Classical Heisenberg Model*

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Exact expressions for the partition function, spin pair correlation function, and susceptibility of the one-dimensional isotropic classical Heisenberg model are obtained in zero external field with cyclic boundary conditions. It is shown that the methods used to derive these results enable the partition functions and susceptibilities of finite clusters of interacting classical spins to be evaluated in terms of the $3n$-j symbols of Wigner. Exact results in one dimension are also obtained for the partition function and susceptibility of a "planar" classical Heisenberg model. In this model the spin vectors interact via a Heisenberg coupling but each spin vector is restricted to lie in a plane.

The anisotropic classical Heisenberg model described by the Hamiltonian

$$\mathcal{H}=-\sum_{(ij)}2(J_{ij}{}^{x}s_i{}^{x}s_j{}^{x}+J_{ij}{}^{y}s_i{}^{y}s_j{}^{y}+J_{ij}{}^{z}s_i{}^{z}s_j{}^{z})-mH\sum_{i=1}^{N}s_i{}^{z},$$

where $s_i{}^{x}$, $s_i{}^{y}$, and $s_i{}^{z}$ are components of the unit vector $\mathbf{s}_i$, is also considered. A perturbation series for the zero-field free energy of the anisotropic model in one dimension with nearest-neighbor interactions $J_{ij}{}^{x}=J_{ij}{}^{y}=J$ and $J_{ij}{}^{z}=\gamma J$ is developed in powers of $\gamma-1$ using the isotropic model as the unperturbed system. Detailed calculations are performed to third order in $\gamma-1$. It is found that the perturbation series for the energy per spin breaks down as $T\to 0$. A high-temperature series expansion for the anisotropic model, which is valid for a general interaction potential and lattice, is derived by generalizing the methods developed by Horwitz and Callen for the Ising model. This series is rearranged to give a simplified diagram expansion. Finally, a practical technique for calculating the high-temperature series expansions of the zero-field free energy and susceptibility of the isotropic classical Heisenberg model is presented.

1. INTRODUCTION

WHEN the magnitude of the spin in the Heisenberg model is allowed to become infinite a classical model of interacting spins is obtained. The Hamiltonian of this model can be written in the form

$$\mathcal{H}=-\sum_{(ij)}2J_{ij}\mathbf{s}_i\cdot\mathbf{s}_j-m\mathbf{H}\cdot\sum_{i=1}^{N}\mathbf{s}_i, \tag{1.1}$$

where $\mathbf{s}_i$ and $\mathbf{s}_j$ are unit vectors, m is the magnetic moment per spin and the first summation is taken over all pairs of spins in the lattice. The partition function of the Heisenberg model

$$Z_N=\text{Trace}\exp(-\beta\mathcal{H}) \tag{1.2}$$

becomes in the classical limit an integral

$$Z_N=\int_{\Omega_1}\cdots\int_{\Omega_N}\prod_{i=1}^{N}(d\Omega_i/4\pi)\exp(-\beta\mathcal{H}), \tag{1.3}$$

where $d\Omega_i$ is the element of solid angle in the direction $\mathbf{s}_i$.

An advantage of the classical Heisenberg model is that its thermodynamic properties can be evaluated exactly in one dimension. Fisher[1] has obtained exact results for the partition function and susceptibility in zero field of an *open chain* of $(N+1)$ classical spins with nearest-neighbor interactions. In Sec. 2 of this paper it is shown by solving an integral equation that exact expressions for the zero-field properties can also be derived for a *ring* of N classical spins with nearest-neighbor interactions. Both results agree in the thermodynamic limit $N\to\infty$, as would be expected intuitively.

For two- and three-dimensional lattices approximate methods must be used. The method of extrapolating high-temperature series expansions has provided the most reliable estimates for the critical behavior $(T>T_c)$ of the Heisenberg model.[2] Recently the high-temperature series for the zero-field free energy and susceptibility of the spin-$\frac{1}{2}$ Heisenberg model have been extended by several authors[3,4] using a technique first proposed by Domb.[5] In this method the free energy of the infinite lattice is expressed as a sum of partition functions of finite clusters of spins.

The author and Bowers[6] have shown that a considerable graphological simplification occurs when the cluster series is applied to the classical Heisenberg model. In particular it has been demonstrated that only star graphs contribute to the zero-field free energy cluster series and that only star graphs and reducible graphs which can be made into star graphs by the addition of one edge contribute to the zero-field susceptibility series. In Secs. 3 and 4 a technique is presented for evaluating the partition functions of star graphs in terms of the $3n$-j symbols of group theory, while in Sec. 5 a similar procedure for evaluating the susceptibilities of finite clusters is discussed. These new results,

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[1] M. E. Fisher, Am. J. Phys. **32**, 343 (1964).
[2] C. Domb and M. F. Sykes, Phys. Rev. **128**, 168 (1962).
[3] C. Domb and D. W. Wood, Proc. Phys. Soc. (London) **86**, 1 (1965).
[4] G. A. Baker, H. E. Gilbert, J. Eve, and G. S. Rushbrooke, Phys. Letters **20**, 146 (1966).
[5] C. Domb, Advan. Phys. **9**, 330 (1960).
[6] G. S. Joyce and R. G. Bowers, Proc. Phys. Soc. (London) **88**, 1053 (1966).

when combined with the simplifications discussed in Ref. 6, provide a powerful method of deriving the high-temperature series expansions for the classical Heisenberg model.

Stanley and Kaplan[7] have derived a new high-temperature series for the spin correlation function

$$\langle \mathbf{s}_i \cdot \mathbf{s}_j \rangle = \mathrm{Trace}\, \mathbf{s}_i \cdot \mathbf{s}_j \exp(-\beta \mathcal{H}) / \mathrm{Trace} \exp(-\beta \mathcal{H}) \quad (1.4)$$

of the Heisenberg model by direct expansion of the exponentials in Eq. (1.4). The terms in the series are given a diagrammatic representation similar to that used by Rushbrooke and Wood,[8] and it is shown that for the classical Heisenberg model the number of contributing diagrams is reduced by roughly an order of magnitude. The specific heat and susceptibility series can be obtained directly from the correlation function. This provides an alternative procedure, to the cluster series method discussed above, for calculating the series expansions for the Heisenberg model. The connection between the diagrammatic simplifications of Stanley and Kaplan and those given in Ref. 6 is established by expanding the finite cluster functions as high-temperature series.

Brown and Luttinger[9] have applied the Bethe-Peierls-Weiss approximation to the classical Heisenberg model. It is interesting to note (although it was not pointed out by these authors) that their results in zero field become exact, in the limit $N \to \infty$, for a one-dimensional lattice and a Bethe lattice. This is immediately seen by applying the star cluster series for the zero-field free energy to these lattices.

Although the classical spin model has unrealistic properties at low temperatures (such as a nonzero specific heat) it does provide an interesting model for studying critical behavior. In some respects the classical Heisenberg model is similar to the spin-$\frac{1}{2}$ Ising model. For example, both models have star graph expansions for the zero-field free energy and inverse susceptibility.[10]

2. THE ONE-DIMENSIONAL SOLUTION

The partition function of a one-dimensional assembly of N systems with a continuous range of energy levels is given by

$$Z_N = \lambda_1^N + \lambda_2^N + \cdots, \quad (2.1)$$

where λ_1, λ_2, $\cdots$ are the eigenvalues of the integral equation[11]

$$\int \exp[-\beta U(\xi_1,\xi_2)] \psi_n(\xi_2) d\xi_2 = \lambda_n \psi_n(\xi_1). \quad (2.2)$$

In this equation $U(\xi_1,\xi_2)$ is the energy of interaction between nearest-neighbor pairs of systems and $\psi_n(\xi)$ is an eigenfunction corresponding to the eigenvalue λ_n. (The variables ξ_1 and ξ_2 may correspond to a set of variables depending on the detailed form of the interaction studied.) For the classical spin assembly in zero field

$$U(\xi_1,\xi_2) = -2J \mathbf{s}_1 \cdot \mathbf{s}_2, \quad (2.3)$$

where $\mathbf{s}_1$ and $\mathbf{s}_2$ are unit vectors. We find by expressing $\mathbf{s}_1 \cdot \mathbf{s}_2$ in terms of polar coordinates that the integral equation becomes

$$\int_0^{2\pi} \int_0^{\pi} K(\theta_1\phi_1,\theta_2\phi_2) \psi_n(\theta_2,\phi_2) (d\Omega_2/4\pi) = \lambda_n \psi_n(\theta_1,\phi_1), \quad (2.4)$$

where

$$K(\theta_1\phi_1,\theta_2\phi_2) = \exp(K \cos\Theta), \quad (2.5)$$

$$\cos\Theta = \cos\theta_1 \cos\theta_2 + \sin\theta_1 \sin\theta_2 \cos(\phi_2 - \phi_1), \quad (2.6)$$

and $K = 2J\beta$. We see that the kernel (2.5) is real and symmetric and is therefore of the Hilbert-Schmidt type. In this case it can be shown that Eq. (2.4) possesses a complete set of mutually orthogonal eigenfunctions and that all the eigenvalues are real.

The correct set of eigenfunctions are the spherical harmonics $(4\pi)^{1/2} Y_{lm}(\theta,\phi)$, which can be expressed in terms of associated Legendre functions as follows:

$$Y_{lm}(\theta,\phi) = (-1)^m \left[\frac{(2l+1)(l-m)!}{4\pi(l+m)!} \right]^{1/2} P_l^m(\cos\theta) \times \exp(im\phi), \quad (2.7)$$

with

$$Y_{l-m}(\theta,\phi) = (-1)^m Y_{lm}^*(\theta,\phi). \quad (2.8)$$

To verify this statement we evaluate the left-hand side of Eq. (2.4) using the expansion

$$\exp(K \cos\Theta) = (\pi/2K)^{1/2} \sum_{l=0}^{\infty} (2l+1) I_{l+\frac{1}{2}}(K) \times P_l(\cos\Theta), \quad (2.9)$$

(where $I_{l+\frac{1}{2}}(x)$ are modified Bessel functions of the first kind) and the addition theorem for spherical harmonics

$$P_l(\cos\Theta) = 4\pi(2l+1)^{-1} \times \sum_{m=-l}^{l} Y_{lm}^*(\theta_2,\phi_2) Y_{lm}(\theta_1,\phi_1). \quad (2.10)$$

The integrations over (θ_2,ϕ_2) can now be easily performed using the standard result

$$\int_0^{2\pi} \int_0^{\pi} Y_{lm}^*(\theta,\phi) Y_{l'm'}(\theta,\phi) d\Omega = \delta_{ll'} \delta_{mm'}. \quad (2.11)$$

It is found that $(4\pi)^{1/2} Y_{lm}(\theta,\phi)$ is an eigenfunction of

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[10] For a proof of the star cluster expansions for the spin-$\frac{1}{2}$ Ising model see, C. Domb and B. J. Hiley, Proc. Roy. Soc. (London) **A268**, 506 (1962).
[11] See Ref. 5, p. 164.

