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Series expansion for an easy-plane spin-one ferromagnet

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Series for susceptibility and zero-field specific heat have been obtained to the fourth order in βJ or J/D for an easy-plane spin-one ferromagnet. The series expansions are for a general lattice and for exchange interaction of arbitrary range. The single-ion anisotropy is treated exactly. We outline the method of series expansion and discuss the critical quantities deduced from the series obtained.

I. INTRODUCTION

Single-ion anisotropies can have a fundamental influence on the behavior of a magnetic system,[1] and prevail in almost all physical systems with spin greater than one half. For systems with spin equal to one, the single-ion anisotropy consists of only second-order terms in spin operators. The uniaxial spin-one systems with one anisotropy parameter thus represent the simplest case for study. Commonly, the mean-field approximation is used in calculations of the thermodynamic quantities for such systems because of the complexities caused by the single-ion anisotropy terms. Only recently have some more advanced methods been extended to treat the simple anisotropy systems. Green's-function theory[2] and the high-temperature series-expansion method[3] have been successfully formulated and applied to the spin-one easy-axis ferromagnets. In this paper we extend the series expansion method to calculate the easy-plane (hard-axis) spin-one system.

The first five terms of the series for the susceptibility and the heat capacity have been found with the single-ion anisotropy treated exactly. An analysis of the susceptibility series yields the critical temperature as a function of the single-ion anisotropy. We show that outside the extremely narrow region where the critical temperature plunges to zero the accuracy of the critical temperatures is within a few percent of the exact values.

Recently, Lines[4] has computed the critical temperature for the uniaxial ferromagnets ($S=1$ to $\frac{7}{2}$) for both the easy-axis and the easy-plane cases using the correlated-effective-field approximation. While the values obtained by such approximation are much improved over the mean-field results, the errors involved can still be as large as 12% when compared with the high-temperature series estimates for the easy-axis case. For an easy-plane system, as we shall see, it is more important to obtain accurate values for the critical temperatures since T_c is reduced to zero for strengths of anisotropy exceeding a critical value.

An RPA Green's-function theory has been given by Egami and Brooks.[5] While the theory has provided much insight into the physics of the system, the validity of the decoupling scheme can only be justified *a posteriori.*

The series-expansion calculation which provides exact results for the coefficients of the series and estimates the critical parameters to high accuracy not only will be of value in its own right but also serve as a gauge for other approximate calculations. In the next section we introduce the spin-one easy-plane ferromagnet and summarize briefly the mean-field results. The series-expansion method which treats the single-ion anisotropy exactly is presented in Sec. III. The results of the series expansion as well as the analyses are presented in the fourth section.

II. SPIN-ONE EASY-PLANE FERROMAGNET

The Hamiltonian of the system is given by

$$\mathcal{H}=D\sum_i (S_i^x)^2-\sum_{i,j} J_{ij}\vec{\mathrm{S}}_i\cdot\vec{\mathrm{S}}_j - g\mu_B h\sum_i S_i^z , \tag{1}$$

where the x axis has been chosen to be along the

anisotropy axis making the yz plane the easy plane. D is positive and measures the strength of the anisotropy. In the absence of an external field ($h=0$), if the system orders ferromagnetically, the spins point along a direction in the easy plane. A Zeeman energy term is included in the Hamiltonian to find the parallel susceptibility.

The Hamiltonian can be split into two parts

$$\mathscr{H}_0=D\sum_i (S_i^x)^2-h_m\sum_i S_i^z+NJ(0)\langle S^z\rangle^2 , \tag{2}$$

$$\mathscr{H}_1=-\sum_{i,j} J_{ij}[(S_i^z-\langle S^z\rangle)(S_j^z-\langle S^z\rangle)+S_i^+S_j^-] , \tag{3}$$

where

$$J(0)=\sum_j J_{ij} \tag{4}$$

and

$$h_m=g\mu_B h+2J(0)\langle S^z\rangle . \tag{5}$$

$\mathscr{H}_0$ is the mean-field Hamiltonian which can be diagonalized exactly yielding the energy eigenstates

$$|\epsilon_1\rangle=\cos\theta\,|1\rangle-\sin\theta\,|-1\rangle , \tag{6}$$

$$|\epsilon_2\rangle=|0\rangle , \tag{7}$$

$$|\epsilon_3\rangle=\sin\theta\,|1\rangle+\cos\theta\,|-1\rangle , \tag{8}$$

and eigenvalues

$$\epsilon_1=D/2-[(D/2)^2+h_m^2]^{1/2} , \tag{9}$$

$$\epsilon_2=D , \tag{10}$$

$$\epsilon_3=D/2+[(D/2)^2+h_m^2]^{1/2} , \tag{11}$$

apart from the constant energy term $J(0)\langle S^z\rangle^2$. In Eqs. (6)–(8) $|m\rangle$ (where $m=\pm1,0$) denotes an eigenstate of the S^z operator with the eigenvalue of S^z equal to m. The mixing angle θ is given by

