1}{128}[T_{+6} + T_{-6} + 6(T_{+4} + T_{-4}) + 15(T_{+2} + T_{-2}) + 20T]$	
G_1	$\frac{1}{4}[T_{+2} - T_{-2}]$	$\frac{1}{8}[T_{+3} - T_{-3} + T_{+1} - T_{-1}]$	$\frac{1}{16}[T_{+4} - T_{-4} + 2(T_{+2} - T_{-2})]$	$\frac{1}{64}[T_{+6} - T_{-6} + 4(T_{+4} - T_{-4}) + 5(T_{+2} - T_{-2})]$	
G_2	$\frac{1}{2}[T_{+2} + T_{-2} - 2T]$	$\frac{1}{4}[T_{+3} + T_{-3} - (T_{+1} + T_{-1})]$	$\frac{1}{8}[T_{+4} + T_{-4} - 2T]$	$\frac{1}{32}[T_{+6} + T_{-6} + 2(T_{+4} + T_{-4}) - (T_{+2} + T_{-2}) - 4T]$	
G_3	0	$\frac{1}{2}[T_{+3} - T_{-3} - 3(T_{+1} - T_{-1})]$	$\frac{1}{2}[\frac{1}{2}(T_{+4} - T_{-4}) - (T_{+2} - T_{-2})]$	$\frac{1}{16}[T_{+6} - T_{-6} - 3(T_{+2} - T_{-2})]$	
G_4	0	0	$\frac{1}{2}[T_{+4} + T_{-4} - 4(T_{+2} + T_{-2}) + 6T]$	$\frac{1}{8}[T_{+6} + T_{-6} - 2(T_{+4} + T_{-4}) - (T_{+2} + T_{-2}) + 4T]$	
G_5	0	0	0	$\frac{1}{4}[T_{+6} - T_{-6} - 4(T_{+4} - T_{-4}) + 5(T_{+2} - T_{-2})]$	
G_6	0	0	0	$\frac{1}{2}[T_{+6} + T_{-6} - 6(T_{+4} + T_{-4}) + 15(T_{+2} + T_{-2}) - 20T]$	

(4.21) and (4.23). The results of Griffiths's²⁰ work on inequalities among the two-spin correlation functions may also be extended to the higher-order cases.

Although we have considered the spin- $\frac{1}{2}$ case for z nearest neighbors in deriving specific results, the formalism of our method enables one to make similar calculations for arbitrary spin, without much additional algebraic complexity.

V. CONCLUSION

The technique of the two-time temperature-dependent Green's functions has been used to analyze the Ising model for a ferromagnet. We have shown that the problem may be reduced to that of solving

a partial differential equation. Although it has not been possible to solve the equation exactly, one easily obtains the results of previous approximate theories. Our method gives an orderly prescription for generating exact relations among correlation functions for an arbitrary number of spins, having arbitrary spin and range of interaction. Some of these exact results have appeared in the literature as already stated.

The obfuscation of the physical approximations resulting from the decoupling procedures is the most disturbing part of the Green's-function analysis. The Tyablikov decoupling leads to molecular-field theory and here the physical assumptions are well understood. However, this is not the case with more elaborate schemes, particularly in the Heisenberg model where the results are noticeably poor in the vicinity of the Curie temperature. It is possible that our procedure for the Ising model might be applied to the Heisenberg model and thus give more insight to the approximations that have been made.

APPENDIX

We now show by using the equations in Sec. II how the BPW relations are obtained. Using Eq. (3.15) for the operator, and Eq. (3.8) for Ω , Eq. (3.2) becomes

$$\sum_{\{n_i\}=0}^{2S} A_{\{n_i\}} \exp\left(\sum_{i=0}^{N-1} a_i(n_i - S)\right)$$