Eq. (2.4) with a corresponding eigenvalue

$$\lambda_l(K)=(\pi/2K)^{1/2}I_{l+\frac{1}{2}}(K). \quad (2.12)$$

Substituting Eq. (2.12) in Eq. (2.1) we have

$$Z_N(K)=(\pi/2K)^{\frac{1}{2}N}\sum_{l=0}^{\infty}(2l+1)I_{l+\frac{1}{2}}{}^N(K), \quad (2.13)$$

where the factor $(2l+1)$ is due to the degeneracy of the eigenvalues. The eigenvalues are conveniently generated by

$$\lambda_l(K)=K^l(d/KdK)^l(\sinh K)/K. \quad (2.14)$$

Thus

$$\lambda_0(K)=(\sinh K)/K, \quad (2.15)$$

$$\lambda_1(K)=\lambda_0(K)u(K), \quad (2.16)$$

and

$$\lambda_2(K)=\lambda_0(K)[1-3K^{-1}u(K)], \quad (2.17)$$

where $u(K)$ is the Langevin function $\coth K-1/K$.

In the thermodynamic limit $N\to\infty$ only the largest eigenvalue ($l=0$) contributes to Eq. (2.13) and the partition function becomes

$$Z_N(K)\sim[(\sinh K)/K]^N, \quad (2.18)$$

which is the result obtained by Fisher[1] for an open chain of $N+1$ spins. As would be expected the particular choice of boundary conditions becomes unimportant in the limit $N\to\infty$.

The above method can be used to solve another closely related continuum spin model. In this model the spin vectors interact via a Heisenberg coupling but each spin vector lies on the surface of a cone $\theta=\alpha$. The integral equation for the model is

$$\exp(K\cos^2\alpha)\int_0^{2\pi}\exp[K\sin^2\alpha\cos(\phi_2-\phi_1)]\times\psi_n(\phi_2)(d\phi_2/2\pi)=\lambda_n\psi_n(\phi_1), \quad (2.19)$$

which has eigenfunctions

$$\psi_n(\phi)=\exp(\pm in\phi)\quad n=0,1,2,\cdots, \quad (2.20)$$

and corresponding eigenvalues

$$\lambda_n(K,\alpha)=\exp(K\cos^2\alpha)I_n(K\sin^2\alpha). \quad (2.21)$$

These results may be verified using the expansion

$$\exp[K\sin^2\alpha\cos(\phi_2-\phi_1)]=\sum_{n=-\infty}^{\infty}I_n(K\sin^2\alpha)\times\exp(in\phi_2)\exp(-in\phi_1). \quad (2.22)$$

In the limit $N\to\infty$ the partition function reduces to

$$Z_N(K,\alpha)\sim\exp(NK\cos^2\alpha)I_0{}^N(K\sin^2\alpha). \quad (2.23)$$

When $\alpha=\frac{1}{2}\pi$ a "planar" classical Heisenberg model is obtained. The specific heat in this case is

$$\lim_{N\to\infty}(C_N/Nk)=K^2\left[1-K^{-1}\frac{I_1(K)}{I_0(K)}-\frac{I_1^2(K)}{I_0^2(K)}\right]. \quad (2.24)$$

Using the asymptotic series for the Bessel functions we find that the behavior at low temperatures is

$$\lim_{N\to\infty}(C_N/Nk)\sim\tfrac{1}{2}+(1/4K)+O(K^{-2}). \quad (2.25)$$

It is interesting to compare this result with that obtained for the "unrestricted" classical Heisenberg model by Fisher.[1]

For studying the effects of anisotropy, in the classical approximation, we can define a Hamiltonian,

$$\mathcal{H}=-\sum_{(ij)}2(J^x s_i{}^x s_j{}^x+J^y s_i{}^y s_j{}^y+J^z s_i{}^z s_j{}^z)-mH\sum_{i=1}^{N}s_i{}^z, \quad (2.26)$$

where the first summation is taken over all nearest-neighbor pairs in the lattice, $s_i{}^x=\sin\theta_i\cos\phi_i$, $s_i{}^y=\sin\theta_i\times\sin\phi_i$, and $s_i{}^z=\cos\theta_i$. The case $J^x=J^y=0$ corresponds to the infinite spin Ising model and $J^x=J^y=J^z=J$ corresponds to the usual isotropic Heisenberg model. (The case $J^x=J^y=J$ and $J^z=0$ should not be confused with the "planar" Heisenberg model discussed above.) The anisotropic model can be solved exactly in one dimension,[12] when $J^x=J^y=-J$ and $J^z=+J$, using the expansion (2.9). The eigenfunctions are $(4\pi)^{1/2}Y_{lm}(\theta,\phi)$ with eigenvalues

$$\lambda_{lm}(K)=(-1)^m(\pi/2K)^{1/2}I_{l+\frac{1}{2}}(K). \quad (2.27)$$

The partition function of a finite ring of spins differs from the isotropic result (2.13), but in the limit $N\to\infty$ both models give the same partition function (2.18). Exact results have not been obtained for the general anisotropic Hamiltonian (2.26). We therefore discuss in Sec. 6 a perturbation expansion in powers of $(\gamma-1)$, for the case $J^x=J^y=J$ and $J^z=\gamma J$, where $\gamma\simeq 1$.

Although exact results have not been derived when $H\neq 0$, expressions will be obtained in Sec. 5 for the zero-field susceptibility of a finite ring of spins. We now show that the techniques developed above can be used to calculate the partition functions of finite clusters of spins.

3. PARTITION FUNCTIONS OF FINITE CLUSTERS

A finite cluster of N interacting classical spins $\mathbf{s}_1\cdots\mathbf{s}_N$ can be simply represented in terms of a graph. A spin $\mathbf{s}_j$ is represented in the graph by a labeled vertex j, while an interaction $-J_{ij}\mathbf{s}_i\cdot\mathbf{s}_j$ between two spins $\mathbf{s}_i$ and $\mathbf{s}_j$ is represented by an edge joining the vertices i

[12] I am grateful to R. G. Bowers for pointing out this result.

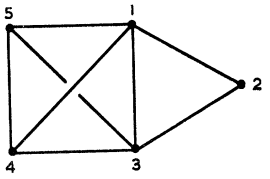

FIG. 1. A graph with a degree 2 vertex.

and j. A cluster is said to be connected (or linked) if the corresponding graph is connected. The same applies for a separated cluster. When the graph of a connected cluster has an articulation point the cluster is called a *reducible* cluster. If the graph of a connected cluster has *no* articulation points then the cluster is said to be a *star* cluster.

The partition function of a finite cluster of classical spins (in zero magnetic field) is

$$Z_N=\int_{\Omega_1}\cdots\int_{\Omega_n}\prod_{i=1}^{N}(d\Omega_i/4\pi)\prod_{(ij)}\exp(K_{ij}\cos\Theta_{ij}), \quad (3.1)$$

where $\cos\Theta_{ij}=\mathbf{s}_i\cdot\mathbf{s}_j$, and the first product is taken over all edges in the graph. For a separated cluster Eq. (3.1) immediately separates into a product of the partition functions of all the connected components. In the case of a reducible cluster Eq. (3.1) becomes a product of the partition functions of all the star clusters obtained by "cutting" the graph at all its articulation points. We see, therefore, that the only partition functions which have to be evaluated are those of star clusters.

The evaluation of Eq. (3.1) for star clusters is carried out by expanding the exponential factors in terms of the eigenfunctions and eigenvalues of the integral equation (2.4) using Eqs. (2.9) and (2.10). This yields

$$Z_N(G)=(4\pi)^{C(G)-1}\sum_{\{l_{ij}\}=0}^{\infty}\prod_{(ij)}\lambda_{l_{ij}}(K_{ij})\times\sum_{\{m_{ij}=-l_{ij}\}}^{\{m_{ij}=+l_{ij}\}}\int_{\Omega_1}\cdots\int_{\Omega_n}\prod_{i=1}^{N}d\Omega_i\times\prod_{(ij)}Y_{l_{ij}m_{ij}}{}^{*}(\theta_i,\phi_i)Y_{l_{ij}m_{ij}}(\theta_j,\phi_j), \quad (3.2)$$

where $\{l_{ij}\}$ and $\{m_{ij}\}$ denote sets of "dummy" summation variables corresponding to the set of edges in the graph G, and $C(G)$ is the cyclomatic number of the graph G.

If the graph G has one or more vertices of *degree two* a considerable simplification of Eq. (3.2) occurs. We take as an example the graph shown in Fig. 1. The contribution to Eq. (3.2) from the edges leaving vertex 2 is

$$\lambda_{l_{12}}(K_{12})\lambda_{l_{23}}(K_{23})Y_{l_{12}m_{12}}{}^{*}(\theta_1,\phi_1)Y_{l_{12}m_{12}}(\theta_2,\phi_2)\times Y_{l_{23}m_{23}}{}^{*}(\theta_2,\phi_2)Y_{l_{23}m_{23}}(\theta_3,\phi_3). \quad (3.3)$$

We find, on integrating over $d\Omega_2$ and summing over l_{23} and m_{23}, that Eq. (3.3) becomes

$$\lambda_{l_{12}}(K_{12})\lambda_{l_{12}}(K_{23})Y_{l_{12}m_{12}}{}^{*}(\theta_1,\phi_1)Y_{l_{12}m_{12}}(\theta_3,\phi_3). \quad (3.4)$$

Thus a vertex of degree two can be eliminated by simply modifying the product of eigenvalues. In general, if the partition function of a graph G is known, then all the partition functions of graphs *homeomorphic* with G can be easily written down.

We can now give a general set of rules for calculating $Z_N(G)$:

(a) Suppress all vertices of degree two in G and label the edges of the resulting graph G' with K_1, $K_2,\cdots$. (This labelling procedure is arbitrary.) An example is given in Fig. 2.