$$\tan\theta=(D/2)\{[(D/2)^2+h_m^2]^{1/2}+h_m\} . \tag{12}$$

In this approximation, the susceptibility and the zero-field heat capacity in the paramagnetic phase are, respectively,

$$\chi_0=\frac{2g^2\mu_B^2}{D}\left[\frac{1-t}{1+2t}\right]\Big/\left[1-\frac{4J(0)}{D}\left[\frac{1-t}{1+2t}\right]\right] , \tag{13}$$

and

$$c_{h=0}=2k_B\beta^2D^2t/(1+2t)^2 , \tag{14}$$

where

$$t=e^{-\beta D}\quad(\beta=1/k_BT) . \tag{15}$$

The critical temperature T_c at which χ_0 becomes divergent is found to be

$$k_BT_c=D\left[\ln\frac{4J(0)+2D}{4J(0)-D}\right]^{-1} . \tag{16}$$

T_c plunges to zero rapidly as D approaches the critical value $D_c=4J(0)$. Near D_c the dependence of T_c on D_c-D is an inverse logarithmic function

$$T_c\sim-(D_c/k_B)[\ln(D_c-D)]^{-1}\quad(D\approx D_c) . \tag{17}$$

The mean-field approximation has ignored entirely the correlations of spin fluctuations which play an essential role in determination of T_c and the critical behavior of the system. To improve the theory, terms describing the interactions of spin fluctuations, $\mathscr{H}_1$ of Eq. (3), should be incorporated in the calculations. The high-temperature series-expansion technique provides a systematic scheme for such calculations.

III. MANY-BODY PERTURBATIVE SERIES EXPANSION

Following Wang and Lee[3] we calculate the free energy in a series expansion treating $\mathscr{H}_1$ [Eq. (3)] as the perturbation. The free-energy function F per spin can be written as

$$F=F_0+\Delta F , \tag{18}$$

with

$$-\beta F_0=\ln\sum_n e^{-\beta\epsilon_n}-\beta J(0)\langle S^z\rangle^2 , \tag{19}$$

and

$$-\beta\Delta F=\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\int_0^\beta d\tau_1\cdots\int_0^\beta d\tau_n\langle T[\mathscr{H}_1(\tau_1)\cdots\mathscr{H}_1(\tau_n)]\rangle_c , \tag{20}$$

where T is Dyson's τ-ordering operator and the angular brackets represent the canonical thermal average over the unperturbed Hamiltonian $\mathscr{H}_0$. The subscript c denotes the cumulant part of the τ-ordered product, or, in the diagrammatic analysis, the contribution of the connected diagrams only. Equations (19) and (20) represent a series expansion of the free energy, the expansion parameter being $\beta J(0)$.

In order to keep the calculation tractable for the high-order terms in the expansion of Eq. (20), it is essential to employ operators whose τ dependence appears only as a c-number factor, as in many-body diagrammatic calculations. This indeed is the case for the spin operators if $\mathscr{H}_0$ contains the Zeeman energy term only, but it is *not* so in the presence of a single-ion anisotropy. To circumvent this difficulty, Wang and Lee[3] have suggested the use of the standard basis operators

$$L_{mn} \equiv |\epsilon_m\rangle\langle\epsilon_n| \ , \tag{21}$$

where $|\epsilon_m\rangle$, $|\epsilon_n\rangle$ are energy eigenstates of $\mathscr{H}_0$. It is easily observed that the τ dependence of a standard basis operator (L operator) in the interaction representation is simply given by

$$L_{mn}(\tau) = e^{(\epsilon_m - \epsilon_n)\tau} L_{mn}(0) \ . \tag{22}$$

Any operator, in particular a spin operator, can be written as a linear combination of the L operators

$$S^\alpha = \sum_{m,n} \langle\epsilon_m | S^\alpha | \epsilon_n\rangle L_{mn} \ . \tag{23}$$

The calculation then involves the evaluation of the thermal average of the τ-ordered products of the L operators instead of the spin operators.

It is convenient to represent the terms in the series expansion by diagrams. While in the actual calculation the spin operators are written in terms of L operators, the first step is to construct the "main diagrams" from the spin-operator cumulants (semi-invariants). Diagrams involving up to four interaction lines are shown in Fig. 1, where a dashed line denotes a longitudinal interaction connecting an S^z operator on one site of the lattice to an S^z operator on another site of the lattice. Similarly, a solid line with an arrow denotes a transverse interaction connecting an S^+ operator to an S^- operator, the convention being that the arrow points from S^+ to S^-. The contribution of a diagram can be obtained as follows:

(1) Assign a τ variable to each interaction line and the two respective spin operators; collect all the spin operators on each site to form the τ-ordered product.