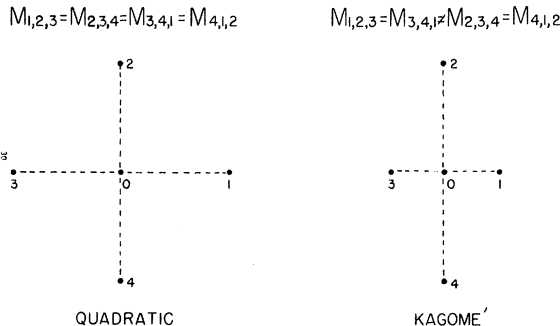


FIG. 1. Three-spin correlation functions in the quadratic and Kagomé lattices.

$$\times \left[(n_0 - 2S)(n_0 + 1) \exp \left(a_0 + h + 2\beta J \sum_{i=1}^z (n_i - S) \right) - (n_0 - 2S - 1)n_0 \right] = 0 \quad (A1)$$

To satisfy the above, one obtains a recursion relation for the coefficients $A_{\{n_i\}}$

$$A_{n_0+1, n_1, n_2, \dots} = \exp \left(h + 2\beta J \sum_{i=1}^z (n_i - S) \right) A_{n_0, n_1, n_2, \dots} \quad (A2)$$

This is easily solved and one has

$$\sum_{\{n_i\}=0}^{2S} A_{0, n_1, n_2, \dots} \exp \left[\sum_{i=0}^{N-1} a_i (n_i - S) + n_0 \left(h + 2\beta J \sum_{i=1}^z (n_i - S) \right) \right] \times \{ (n_1 - S)(n_1 + 1) \exp [a_1 + h + 2\beta J(n_0 - S) + h_1(z - 1)] - (n_1 - 2S - 1)n_1 \} = 0 \quad (A5)$$

Again, a recursion relation for the A_{0, n_1, n_2} is obtained

$$A_{0, n_1+1, n_2, \dots} = e^{h+h_1(z-1)-2\beta JS} A_{0, n_1, n_2, \dots} \quad (A6)$$

whose solution is

$$A_{0, n_1, n_2, \dots} = e^{n_1[h+h_1(z-1)-2\beta JS]} A_{0, 0, n_2, \dots} \quad (A7)$$

Using the above expression in Eq. (A4), Ω becomes

$$\Omega = \sum_{\{n_i\}=0}^{2S} A_{0, 0, n_2, n_3, \dots} \exp \left[\sum_{i=0}^{N-1} a_i (n_i - S) + n_0 \left(h + 2\beta J \sum_{i=1}^z (n_i - S) \right) + n_1 (h + h_1(z - 1) - 2\beta JS) \right] \quad (A8)$$

The same procedure follows for $g = 2, 3, \dots, z$, so one may immediately write Ω as

$$\Omega = \sum_{\{n_i\}=0}^{2S} A_{0, 0, 0, \dots, n_{z+1}, n_{z+2}, \dots} \times \exp \left[\sum_{i=0}^{N-1} a_i (n_i - S) + n_0 \left(h + 2\beta J \sum_{i=1}^z (n_i - S) \right) + \sum_{i=1}^z n_i [h + h_1(z - 1) - 2\beta JS] \right] \quad (A9)$$

where we have now determined the coefficients A_{n_0, n_1, \dots, n_z} within the cluster. The remaining coefficients may be found by using Eq. (3.17) in Eq. (3.2) and Ω given by Eq. (A9). Letting $g = z + 1$, for example, one obtains the following recursion rela-

$$A_{n_0, n_1, n_2, \dots} = \exp \left[n_0 \left(h + 2\beta J \sum_{i=1}^z (n_i - S) \right) \right] A_{0, n_1, n_2, \dots} \quad (A3)$$

Putting this expression back into Eq. (3.8) for Ω yields

$$\Omega = \sum_{\{n_i\}=0}^{2S} A_{0, n_1, n_2, \dots} \exp \left[\sum_{i=0}^{N-1} a_i (n_i - S) + n_0 \left(h + 2\beta J \sum_{i=1}^z (n_i - S) \right) \right] \quad (A4)$$