(b) Calculate $Z_{N'}(G')$ by applying Eq. (3.2) to the graph G'. After changing the notation, so that the sets of summation variables $\{l_{ij}\}$ and $\{m_{ij}\}$ are replaced by the sets $\{l_i\}$ and $\{m_i\}$, and rearranging the product of eigenfunctions we find

$$Z_{N'}(G')=(4\pi)^{C(G)-1}\sum_{\{l_i\}}\sum_{\{m_i\}}\prod_{i}\lambda_{l_i}(K_i)\times\prod_{\left[\begin{smallmatrix}\text{all vertices}\\ v\text{ in }G'\end{smallmatrix}\right]}\left[\int_{\Omega}\{\prod_{\left[\begin{smallmatrix}\text{all }\delta\text{ at}\\ \text{vertex }v\end{smallmatrix}\right]}Y_{l_im_i}(\theta,\phi)\}d\Omega\right]. \quad (3.5)$$

The labeled edges incident at a given vertex in G' form a vertex set $\{K_i\}_v$ and the parameter δ at vertex v takes the values of all the subscripts i of the elements K_i in this set $\{K_i\}_v$. The correct complex conjugates can be assigned to the eigenfunctions in Eq. (3.5) by making *one* of every pair of spherical harmonics with the *same* subscripts a complex conjugate function. [Since all homeomorphic graphs have the same cyclomatic number, $C(G')=C(G)$.] For the example shown in Fig. 2 Eq. (3.5) becomes

$$Z_2(G')=4\pi\sum_{l_1l_2l_3}\sum_{m_1m_2m_3}\lambda_{l_1}(K_1)\lambda_{l_2}(K_2)\lambda_{l_3}(K_3)\times\int_{\Omega}Y_{l_1m_1}(\theta,\phi)Y_{l_2m_2}(\theta,\phi)Y_{l_3m_3}(\theta,\phi)d\Omega\times\int_{\Omega}Y_{l_1m_1}{}^{*}(\theta,\phi)Y_{l_2m_2}{}^{*}(\theta,\phi)Y_{l_3m_3}{}^{*}(\theta,\phi)d\Omega. \quad (3.6)$$

(c) $Z_N(G)$ is finally obtained by replacing each $\lambda_{l_i}(K_i)$ in Eq. (3.5) by a suitable product $\prod_{(p,q)}\lambda_{l_i}(K_{pq})$, where K_{pq} are the labels of edges in G which are incident at degree two vertices. For the example given above

$$\begin{aligned}&\lambda_{l_1}(K_1)\rightarrow\lambda_{l_1}(K_{12})\lambda_{l_1}(K_{23})\lambda_{l_1}(K_{34}),\\&\lambda_{l_2}(K_2)\rightarrow\lambda_{l_2}(K_{14}),\\&\lambda_{l_3}(K_3)\rightarrow\lambda_{l_3}(K_{15})\lambda_{l_3}(K_{54}).\end{aligned} \quad (3.7)$$

The above rules enable formal expressions for any star cluster partition function to be written down in terms of integrals of products of spherical harmonics.

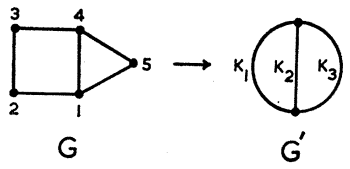

FIG. 2. An illustration of the suppression of degree 2 vertices.

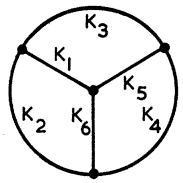

FIG. 3. The basic α graph.

4. APPLICATION OF THE $3n$-j SYMBOLS

The integral over three spherical harmonics, which is expressible in terms of the $3n$-j symbols of Wigner, is well known[13]:

$$\int_0^{2\pi}\int_0^{\pi} Y_{l_1m_1}(\theta,\phi)Y_{l_2m_2}(\theta,\phi)Y_{l_3m_3}(\theta,\phi)\sin\theta d\theta d\phi=\left[\frac{(2l_1+1)(2l_2+1)(2l_3+1)}{4\pi}\right]^{1/2}\begin{pmatrix}l_1 & l_2 & l_3\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_1 & l_2 & l_3\\ m_1 & m_2 & m_3\end{pmatrix}. \quad (4.1)$$

Little work appears to have been done on integrals over four or more spherical harmonics. Suppose we have an integral over N spherical harmonics, then the formula

$$Y_{l_1m_1}(\theta,\phi)Y_{l_2m_2}(\theta,\phi)=\sum_{lm}\left[\frac{(2l_1+1)(2l_2+1)(2l+1)}{4\pi}\right]^{1/2}\begin{pmatrix}l_1 & l_2 & l\\ m_1 & m_2 & m\end{pmatrix}Y_{lm}^*(\theta,\phi)\begin{pmatrix}l_1 & l_2 & l\\ 0 & 0 & 0\end{pmatrix} \quad (4.2)$$

may be applied to any pair of spherical harmonics in the integrand, and the original integral becomes a sum of integrals over $(N-1)$ spherical harmonics. Repeated application of Eq. (4.2) yields a sum of products of 3-j symbols. In the case of four spherical harmonics we find that

$$\int_0^{2\pi}\int_0^{\pi} Y_{l_1m_1}(\theta,\phi)Y_{l_2m_2}(\theta,\phi)Y_{l_3m_3}(\theta,\phi)Y_{l_4m_4}(\theta,\phi)\sin\theta d\theta d\phi=(4\pi)^{-1}\sum_{lm}[(2l_1+1)(2l_2+1)(2l+1)^2(2l_3+1)(2l_4+1)]^{1/2}$$
$$\times(-1)^m\begin{pmatrix}l_1 & l_2 & l\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_3 & l_4 & l\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_1 & l_2 & l\\ m_1 & m_2 & m\end{pmatrix}\begin{pmatrix}l_3 & l_4 & l\\ m_3 & m_4 & -m\end{pmatrix}. \quad (4.3)$$

When the integrals in Eq. (3.5) have been evaluated, using the above results, it is usually possible to sum over *all* the summation variables $\{m_i\}$ using the sum rules, contraction formulas and orthogonality relations of the $3n$-j symbols.[14] Some examples are now given.

The expression (3.6), for the partition function of the graph G' shown in Fig. 2, may be reduced, using Eq. (4.1) and (2.8), to

$$Z_2(G')=\sum_{l_1l_2l_3}\prod_{i=1}^{3}\lambda_{l_i}(K_i)(2l_i+1)\begin{pmatrix}l_1 & l_2 & l_3\\ 0 & 0 & 0\end{pmatrix}^2\sum_{m_1m_2m_3}(-1)^{m_1+m_2+m_3}\begin{pmatrix}l_1 & l_2 & l_3\\ m_1 & m_2 & m_3\end{pmatrix}\begin{pmatrix}l_1 & l_2 & l_3\\ -m_1 & -m_2 & -m_3\end{pmatrix}. \quad (4.4)$$

From the symmetry properties and orthogonality properties of the 3-j symbol we find

$$Z_2(G')=\sum_{l_1l_2l_3}\prod_{i=1}^{3}(2l_i+1)\lambda_{l_i}(K_i)\begin{pmatrix}l_1 & l_2 & l_3\\ 0 & 0 & 0\end{pmatrix}^2. \quad (4.5)$$

Partition functions of graphs homeomorphic with G' can be immediately written down from Eq. (4.5).

As a second example we consider the basic 'suppressed' α graph[15] shown in Fig. 3. The application of Eqs. (3.5) and (4.1) to this graph gives

$$Z_4(\alpha)=\sum_{l_1\cdots l_6}\prod_{i=1}^{6}\lambda_{l_i}(K_i)(2l_i+1)\begin{pmatrix}l_1 & l_2 & l_3\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_1 & l_5 & l_6\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_4 & l_2 & l_6\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_4 & l_5 & l_3\\ 0 & 0 & 0\end{pmatrix}$$
$$\times\sum_{m_1\cdots m_6}\begin{pmatrix}l_1 & l_2 & l_3\\ m_1 & m_2 & m_3\end{pmatrix}\begin{pmatrix}l_1 & l_5 & l_6\\ -m_1 & -m_5 & m_6\end{pmatrix}\begin{pmatrix}l_4 & l_2 & l_6\\ m_4 & -m_2 & -m_6\end{pmatrix}\begin{pmatrix}l_4 & l_5 & l_3\\ -m_4 & m_5 & -m_3\end{pmatrix}\prod_{i=1}^{6}(-1)^{m_i}. \quad (4.6)$$

[13] See A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, New Jersey, 1957), p. 63.

[14] An excellent summary of the main results is given in M. Rotenberg, B. Rivins, N. Metropolis, and J. K. Wooten, *The 3-j and 6-j Symbols* (M.I.T. Press, Cambridge, Massachusetts, 1959).

[15] The notation for labeling the basic topological types of graphs is that given in M. F. Sykes, J. W. Essam, B. R. Heap, and B. J. Hiley, J. Math. Phys. 7, 1557 (1966).

TABLE I. Zero-field partition functions of the graphs shown in Fig. 3.

Graph G	$Z(G)$
γ	$\sum_{l_1\cdots l_5}\prod_{i=1}^{5}(2l_i+1)\lambda_{l_i}(K_i)\begin{pmatrix}l_1 & l_2 & l_5\\ 0 & 0 & 0\end{pmatrix}^2\begin{pmatrix}l_3 & l_4 & l_5\\ 0 & 0 & 0\end{pmatrix}^2$.
δ	$\sum_{l_1\cdots l_4}\prod_{i=1}^{4}(2l_i+1)\lambda_{l_i}(K_i)\sum_{l}(2l+1)\begin{pmatrix}l_1 & l_2 & l\\ 0 & 0 & 0\end{pmatrix}^2\begin{pmatrix}l_3 & l_4 & l\\ 0 & 0 & 0\end{pmatrix}^2$.
A	$\sum_{l_1\cdots l_9}\prod_{i=1}^{9}(2l_i+1)\lambda_{l_i}(K_i)\begin{pmatrix}l_1 & l_2 & l_3\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_4 & l_5 & l_6\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_7 & l_8 & l_9\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_1 & l_4 & l_7\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2 & l_5 & l_8\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_3 & l_6 & l_9\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix}l_1 & l_2 & l_3\\ l_4 & l_5 & l_6\\ l_7 & l_8 & l_9\end{Bmatrix}$.
B	$\sum_{l_1\cdots l_9}\prod_{i=1}^{9}(2l_i+1)\lambda_{l_i}(K_i)\begin{pmatrix}l_1 & l_2 & l_5\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_1 & l_3 & l_4\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2 & l_3 & l_9\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_6 & l_7 & l_9\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_4 & l_6 & l_8\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_5 & l_7 & l_8\\ 0 & 0 & 0\end{pmatrix}$ $\times\begin{Bmatrix}l_4 & l_5 & l_9\\ l_2 & l_3 & l_1\end{Bmatrix}\begin{Bmatrix}l_4 & l_5 & l_9\\ l_7 & l_6 & l_8\end{Bmatrix}\prod_{i=1}^{9}(-1)^{l_i}$.
N	$\sum_{l_1\cdots l_7}\prod_{i=1}^{7}(2l_i+1)\lambda_{l_i}(K_i)\begin{pmatrix}l_1 & l_2 & l_5\\ 0 & 0 & 0\end{pmatrix}^2\begin{pmatrix}l_3 & l_4 & l_6\\ 0 & 0 & 0\end{pmatrix}^2\begin{pmatrix}l_5 & l_6 & l_7\\ 0 & 0 & 0\end{pmatrix}^2$.
O	$\sum_{l_1\cdots l_6}\prod_{i=1}^{6}(2l_i+1)\lambda_{l_i}(K_i)\sum_{l}(2l+1)\begin{pmatrix}l_1 & l_2 & l\\ 0 & 0 & 0\end{pmatrix}^2\begin{pmatrix}l_3 & l_4 & l\\ 0 & 0 & 0\end{pmatrix}^2\begin{pmatrix}l_5 & l_6 & l\\ 0 & 0 & 0\end{pmatrix}^2$.

Using the symmetry properties of the 3-j symbol and the definition of the 6-j symbol it is found that

$$Z_4(\alpha)=\sum_{l_1\cdots l_6}\prod_{i=1}^{6}\lambda_{l_i}(K_i)(2l_i+1)(-1)^{l_4+l_5+l_6}\begin{pmatrix}l_1 & l_2 & l_3\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_1 & l_5 & l_6\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_4 & l_2 & l_6\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_4 & l_5 & l_3\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix}l_1 & l_2 & l_3\\ l_4 & l_5 & l_6\end{Bmatrix}. \tag{4.7}$$

Similar methods have been used to calculate the partition functions of all topologically distinct types of graphs with cyclomatic number $C(G)\leqslant 4$. (A total of 23 graph types are involved.) We list in Table I the partition functions of the finite graphs shown in Fig. 4 as further examples.

The partition functions of finite star graphs for the "planar" classical Heisenberg model can be evaluated using the rules (a), (b), and (c), except that (3.5) is now replaced by

$$Z_{N'}(G')=\sum_{\{l_i\}=-\infty}^{\infty}\prod_{i}\lambda_{l_i}(K_i)\prod_{\binom{\text{all vertices}}{v\text{ in }G'}}\left[\int_0^{2\pi}\{\prod_{\delta}\exp(il_\delta\phi)\}\frac{d\phi}{2\pi}\right]. \tag{4.8}$$

The definition of the product $\prod_\delta$ and the assignment of the complex conjugates is the same as in (3.5). For example the application of Eq. (4.8) to the graph G', shown in Fig. 2, leads to

$$Z_2(G')=\sum_{-\infty}^{\infty}{}_{l_1l_2}\lambda_{l_1}(K_1)\lambda_{l_2}(K_2)\lambda_{l_1+l_2}(K_3), \tag{4.9}$$

where

$$\lambda_n(K)=I_n(K). \tag{4.10}$$

The techniques developed above can in principle be easily extended to deal with the case $H\neq 0$, although the calculations soon become complicated. To describe a cluster of spins in a field we must extend the definition of the graph respresentation. A labeled vertex H is introduced and the interaction of a spin $\mathbf{s}_j$ with the field is represented by a dotted edge joining vertex j to vertex H. The partition function of a separated cluster in a field is still equal to the product of the partition functions of the connected components, but for a connected reducible cluster in a field this "product" property no longer holds.

To find the partition function of a cluster G in a field, we draw the dotted edge graph, label the dotted lines with $L=\beta mH$ and treat the whole graph as a zero field graph of interacting spins. This general result is seen by writing the spin-field interaction as $mH\mathbf{s}_H\cdot\mathbf{s}_i$, where $\mathbf{s}_H$ is a unit vector in the field direction. An example is given in Fig. 5. After suppressing the degree two vertices in the dotted line graph of Fig. 5 we obtain a γ graph. The partition function of a chain of 4 spins in a field can therefore be written down from Table I as

$$Z=\sum_{l_1\cdots l_5}\lambda_{l_1}(L)\lambda_{l_2}(L)\lambda_{l_3}(L)\lambda_{l_4}(L)\lambda_{l_1}(K_1)\lambda_{l_4}(K_3)\lambda_{l_5}(K_2)\begin{pmatrix}l_1 & l_2 & l_5\\ 0 & 0 & 0\end{pmatrix}^2\begin{pmatrix}l_3 & l_4 & l_5\\ 0 & 0 & 0\end{pmatrix}^2\prod_{i=1}^{5}(2l_i+1). \tag{4.11}$$

An alternative direct method of evaluating partition functions in a field is to use the field direction as a polar axis for the spherical polar coordinates of the spins. The application of the expansion

$$\exp(L\cos\theta_i)=\sum_q \lambda_q(L)(2q+1)^{1/2}(4\pi)^{1/2}Y_{q0}(\theta_i,\phi_i)\,, \tag{4.12}$$

enables the following general expression to be obtained for the partition function of any graph G in a field:

$$Z_N(G)=(4\pi)^{C(G)-1+\frac{1}{2}N}\sum_{\{l_i\}}\sum_{\{m_i\}}\prod_i \lambda_{l_i}(K_i)\sum_{\{q_i\}=0}^{\infty}\prod_{i=1}^{N}(2q_i+1)^{1/2}\lambda_{q_i}(L)$$
$$\times\prod_{(\substack{\text{all vertices}\\ v_i \text{ in } G})}\left[\int_\Omega\{\prod_\delta Y_{l_\delta m_\delta}(\theta,\phi)\}Y_{q_i0}(\theta,\phi)d\Omega\right]. \tag{4.13}$$

The graph G is the "full" edge graph with N-spin vertices. The notation in Eq. (4.13) is similar to that in Eq. (3.5) except that each spin vertex v_i is now associated with a new summation variable q_i. As an example we apply Eq. (4.13) to the triangular cluster shown in Fig. 6. It is found using Eq. (4.1) that

$$Z_3(G)=\sum_{l_1l_2l_3}\sum_{q_1q_2q_3}\prod_{i=1}^{3}(2l_i+1)(2q_i+1)\lambda_{l_i}(K_i)\lambda_{q_i}(L)\begin{pmatrix}l_1 & l_3 & q_1\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_1 & l_2 & q_2\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_2 & l_3 & q_3\\ 0 & 0 & 0\end{pmatrix}$$
$$\times\sum_\nu(-1)^{3\nu}\begin{pmatrix}q_1 & l_1 & l_3\\ 0 & \nu & -\nu\end{pmatrix}\begin{pmatrix}l_2 & q_3 & l_3\\ -\nu & 0 & \nu\end{pmatrix}\begin{pmatrix}l_2 & l_1 & q_2\\ \nu & -\nu & 0\end{pmatrix}. \tag{4.14}$$

The last summation is performed using the standard result[14]:

$$\sum_\nu(-1)^{3\nu}\begin{pmatrix}q_1 & l_1 & l_3\\ 0 & \nu & -\nu\end{pmatrix}\begin{pmatrix}l_2 & q_3 & l_3\\ -\nu & 0 & \nu\end{pmatrix}\begin{pmatrix}l_2 & l_1 & q_2\\ \nu & -\nu & 0\end{pmatrix}=\begin{pmatrix}q_1 & q_2 & q_3\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix}q_1 & q_3 & q_2\\ l_2 & l_1 & l_3\end{Bmatrix}(-1)^{l_1+l_2+l_3}. \tag{4.15}$$

We finally obtain

$$Z_3(G)=\sum_{l_1l_2l_3}\sum_{q_1q_2q_3}\prod_{i=1}^{3}(2l_i+1)(2q_i+1)\lambda_{l_i}(K_i)\lambda_{q_i}(L)(-1)^{l_1+l_2+l_3}\begin{pmatrix}l_1 & l_3 & q_1\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_1 & l_2 & q_2\\ 0 & 0 & 0\end{pmatrix}$$
$$\times\begin{pmatrix}l_2 & l_3 & q_3\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}q_1 & q_2 & q_3\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix}q_1 & q_3 & q_2\\ l_2 & l_1 & l_3\end{Bmatrix}, \tag{4.16}$$

which is the partition function of an α graph (4.7) with various $K_i=L$. This would be expected from the discussion above, since the dotted line graph for the triangle is an α graph.

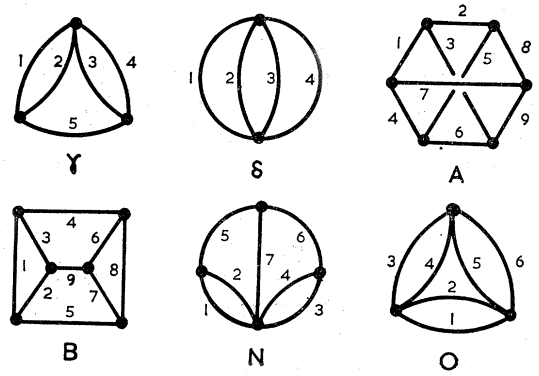

FIG. 4. Some basic topological types of graphs with $C(G)\leqslant 4$.

The Bethe-Peierls-Weiss approximation, when applied to the classical Heisenberg model, leads to integrals which can be evaluated using the methods discussed above. The approximation treats the interaction of a central spin $\mathbf{s}_0$ with its nearest-neighbor spins $\mathbf{s}_i$ $(i=1\cdots q)$ exactly and represents the interaction of the spins $\mathbf{s}_i$ with the rest of the crystal by an internal field $\mathbf{H}_1$ (which is assumed parallel to the external field $\mathbf{H}$). The Hamiltonian (1.1) is replaced by the cluster Hamiltonian

$$\mathcal{H}_{cl}=-2J\sum_{i=1}^{q}\mathbf{s}_0\cdot\mathbf{s}_i-m\mathbf{H}\cdot\mathbf{s}_0-m\mathbf{H}_1\cdot\sum_{i=1}^{q}\mathbf{s}_i. \tag{4.17}$$

Following Brown and Luttinger[9] we can write the cluster partition function as

$$Z_{cl}=\int_{\Omega_0}(d\Omega_0/4\pi)[\exp(L\cos\theta_0)]D^q, \tag{4.18}$$

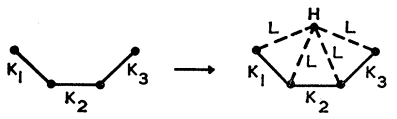

FIG. 5. An example showing the graphical representation of a finite cluster of spins in a field.

where

$$D=\int_{\Omega_i}(d\Omega_i/4\pi)\exp(K\mathbf{s}_0\cdot\mathbf{s}_i+L_1\cos\theta_i), \quad (4.19)$$

and $L_1=\beta mH_1$. The field direction has been taken as the polar axis. The basic integral (4.19) is evaluated using Eqs. (2.9), (2.10), and (4.12) which gives

$$D=\sum_l (2l+1)\lambda_l(K)\lambda_l(L_1)P_l(\cos\theta_0). \quad (4.20)$$

The application of the expansion (4.12) to the integrand of (4.18) enables Z_{cl} to be evaluated. For the one-dimensional lattice it is found that

$$Z_{cl}=\sum_{l_1l_2l_3}(2l_1+1)(2l_2+1)(2l_3+1)\lambda_{l_1}(L_1)\lambda_{l_1}(K)\times\lambda_{l_2}(L_1)\lambda_{l_2}(K)\lambda_{l_3}(L)\begin{pmatrix}l_1 & l_2 & l_3\\ 0 & 0 & 0\end{pmatrix}^2. \quad (4.21)$$