Let us next take g to be one of the cluster spins $g \neq 0$, then use Eq. (3.16) for the operator in the differential equation, Eq. (3.2), and use Eq. (A4) for Ω . Taking $g = 1$, for example, one has

tion:

$$A_{0, 0, \dots, n_{z+1}+1, \dots} = e^{h+h_1z} A_{0, 0, n_{z+1}, \dots} \quad (A10)$$

whose solution is

$$A_{0, 0, \dots, n_{z+1}, \dots} = e^{n_{z+1}(h+h_1z)} A_{0, 0, \dots, 0, \dots} \quad (A11)$$

An identical form obtains for all of the spins outside the cluster, so one may now write the total solution to Ω as

$$\Omega = A_{\{0\}} \sum_{\{n_i\}=0}^{2S} \exp \left[\sum_{i=0}^{N-1} a_i (n_i - S) + n_0 \left(h + 2\beta J \sum_{i=1}^z (n_i - S) \right) \right] \times \exp \left[\sum_{i=1}^z n_i [h + h_1(z - 1) - 2\beta JS] + \sum_{i=z+1}^{N-1} n_i (h + h_1z) \right] \quad (A12)$$

The sums over n_i are easily done, and we have for the solution

$$\Omega = \Omega(0) \sum_{n_0=0}^{2S} e^{(a_0+h)(n_0-S)} \times \prod_{i=1}^z \Omega_1 [a_i + h + h_1(z - 1) + 2\beta J(n_0 - S)] \times \prod_{i=z+1}^{N-1} \Omega_1 (a_i + h + h_1z) \quad (A13)$$

where

$$\Omega_1(x) = \sinh x(S + \frac{1}{2}) / \sinh \frac{1}{2}x \quad (\text{A14})$$

and $\Omega(0)$ is the value of Ω for $\{a_i\}=0$. To find the magnetization, one differentiates Eq. (A13) with respect to one of the variables a_i , and then sets

$\{a_i\}=0$. Self-consistently we require

$$\langle S_0^* \rangle = \langle S_i^* \rangle, \quad i=1, 2, \dots, N-1 \quad (\text{A15})$$

which will then determine both the magnetization and effective field h_1 . Proceeding as described one obtains

$$\langle S_0^* \rangle = \frac{\sum_{n_0=0}^{2S} (n_0 - S) e^{h(n_0 - S)} \Omega_1^* [h + h_1(z-1) + 2\beta J(n_0 - S)]}{\sum_{n_0=0}^{2S} e^{h(n_0 - S)} \Omega_1^* [h + h_1(z-1) + 2\beta J(n_0 - S)]}, \quad (\text{A16})$$

$$\langle S_i^* \rangle = \frac{\sum_{n_0=0}^{2S} e^{h(n_0 - S)} \Omega_1^{*-1} [h + h_1(z-1) + 2\beta J(n_0 - S)] \{D_i \Omega_i [a_i + h + h_1(z-1) + 2\beta J(n_0 - S)]\}_{a_i=0}}{\sum_{n_0=0}^{2S} e^{h(n_0 - S)} \Omega_1^* [h + h_1(z-1) + 2\beta J(n_0 - S)]}, \quad (\text{A17})$$

$$\langle S_i^* \rangle = SB_S[S(h + h_1 z)], \quad (\text{A18})$$

where B_S is the Brillouin function defined by Eq. (3.14). For completeness we also give the expression for the nearest-neighbor spin-spin correlation function

$$\langle S_0^* S_1^* \rangle = \frac{\sum_{n_0=0}^{2S} (n_0 - S) e^{h(n_0 - S)} \Omega_1^{*-1} [h + h_1(z-1) + 2\beta J(n_0 - S)] \{D_i \Omega_i [a_i + h + h_1(z-1) + 2\beta J(n_0 - S)]\}_{a_i=0}}{\sum_{n_0=0}^{2S} e^{h(n_0 - S)} \Omega_1^* [h + h_1(z-1) + 2\beta J(n_0 - S)]}. \quad (\text{A19})$$

Equations (A16)–(A19) are the BPW equations for spin S , and nearest-neighbor interactions.

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