The internal field H_1 is determined by a self-consistent procedure.[9]

5. SUSCEPTIBILITY OF FINITE CLUSTERS

The most convenient method for calculating the zero-field susceptibility

$$\chi_N(G)=\lim_{H\to 0} kT(\partial^2/\partial H^2)\ln Z_N(G) \quad (5.1)$$

of a finite graph G is to use the fluctuation relation

$$(3kT/m^2N)\chi_N(G)=1+(2/N)\sum_{(ij)}\langle\mathbf{s}_i\cdot\mathbf{s}_j\rangle, \quad (5.2)$$

where the spin correlation function $\langle\mathbf{s}_i\cdot\mathbf{s}_j\rangle$ is defined by

$$\langle\mathbf{s}_i\cdot\mathbf{s}_j\rangle=Z_N^{-1}(G)\int_{\Omega_1}\cdots\int_{\Omega_N}\mathbf{s}_i\cdot\mathbf{s}_j\exp(-\beta\mathcal{H})\times\prod_{i=1}^{N}(d\Omega_i/4\pi), \quad (5.3)$$

and the summation in (5.2) is taken over all pairs of vertices in the graph G. The results $\langle s_i^z s_j^z\rangle=\frac{1}{3}\langle\mathbf{s}_i\cdot\mathbf{s}_j\rangle$ and $\langle(s_i^z)^2\rangle=\frac{1}{3}$ have been used in the derivation of (5.2).

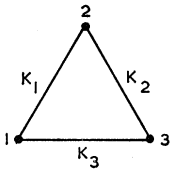

FIG. 6. A triangular cluster of spins.

The spin correlation function, between two spins i and j in a graph G, is readily determined by introducing an interaction edge K_{ij} between the vertices i and j. If $Z_N(G_{ij})$ is the partition function, in zero field, of the resulting graph G_{ij} then

$$\langle\mathbf{s}_i\cdot\mathbf{s}_j\rangle=\lim_{K_{ij}\to 0}(\partial/\partial K_{ij})\ln Z_N(G_{ij}). \quad (5.4)$$

When there is a *direct* interaction edge between the vertices i and j in the graph G, the introduction of a further edge K_{ij} is not necessary. The zero-field partition functions $Z_N(G_{ij})$ are calculated using the methods of Secs. 3 and 4.

To find the correlation function between two spins i and j on a ring of N spins we require the partition function of the graph G_{ij} shown in Fig. 7, which can be written down from Eq. (4.5) as

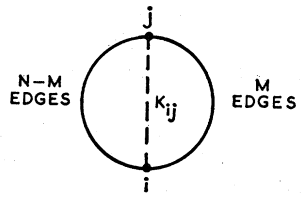

FIG. 7. The graph G_{ij} whose partition function is required for the calculation of the correlation function $\langle\mathbf{s}_i\cdot\mathbf{s}_j\rangle$ in a ring of N spins.

$$Z_N(G_{ij})=\sum_{l_1l_2l_3}(2l_1+1)(2l_2+1)(2l_3+1)\lambda_{l_1}{}^M(K)\times\lambda_{l_2}{}^{N-M}(K)\lambda_{l_3}(K_{ij})\begin{pmatrix}l_1 & l_2 & l_3\\ 0 & 0 & 0\end{pmatrix}^2. \quad (5.5)$$

The application of Eq. (5.4) to Eq. (5.5) gives

$$\langle\mathbf{s}_i\cdot\mathbf{s}_j\rangle=Z_N^{-1}(G)\sum_{l_1l_2}(2l_1+1)(2l_2+1)\lambda_{l_1}{}^M(K)\lambda_{l_2}{}^{N-M}(K)\times\begin{pmatrix}l_1 & l_2 & 1\\ 0 & 0 & 0\end{pmatrix}^2. \quad (5.6)$$

We substitute Eq. (5.6) in Eq. (5.2) and simplify the resulting expression using the formula[14]

$$\begin{aligned}\begin{pmatrix}l & l+1 & 1\\ 0 & 0 & 0\end{pmatrix}^2&=\begin{pmatrix}l+1 & l & 1\\ 0 & 0 & 0\end{pmatrix}^2\\ &=(l+1)/(2l+1)(2l+3), \quad (5.7)\\ &=0, \quad \text{otherwise}.\end{aligned}$$

The final result, for the susceptibility of a ring of N spins, is

$$(3kT/m^2N)\chi_N(G)=1+\Big[\sum_{l=0}^{\infty}(2l+1)\lambda_l{}^N(K)\Big]^{-1}2\sum_{l=0}^{\infty}(l+1)\times\left[\frac{\lambda_l(K)\lambda_{l+1}{}^N(K)-\lambda_{l+1}(K)\lambda_l{}^N(K)}{\lambda_{l+1}(K)-\lambda_l(K)}\right]. \quad (5.8)$$

In the thermodynamic limit $N\to\infty$ we obtain

$$\lim_{N\to\infty}(3kT/m^2N)\chi_N(G)=[1+u(K)]/[1-u(K)], \quad (5.9)$$

which is the result derived by Fisher[1] for an open chain of $N+1$ spins.

For the "planar" classical Heisenberg model, with the external field in the plane of the spins, it can be shown that the zero-field susceptibility in one dimension is given by

$$\lim_{N\to\infty}(2kT/m^2N)\chi_N=[I_0(K)+I_1(K)]/[I_0(K)-I_1(K)]. \quad (5.10)$$

The ferromagnetic susceptibility diverges as $1/T$ as $T\to 0$, whereas the susceptibility of the usual classical spin model (5.9) diverges as $1/T^2$.

The correlation function between two spins in a reducible graph can be evaluated in terms of star graph correlation functions. Suppose we have a reducible graph G made up of n star graphs $G^{(1)}\cdots G^{(n)}$ linked together by articulation points then the correlation function between two spins $\mathbf{s}_i$ and $\mathbf{s}_j$ in the same star component $G^{(r)}$ is independent of the other star graphs and is given by

$$\langle \mathbf{s}_i\cdot\mathbf{s}_j\rangle=\lim_{K_{ij}\to 0}(\partial/\partial K_{ij})\ln Z(G_{ij}{}^{(r)}). \quad (5.11)$$

This result is readily seen by applying (5.4) to the graph G_{ij}.

If we have a reducible cluster G consisting of two star graphs G_1 and G_2 linked by an articulation point then it can be shown from (5.3), using the spin $\mathbf{s}_0$ at the articulation point as a polar axis, that the correlation function between two spins $\mathbf{s}_i$ and $\mathbf{s}_j$ in the graphs G_1 and G_2, respectively, can be written as

$$\langle \mathbf{s}_i\cdot\mathbf{s}_j\rangle_G=\langle \mathbf{s}_i\cdot\mathbf{s}_0\rangle_{G_1}\langle \mathbf{s}_j\cdot\mathbf{s}_0\rangle_{G_2}. \quad (5.12)$$

This result can be simply generalized to deal with correlation functions in a reducible graph with more than two star-graph components. We see therefore that a knowledge of the star-graph correlation functions enables the zero-field susceptibility of reducible and star graphs to be calculated. These correlation functions are calculated from the partition functions of star graphs using Eq. (5.4). For example, to find the susceptibility of the general θ graph (shown in Fig. 2 as the graph G') we require three distinct types of correlation functions,[15a] which can be calculated from the zero-field partition functions of the three graphs shown in Fig. 8. The graphs (a), (b), and (c) are α, γ, and δ graphs, respectively, and their partition functions can be written down from Eq. (4.7) and Table I.

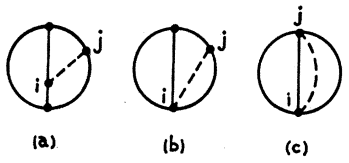

FIG. 8. The graphs (a), (b), and (c) are those whose partition functions are required for the calculation of correlation functions in a θ graph.

6. PERTURBATION SERIES FOR THE ANISOTROPIC MODEL IN ONE DIMENSION

In this Section we derive a perturbation series for the zero-field free energy of the one-dimensional classical Heisenberg model, with small anisotropy, using the isotropic model as the unperturbed system. We consider an open chain of $N+1$ spins and take N to be large so that finite size effects can be ignored. The Hamiltonian is written in the form

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_1, \quad (6.1)$$

where

$$\mathcal{H}_0=-\sum_{i=0}^{N-1}2J\mathbf{s}_i\cdot\mathbf{s}_{i+1}, \quad (6.2)$$

$$\mathcal{H}_1=-\sum_{i=0}^{N-1}2J(\gamma-1)s_i{}^z s_{i+1}{}^z, \quad (6.3)$$

and $(\gamma-1)$ is small. The free energy is

$$-\beta F_{N+1}=-\beta F^{(0)}-\beta F^{(1)}, \quad (6.4)$$

where

$$-\beta F^{(0)}=N\ln[(\sinh K)/K], \quad (6.5)$$

$$-\beta F^{(1)}=\ln\langle\exp(-\beta\mathcal{H}_1)\rangle_0, \quad (6.6)$$

and $\langle A\rangle_0$ denotes the average

$$\langle A\rangle_0=\int_{\Omega_0}\cdots\int_{\Omega_N}\prod_{i=0}^{N}\left(\frac{d\Omega_i}{4\pi}\right)A\exp(-\beta\mathcal{H}_0)\Big/\int_{\Omega_0}\cdots\int_{\Omega_N}\prod_{i=0}^{N}\left(\frac{d\Omega_i}{4\pi}\right)\exp(-\beta\mathcal{H}_0). \quad (6.7)$$

The method developed by Horwitz and Callen[16] for deriving the high-temperature series expansion of the free energy of the Ising model can now be applied to expand $-\beta F^{(1)}$ in powers of $(\gamma-1)$. It is found

$$-\beta F^{(1)}=\sum_{\{p_{i,i+1}\}}\Big[\prod_{i=0}^{N-1}(p_{i,i+1}!)^{-1}(K\delta)^{p_{i,i+1}}\Big]M_{\{p_{i,i+1}\}}, \quad (6.8)$$

where $\delta=\gamma-1$. The summation in Eq. (6.8) is taken over all sets of non-negative integers $p_{i,i+1}$ and $M_{\{p_{i,i+1}\}}$ is conveniently generated by

$$M_{\{p_{i,i+1}\}}=\lim_{\{\alpha_{i,i+1}\}\to 0}\prod_{i=0}^{N-1}(D_{i,i+1})^{p_{i,i+1}}\times\ln\Big\langle\prod_{i=0}^{N-1}\exp(\alpha_{i,i+1}s_i{}^z s_{i+1}{}^z)\Big\rangle_0, \quad (6.9)$$

[15a] *Note added in proof.* Four distinct types of correlation function are in fact needed. The omitted correlation function can be found from the partition function of a β graph. (The definition of a β graph is given in Ref. 15.)

[16] G. Horwitz and H. B. Callen, Phys. Rev. 124, 1757 (1961).

where $D_{i,i+1}=\partial/\partial\alpha_{i,i+1}$. Each term in Eq. (6.8) corresponding to a particular set $\{p_{i,i+1}\}$ is given a graphical representation by drawing $p_{i,i+1}$ edges between the nearest-neighbor pair $(i, i+1)$ for each integer $p_{i,i+1}$ in the set.

It is usual when deriving perturbation expansions in the theory of ferromagnetism to take a lattice of noninteracting spins in a field as the unperturbed system. In this case a considerable simplification occurs and only linked graphs contribute to the free-energy expansion. The unperturbed system in our case consists of interacting spins and separated or unlinked graphs also contribute to Eq. (6.8).

It is convenient to group all graphs with the same topology together. The different topological types of graph with n edges are labeled (n,t) where $t=1, 2, \cdots$. We can write

$$\prod_{i=0}^{N-1}(p_{i,i+1}!)^{-1}=P_{(n,t)}, \tag{6.10}$$

since this product is the same for all graphs in the set (n,t). Using this graphical representation, Eq. (6.8) becomes

$$-\beta F^{(1)}=\sum_{(n,t)}(K\delta)^n P_{(n,t)}\sum_{\{p_{i,i+1}\}}M_{\{p_{i,i+1}\}}, \tag{6.11}$$

where the second summation is taken over all sets of integers $\{p_{i,i+1}\}$ which give graphs in the set (n,t).

All *linked* graphs in the set (n,t) have the same graph cumulant, which we denote by $M_{(n,t)}$. But $M_{\{p_{i,i+1}\}}$ is not the same for all *unlinked* graphs in the set (n,t). We therefore label the graphs in the set (n,t) by $G_q^{n,t}$, where $q=1, 2, \cdots$, and define the graph cumulant for the graph $G_q^{n,t}$ by $M(G_q^{n,t})$. We can rewrite Eq. (6.11) as

$$-\beta F^{(1)}=2N\sum_{\substack{(n,t)\\ \text{linked}}}(\delta K)^n W_{(n,t)}^{-1}M_{(n,t)}P_{(n,t)} + \sum_{\substack{(n,t)\\ \text{unlinked}}}(\delta K)^n P_{(n,t)}\sum_q M(G_q^{n,t}), \tag{6.12}$$

where $W_{(n,t)}$ is the number of ways in which the vertices of a graph in the set (n,t) can be labeled keeping the connectivity of the graph unaltered. The contributing sets of graphs for $n\leqslant 3$ are shown in Fig. 9.

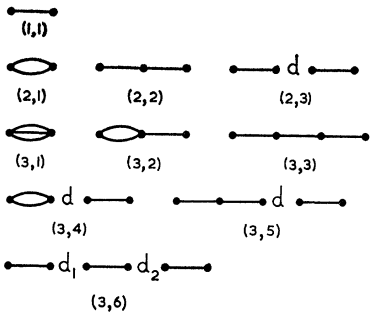

FIG. 9. The sets of graphs $n\leq 3$ which contribute to the perturbation series for the free energy of the one-dimensional anisotropic classical Heisenberg model.

The cumulant for the graph set (1,1), which can be found from Eq. (6.9), is

$$M_{(1,1)}=\langle s_i^z s_{i+1}^z\rangle_0. \tag{6.13}$$

This nearest-neighbor correlation function was evaluated by Fisher[1] as $\frac{1}{3}u(K)$. Thus for large N

$$-\beta F_N/N=\ln[(\sinh K)/K]+\tfrac{1}{3}\delta K u(K)+0(\delta^2). \tag{6.14}$$

The second-order graph cumulants are

$$\begin{aligned}
M_{(2,1)}&=\langle(s_i^z)^2(s_{i+1}^z)^2\rangle_0-\langle s_i^z s_{i+1}^z\rangle_0^2,\\
M_{(2,2)}&=\langle s_i^z(s_{i+1}^z)^2 s_{i+2}^z\rangle_0-\langle s_i^z s_{i+1}^z\rangle_0\langle s_{i+1}^z s_{i+2}^z\rangle_0,\\
M_{(2,3)}&=\langle s_i^z s_{i+1}^z s_j^z s_{j+1}^z\rangle_0-\langle s_i^z s_{i+1}^z\rangle_0\langle s_j^z s_{j+1}^z\rangle_0.
\end{aligned} \tag{6.15}$$

The higher-order correlation functions in (6.15) can be evaluated using the methods discussed in Secs. 2 and 3. For example, to calculate the correlation function required for $M_{(2,1)}$ we perform the integrations over all spins $j<i$ and $j>i+1$, leaving

$$\langle(s_i^z)^2(s_{i+1}^z)^2\rangle_0=\lambda_0^{-1}(K)\int_{\Omega_i}\int_{\Omega_{i+1}}d\Omega_i d\Omega_{i+1}(4\pi)^{-2} \times\cos^2\theta_i\cos^2\theta_{i+1}\exp(K\cos\Theta_{i,i+1}). \tag{6.16}$$

The polar axis for the spherical polar coordinates has been taken in an arbitrary direction. After applying the expansion (2.9) to Eq. (6.16) the integrations can be readily performed. We find

$$M_{(2,1)}=\tfrac{1}{9}(1-u_1^2+\tfrac{4}{5}u_2), \tag{6.17}$$

where $u_n=\lambda_n(K)/\lambda_0(K)$. A similar procedure enables the other cumulants in Eq. (6.15) to be evaluated as

$$M_{(2,2)}=(4/45)u_1^2, \tag{6.18}$$

$$M_{(2,3)}=(4/45)u_1^2u_2^d, \tag{6.19}$$

where $d=1, 2, \cdots$ is the number of edges between the two components of the unlinked graph (2,3). The summation over all unlinked graphs in the set (2,3) is

$$\sum_q M(G_q^{2,3})=(4N/45)u_1^2\sum_{d=1}^{\infty}u_2^d. \tag{6.20}$$

The substitution of (6.18), (6.19) and (6.20) in (6.12) leads to

$$-\beta F_N/N=\ln[(\sinh K)/K]+\tfrac{1}{3}\delta K u_1+(1/90)(\delta K)^2 \times(1-u_2)^{-1}(5-u_2+3u_1^2-4u_2^2+5u_1^2u_2). \tag{6.21}$$

We list below the graph cumulants for the third-order graphs shown in Fig. 9:

$$\begin{aligned}
M_{(3,1)}&=(2/4725)(21u_1+54u_3+175u_1^3-210u_1u_2),\\
M_{(3,2)}&=(20/4725)(7u_1+11u_1u_2-14u_1^3),\\
M_{(3,3)}&=(4/4725)(27u_1^2u_3+28u_1^3-35u_1^3u_2),\\
M_{(3,4)}&=u_2^d M_{(3,2)},\\
M_{(3,5)}&=u_2^d M_{(3,3)},\\
M_{(3,6)}&=u_2^{d_1+d_2}M_{(3,3)}.
\end{aligned} \tag{6.22}$$

We find on substituting (6.22) in Eq. (6.12) that the third-order term in the perturbation series is

$$(1/14175)(K\delta)^3(1-u_2)^{-2}[441u_1+54u_3-12u_1u_2-329u_1^3 -108u_2u_3-219u_1u_2^2+70u_1^3u_2+324u_1^2u_3 +54u_2^2u_3+175u_1^3u_2^2-210u_1u_2^3]. \quad (6.23)$$

The perturbation series for the energy per spin

$$(E_N/N)=-2J(\partial/\partial K)(-\beta F_N/N) \quad (6.24)$$

derived from Eqs. (6.21) and (6.23) breaks down at low temperatures indicating that $E_N(K,\delta)$ cannot be expanded as a Taylor series in δ when $T=0$. It is interesting to compare these results with those obtained by Katsura and Inawashiro[17] for the one-dimesnional spin-$\frac{1}{2}$ anisotropic Heisenberg model. A linked cluster series in powers of γ, where γ is small, was developed by these authors and detailed calculations were performed up to third order in γ. The perturbation series gave results for the ground-state energy of the system which were in good agreement with known exact results.

A partial check on the above results can be made by deriving terms in the high-temperature series of the anisotropic classical Heisenberg model.

7. DIAGRAM EXPANSIONS FOR CLASSICAL ANISOTROPIC HEISENBERG MODEL

We derive in this section a high-temperature series expansion for the free energy of the anisotropic Heisenberg model by generalizing the method used by Horwitz and Callen[16] for the Ising model. The Hamiltonian is written as

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_1, \quad (7.1)$$

where

$$\mathcal{H}_0=-mH\sum_{i=1}^{N}s_i^z \quad (7.2)$$

and

$$\mathcal{H}_1=-\sum_{(ij)}\sum_{\epsilon}2J_{ij}^{\epsilon}s_i^{\epsilon}s_j^{\epsilon}. \quad (7.3)$$

In the second summation of (7.3), ϵ runs over the x, y and z components of the spin vectors. (The following derivation is not restricted to one-dimensional systems or nearest-neighbor interactions.) The free energy can be expressed in the form

$$-\beta F_N=N\ln[(\sinh L)/L]-\beta F_N^{(1)}, \quad (7.4)$$

where

$$-\beta F_N^{(1)}\ln\langle\exp(-\beta\mathcal{H}_1)\rangle_0, \quad (7.5)$$

and $\langle A\rangle_0$ denotes the average given in (6.7). We now introduce three parameters α_{ij}^{ϵ}, with $\epsilon=x$, y and z, for each pair of spins (ij) in the lattice and rewrite (7.5) as

$$-\beta F_N^{(1)}=\lim_{\{\alpha_{ij}^{\epsilon}\}\to 0}\ln\langle\exp\sum_{(ij)}\sum_{\epsilon}(2J_{ij}^{\epsilon}\beta+\alpha_{ij}^{\epsilon})s_i^{\epsilon}s_j^{\epsilon}\rangle_0. \quad (7.6)$$

[17] S. Katsura and S. Inawashiro, J. Math. Phys. 5, 1091 (1964).

Using the operator expression

$$\phi(2\beta J_{ij}+\alpha_{ij})=\exp(2\beta J_{ij}D_{ij})\phi(\alpha_{ij}), \quad (7.7)$$

where $D_{ij}=\partial/\partial\alpha_{ij}$, we find

$$-\beta F_N^{(1)}=\lim_{\{\alpha_{ij}^{\epsilon}\}\to 0}\prod_{\epsilon}[\exp(2\beta\sum_{(ij)}D_{ij}^{\epsilon}J_{ij}^{\epsilon})] \times\ln\langle\exp\sum_{(ij)}\sum_{\epsilon}\alpha_{ij}^{\epsilon}s_i^{\epsilon}s_j^{\epsilon}\rangle_0. \quad (7.8)$$

The three exponentials in the product of Eq. (7.8) are expanded as high-temperature series. The application of the multinomial theorem to the resulting expressions leads to

$$-\beta F_N^{(1)}=\lim_{\{\alpha_{ij}^{\epsilon}\}\to 0}\sum_{\{p_{ij}^x\}}\sum_{\{p_{ij}^y\}}\sum_{\{p_{ij}^z\}}\prod_{(ij)}\prod_{\epsilon}(2J_{ij}^{\epsilon}\beta)^{p_{ij}^{\epsilon}} \times(p_{ij}^{\epsilon}!)^{-1}\prod_{(ij)}\prod_{\epsilon}(D_{ij}^{\epsilon})^{p_{ij}^{\epsilon}} \times\ln\langle\prod_{(ij)}\prod_{\epsilon}\exp(\alpha_{ij}^{\epsilon}s_i^{\epsilon}s_j^{\epsilon})\rangle_0, \quad (7.9)$$

where the summations are taken over all possible sets of non-negative integers $\{p_{ij}^{\epsilon}\}$, $\epsilon=x$, y, and z. Each term in Eq. (7.9), corresponding to a particular choice of the sets $\{p_{ij}^{\epsilon}\}$, is represented by a *labeled* graph by drawing p_{ij}^x lines labeled x between i and j for all integers in $\{p_{ij}^x\}$ and repeating the procedure for the sets $\{p_{ij}^y\}$ and $\{p_{ij}^z\}$. It can be shown that unlinked or separated labeled graphs give zero contribution. (The method of proof follows that given by Horwitz and Callen[16] for the Ising model.)

We classify all the labeled graphs with a total number of n lines into sets of graphs (n,t) which have the same topology. The parameter t runs over all the different topologically distinct sets of labeled graphs with n lines. (In this classification the labeling of the edges must be taken into account.) For all graphs in the set (n,t) we can define

$$P_{(n,t)}=\prod_{(ij)}\prod_{\epsilon}(p_{ij}^{\epsilon}!)^{-1} \quad (7.10)$$

and

$$M_{(n,t)}=\lim_{\{\alpha_{ij}^{\epsilon}\}\to 0}\prod_{(ij)}\prod_{\epsilon}(D_{ij}^{\epsilon})^{p_{ij}^{\epsilon}} \times\ln\langle\prod_{(ij)}\prod_{\epsilon}\exp(\alpha_{ij}^{\epsilon}s_i^{\epsilon}s_j^{\epsilon})\rangle_0, \quad (7.11)$$

since these quantities are the same for all graphs in the set (n,t). [The notation used in Eqs. (7.10) and (7.11) should not be confused with that used in Sec. 6.]

The summations in Eq. (7.9) are replaced by a summation over all possible sets of labeled graphs (n,t) and it is found, using Eqs. (7.10) and (7.11), that

$$-\beta F_N^{(1)}=\sum_{(n,t)}(2\beta)^nP_{(n,t)}M_{(n,t)}W_{(n,t)}^{-1} \times\sum_{ijk\cdots}{}'\prod_{(ij)}\prod_{\epsilon}(J_{ij}^{\epsilon})^{p_{ij}^{\epsilon}}, \quad (7.12)$$

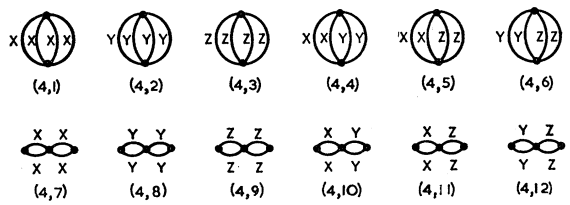

FIG. 10. The sets of fourth-order graphs which contribute to the high-temperature series expansion of the free energy of the one-dimensional anisotropic classical Heisenberg model.

where $W_{(n,t)}$ is the number of ways in which the vertices of a graph of the type (n,t) can be numbered 1, 2, $\cdots$ keeping the connectivity of the indices unaltered. (In the calculation of $W_{(n,t)}$ the labeling of the edges must be taken into account.) The summation indices in the second summation of Eq. (7.12) are restricted so that each term in the summation corresponds only to graphs in the set (n,t).

For nearest-neighbor interactions, with $J_{ij}^{\epsilon}=J^{\epsilon}$, we can simplify the lattice summation in Eq. (7.12) by following a procedure developed by Rushbrooke,[18] which involves the concept of graphs of a given *basic type*. Two graphs are said to be of the same basic type if they differ only in the *labeling* and multiplicities of their edges. The basic type of graph corresponding to a labeled graph of type (n,t) is obtained from the labeled graph by replacing all the multiple edges by single edges and ignoring the labeling of the edges. The basic graphs, with a total of m *edges*, are classified into sets of basic graphs (m,τ), which have the same topology.

We define $W_{(m,\tau)}$ to be the vertex labeling factor for the basic type of graph (m,τ) corresponding to the graph type (n,t), and $N_{(m,\tau)}$ to be the number of independent graphs of the type (m,τ) that can be made up of nearest-neighbor edges in a given lattice. It can be shown[19] from the above definitions that

$$\sum_{ijk,\cdots}{}' \prod_{(ij)} \prod_{\epsilon} (J_{ij}^{\epsilon})^{p_{ij}^{\epsilon}} = W_{(m,\tau)} N_{(m,\tau)} \prod_{\epsilon} (J^{\epsilon})^{n_{\epsilon}}, \quad (7.13)$$

where n_x, n_y, and n_z are the total number of x, y, and z edges, respectively, in a labeled graph of type (n,t). Thus Eq. (7.12) becomes

$$-\beta F_N^{(1)} = \sum_{(n,t)} (2\beta)^n \prod_{\epsilon} (J^{\epsilon})^{n_{\epsilon}} P_{(n,t)} M_{(n,t)} \times W_{(n,t)}^{-1} W_{(m,\tau)} N_{(m,\tau)}. \quad (7.14)$$

This expansion has been applied to the one-dimensional system for the case $J^x=J^y=J$ and $J^z=\gamma J$. The basic graphs for this system are just simple chains which have $N_{(m,\tau)}=N$ and $W_{(m,\tau)}=2$. The labeled sets of graphs for $n=4$ which contribute to the zero-field free-energy series in one dimension are shown in Fig. 10. The graph cumulants $M_{(n,t)}$ are calculated from Eq. (7.11) while $P_{(n,t)}$ and $W_{(n,t)}$ are found by inspection. For example, $P_{(4,4)}=(2!2!)^{-1}$ and $W_{(4,4)}=2$. We given below the final results for $n\leqslant 6$:

$$-\beta F_N/N = \sum_{n=1} a_{2n} K^{2n}, \quad (7.15)$$

where

$$\begin{aligned} a_2 &= (1/18)(2+\gamma^2), \\ a_4 &= (1/2700)(2-24\gamma^2+7\gamma^4), \\ a_6 &= (1/2679075)(107\gamma^6-636\gamma^4+1896\gamma^2-422). \end{aligned} \quad (7.16)$$

If we substitute $\gamma=1+\delta$ into (7.16), where δ is considered small, we find

$$\begin{aligned} a_2 &= [(1/6)+(1/9)\delta+(1/18)\delta^2], \\ a_4 &= [(-1/180)-(1/135)\delta+(1/150)\delta^2 \\ &\qquad +(7/675)\delta^3+\cdots], \\ a_6 &= [(1/2835)+(2/2835)\delta-(1/8505)\delta^2 \\ &\qquad -(404/2679075)\delta^3+\cdots]. \end{aligned} \quad (7.17)$$

These results can be checked by expanding the perturbation series (6.21) and (6.23) as a high-temperature series. Agreement was found.

A cluster series for the anisotropic Heisenberg model similar to that developed by Domb[5] and Domb and Wood[3] for the isotropic Heisenberg model is readily obtained from Eq. (7.14) using a method given by Rushbrooke.[18] We perform a formal partial summation over all sets of labeled graphs (n,t) which are of the same basic type (m,τ), and write Eq. (7.14) in the form

$$-\beta F_N^{(1)} = \sum_{(m,\tau)} N_{(m,\tau)} \phi_{(m,\tau)}(K^x,K^y,K^z,L), \quad (7.18)$$

where $K^{\epsilon}=2\beta J^{\epsilon}$ and

$$\phi_{(m,\tau)}(K^x,K^y,K^z,L) = \sum_{(n,t)} \prod_{\epsilon} (K^{\epsilon})^{n_{\epsilon}} P_{(n,t)} M_{(n,t)} W_{(n,t)}^{-1} W_{(m,\tau)}. \quad (7.19)$$

The summation in Eq. (7.19) is over all sets of graphs (n,t) which are of the same basic type (m,τ). The $\phi_{(m,\tau)}$ functions are found in terms of partition functions of finite clusters of spins by successively applying (7.18) to finite graphs. For the spin-$\frac{1}{2}$ isotropic Heisenberg model this method has provided a powerful method for calculating high-temperature series expansions.[3,4] For the classical anisotropic model the cluster series (7.19) is not very useful because of the difficulty of evaluating finite cluster partition functions with anisotropy present.

The diagram expansion (7.12) suffers from two disadvantages. The calculation of the graph cumulants soon becomes very tedious and the restrictions on the summation indices have to be carefully analyzed. Horwitz and Callen[16] avoided these difficulties for the Ising model by removing the restrictions on the lattice sums and expressing the graph cumulants as sums of

[18] G. S. Rushbrooke, J. Math. Phys. 5, 1106 (1964).
[19] For details see Ref. 18.

products of single-spin cumulants. A simpler diagrammatic expansion results. This procedure can be generalized to the anisotropic classical Heisenberg model. The single-spin cumulants $M(n_x,n_y,n_z)$ in this case are defined by

$$\ln\langle\exp(xs_i^x+ys_i^y+zs_i^z)\rangle_0 = \sum_{n_xn_yn_z}{}_0' \frac{x^{n_x}y^{n_y}z^{n_z}}{n_x!n_y!n_z!}M(n_x,n_y,n_z), \quad (7.20)$$

where the prime denotes the exclusion of the case $n_x=n_y=n_z=0$. It can be readily shown using the operator "trick" (7.7) that

$$M(n_x,n_y,n_z)=\lim_{\substack{\alpha_x\to 0,\alpha_y\to 0,\\ \alpha_z\to L}}\prod_\epsilon(\partial/\partial\alpha_\epsilon)^{n_\epsilon} \times\ln\int_{\Omega_i}\exp\Big(\sum_\epsilon\alpha_\epsilon s_i^\epsilon\Big)\Big(\frac{d\Omega_i}{4\pi}\Big). \quad (7.21)$$

By direct differentiation of Eq. (7.21) the single-spin average $\langle(s_i^x)^{\nu_1}(s_i^y)^{\nu_2}(s_i^z)^{\nu_3}\rangle_0$ can be expressed as a sum of products of single-spin cumulants. For example,

$$\begin{aligned}\langle s_i^x\rangle_0&=M(100),\\ \langle s_i^xs_i^y\rangle_0&=M(110)+M(100)M(010),\\ \langle s_i^xs_i^ys_i^z\rangle_0&=M(111)+M(001)M(110)+M(100)M(011)\\ &\quad+M(010)M(101)+M(100)M(010)M(001).\end{aligned} \quad (7.22)$$

We see therefore that the graph cumulants, defined by (7.11), are also expressible as sums of products of single-spin cumulants. When all the graph cumulants at a given order n have been expressed in terms of the single-spin cumulants and the restrictions on the summations in (7.12) have been removed it is found that the following rearranged diagram expansion results:

$$-\beta F_N^{(1)}=\sum_{(n,t)}(2\beta)^nP_{(n,t)}\tilde{M}_{(n,t)}W_{(n,t)}^{-1} \times\sum_{ijk\cdots}\prod_{(ij)}\prod_\epsilon(J_{ij}^\epsilon)^{p_{ij}\epsilon}, \quad (7.23)$$

where

$$\tilde{M}_{(n,t)}=\prod_v M(n_x^v,n_y^v,n_z^v). \quad (7.24)$$

At each vertex v of a graph in the set (n,t) we associate a single-spin cumulant $M(n_x^v,n_y^v,n_z^v)$, where n_x^v, n_y^v, and n_z^v are the number of edges labeled x, y, and z, respectively, which are incident at the vertex v. The product in Eq. (7.24) is taken over all vertices of a graph in the set (n,t). The lattice summation in Eq. (7.23) is, now *unrestricted* with $J_{ii}=0$. Although a proof of Eq. (7.23) can be given by generalizing the arguments of Horwitz and Callen,[16] it is simpler and more direct to follow the methods developed by Englert[20] and Stinchcombe *et al.*[21] This alternative approach has the advantage that expansions similar to Eq. (7.23) can be established for the spin correlation functions.

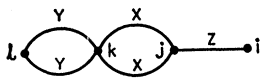

FIG. 11. Graphical representation of the term $(2\beta)^5\frac{1}{4}M(001)M(201)M(220)M(020)[\sum_l(J_{lk}{}^y)^2]\times[\sum_k(J_{jk}{}^x)^2][\sum_j(J_{ij}{}^z)]$.

An example is given in Fig. 11 of the graphical representation of a typical term in the linked graph expansion (7.23). The single-spin cumulants are conveniently found, in zero field or as a power series in the field, by evaluating the integral in Eq. (7.21) as

$$\int_{\Omega_i}(d\Omega_i/4\pi)\exp(\sum_\epsilon\alpha_\epsilon s_i^\epsilon)=(\sum_\epsilon\alpha_\epsilon{}^2)^{-1}\sinh(\sum_\epsilon\alpha_\epsilon{}^2). \quad (7.25)$$

Using a standard result we can write

$$M(n_x,n_y,n_z)=\lim_{\substack{\alpha_x\to 0,\alpha_y\to 0,\\ \alpha_z\to L}}\prod_\epsilon(\partial/\partial\alpha_\epsilon)^{n_\epsilon} \times\sum_{n=1}^\infty\frac{2^{2n-1}B_n(-1)^{n+1}}{n(2n)!}(\sum_\epsilon\alpha_\epsilon{}^2)^n, \quad (7.26)$$

where B_n are the Bernoulli numbers. In zero field it is seen that $M(n_x,n_y,n_z)=0$ if one or more of n_ϵ are odd. Thus the linked graphs which contribute to the zero-field free-energy series all have an *even* number of x, y, and z edges incident at each vertex. A similar result holds for the original expansion (7.12). The contributing graphs for $H\neq 0$ have an even number of x and y edges incident at every vertex and an arbitrary number of z edges.

The expansions (7.14) and (7.23) are at present being used to investigate the effects of anisotropy on the critical properties of the three-dimensional classical model. Diagram expansions similar to those given above can be derived for the "planar" anisotropic Heisenberg model defined in Sec. 2.

It should be pointed out that the expansion (7.14) is not very convenient for deriving series expansions for the isotropic model. This case can be treated in terms of unlabeled graphs by rewriting Eq. (7.6) in the form

$$-\beta F^{(1)}=\lim_{\{\alpha_{ij}\}\to 0}\ln\langle\exp\sum_{(ij)}(2J_{ij}\beta+\alpha_{ij})\mathbf{s}_i\cdot\mathbf{s}_j\rangle_0. \quad (7.27)$$

Analogous expressions to (7.12) and (7.14) can then be derived by repeating the arguments given above.

8. CONCLUDING REMARKS

It was stated in Sec. 1 that the cluster series method of Domb and Wood,[3] when combined with the results of Secs. 3 and 4, provides a powerful method of deriving high-temperature series expansions for the isotropic

[20] F. Englert, Phys. Rev. **129**, 567 (1963).
[21] R. B. Stinchcombe, G. Horwitz, F. Englert and R. Brout, Phys. Rev. **130**, 155 (1963).

classical Heisenberg model. We now discuss this application in more detail. The cluster series, which may be obtained from Eq. (7.18), is

$$\ln Z_N = N \ln[(\sinh L)/L] + \sum_{(m,\tau)} N_{(m,\tau)} \phi_{(m,\tau)}(K,L). \quad (8.1)$$

It has been shown that, in zero field, only star graphs contribute to this cluster series.[3,6] The $\phi_{(m,\tau)}(K,0)$ functions for these graphs are found in terms of partition functions of finite clusters by applying Eq. (8.1) to finite star graphs. For example, the application of Eq. (8.1) to a single edge gives $\phi_{(\backslash)}(K,0) = \ln\lambda_0(K)$, and the application to an n-sided polygon $(n)_p$ yields

$$\phi_{(n)_p} = \ln[1 + \sum_{l=1}^{\infty} (2l+1) u_l{}^n]. \quad (8.2)$$

For an $(r,s,t)_\theta$ graph[15] with r, s, and t edges along the three "bridges" (see graph G' in Fig. 2) we find, using Eq. (4.5), that

$$\phi_{(r,s,t)_\theta} = \ln\Bigg[\sum_{l_1 l_2 l_3}{}^{\infty}{}_{\theta} (2l_1+1)(2l_2+1)(2l_3+1) \times u_{l_1}{}^r u_{l_2}{}^s u_{l_3}{}^t \begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix}^2 \Bigg] - \phi_{(r+s)_p} - \phi_{(s+t)_p} - \phi_{(r+t)_p}. \quad (8.3)$$

Similar expressions can be found for the $\phi_{(m,\tau)}$ functions of graphs with higher cyclomatic number (such as α, β, δ graphs) by using the formulas given in Secs. 3 and 4.

A formal expression for the free energy which takes into account all star graphs with cyclomatic number $C(G) \leqslant 2$ is obtained by substituting Eqs. (8.2) and (8.3) into Eq. (8.1). We find

$$\ln Z_N = \tfrac{1}{2} N q \ln\lambda_0(K) + \sum_{n=3}^{\infty} N_{(n)_p} \phi_{(n)_p} + \sum_{r=1}^{\infty} \sum_{\substack{s=2 \\ (r \leqslant s \leqslant t)}}^{\infty} \sum_{t=2}^{\infty} N_{(r,s,t)_\theta} \phi_{(r,s,t)_\theta} + \cdots, \quad (8.4)$$

where q is the coordination number of the lattice, and the restrictions on the second summations ensure that the $(r,s,t)_\theta$ graphs are not "overcounted".

The $\phi_{(m,\tau)}(K,0)$ functions, when expanded as high-temperature series, have a leading term of $O(K^{m+\lambda_{(m,\tau)}})$, where $\lambda_{(m,\tau)} \geqslant 0$, is called the entry parameter[3] for a graph of the type (m,τ). (A simple general rule has been given for finding the entry parameters of the star graphs.)[6] Thus if the $\phi_{(m,\tau)}(K,0)$ functions, for all the star graphs which satisfy $m + \lambda_{(m,\tau)} \leqslant M$, are expanded to $O(K^M)$, then the high-temperature series expansion for $\ln Z_N$ is given correctly to $O(K^M)$. For example, the expansion of the expression

$$\ln Z_N = \tfrac{1}{2} N q \ln\lambda_0(K) + \sum_{n=3}^{6} N_{(n)_p} \phi_{(n)_p} + N_{(1,2,2)_\theta} \phi_{(1,2,2)_\theta} \quad (8.5)$$

gives the series for $\ln Z_N$ correct to $O(K^6)$.

The advantage of this approach over the usual Brout-Horwitz-Callen type of expansion (7.14) is that a computer can be used to perform the algebra required to expand expressions such as (8.4) and (8.5) into high-temperature series. Thus the detailed calculation of graph cumulants of multiple edge graphs is avoided.

A similar technique can be used to derive the high-temperature series expansion for the zero-field susceptibility. The cluster series in this case is

$$(3kT/m^2)\chi_N = N + \sum_{(m,\tau)} N_{(m,\tau)} g_{(m,\tau)}(K,0), \quad (8.6)$$

where

$$g_{(m,\tau)}(K,0) = \lim_{L \to 0} 3(\partial^2/\partial L^2) \phi_{(m,\tau)}(K,L). \quad (8.7)$$

The application of Eq. (8.6) to finite graphs enables the $g_{(m,\tau)}(K,0)$ functions to be expressed in terms of the zero-field susceptibility of finite clusters. The latter can be determined using the methods given in Sec. 5.

The high-temperature series expansions for the free energy and susceptibility (in zero field) of the isotropic classical Heisenberg model are at present being extended by the author in collaboration with R. G. Bowers, using the techniques discussed above. It is hoped to give the results in a future publication.[22]

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[22] Preliminary results for the specific heat and susceptibility series have already been published in G. S. Joyce and R. G. Bowers, Proc. Phys. Soc. (London) **89**, 776 (1966). The susceptibility series has also been extended independently by P. J. Wood and G. S. Rushbrooke using a different procedure. See Phys. Rev. Letters **17**, 307 (1966).