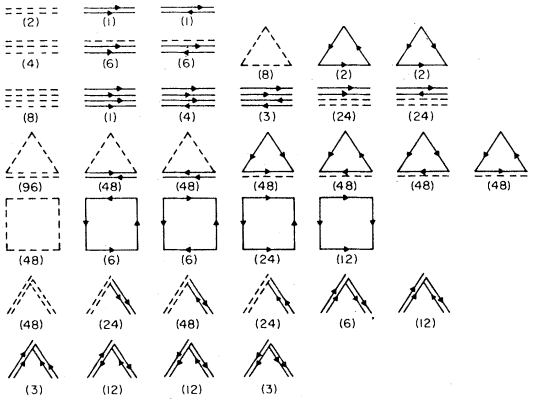

FIG. 1. Free-energy diagrams. Diagrams involving up to four interaction lines are shown. Longitudinal interactions are represented by dashed lines; transverse interactions are represented by solid lines. The arrow on a transverse interaction line points from S^+ to S^-. The weight factors P of the diagrams are also shown (in parenthesis).

(2) Attach a factor $J(\vec{q})$ to each interaction line, $J(\vec{q})$ being the Fourier transform of the exchange interaction J_{ij}. The $\vec{q}$ vectors are so assigned that the sum of $\vec{q}$ vectors is conserved on each site.

(3) Multiply together the τ-ordered products and the interaction $J(\vec{q})$ factors.

(4) Integrate over all τ from zero to β and sum over all $\vec{q}$ variables.

(5) Finally, multiply the result by the weight factor $P/n!$, where P is number of topologically distinct diagrams obtainable by permuting the indices of the spin operators, and n is the number of the interaction lines.

As can be verified, each diagram represents a term in the expansion of $-\beta\Delta F$ [Eq. (20)]. As mentioned, to evaluate the main diagrams, it is necessary to transform the spin operators into the L operators. As a consequence, each main diagram generates a set of subdiagrams with L-operator cumulants. The evaluation is done on the subdiagrams because of the simple τ dependence of the L operators in the interaction picture as discussed above.

While the sums over $\vec{q}$ for the subdiagrams remain the same as the sums for their respective parent main diagrams, the τ integrations are in general different for each subdiagram and must be evaluated separately.

A general formula has been found to evaluate the multiple τ integrals.[6] We first note that the integral can be written in the form

$$I=\sum_P A_{12\cdots m}\int_0^\beta d\tau_1\int_0^{\tau_1}d\tau_2\cdots\int_0^{\tau_{m-1}}d\tau_m\exp(\zeta_1\tau_1+\zeta_2\tau_2+\cdots+\zeta_m\tau_m)\,, \tag{24}$$

where $A_{12\cdots m}$ denotes a product of two or more L-operator cumulants with a total number of $2m$ L operators. For example, a fourth-order diagram may consist of two fourth-order cumulants,

$$\langle L^i_{\alpha_1\beta_1}(\tau_1)L^i_{\alpha_2\beta_2}(\tau_2)L^i_{\alpha_3\beta_3}(\tau_3)L^i_{\alpha_4\beta_4}(\tau_4)\rangle_c\,,$$

and

$$\langle L^j_{a_1b_1}(\tau_1)L^j_{a_2b_2}(\tau_2)L^j_{a_3b_3}(\tau_3)L^j_{a_4b_4}(\tau_4)\rangle_c\,,$$

Then

$$A_{1234}=\langle L_{\alpha_1\beta_1}L_{\alpha_2\beta_2}L_{\alpha_3\beta_3}L_{\alpha_4\beta_4}\rangle_c \times\langle L_{a_1b_1}L_{a_2b_2}L_{a_3b_3}L_{a_4b_4}\rangle_c\,, \tag{25}$$

$\zeta_1\cdots\zeta_m$ are energies associated with the interaction lines. Here, for example, $\zeta_1=\epsilon_{\alpha_1\beta_1}+\epsilon_{a_1b_1}$ where $\epsilon_{\alpha_1\beta_1}=\epsilon_{\alpha_1}-\epsilon_{\beta_1}$ and ϵ_m is the eigenenergy of the mth energy level of $\mathscr{H}_0$. Finally, the summation is over all possible permutations of the indices.

To evaluate the integral, we first note that all A's obtainable from each other by cyclic permutations are related

$$\exp(\beta\epsilon_{n_1})A_{n_1n_2\cdots n_m}=A_{n_2n_3\cdots n_mn_1}\,. \tag{26}$$

Therefore there are $(m-1)!$ independent A's in general. Secondly, it can be shown that a partial summation of the m terms that are related through cyclic permutations gives the result

$$\beta\sum_{P_c}\left[\frac{(-1)^{m-1}A_{n_1n_2\cdots n_m}}{\epsilon_{n_1}(\epsilon_{n_1}+\epsilon_{n_2})\cdots(\epsilon_{n_1}+\epsilon_{n_2}+\cdots+\epsilon_{n_{m-1}})}\right], \tag{27}$$

where the sum is over the cyclic permutations of the indices of A and ϵ. Equation (24) can now be written as

$$I=\beta\sum_P\left[\frac{(-1)^{m-1}A_{n_1n_2\cdots n_m}}{\epsilon_{n_1}(\epsilon_{n_1}+\epsilon_{n_2})\cdots(\epsilon_{n_1}+\epsilon_{n_2}+\cdots+\epsilon_{n_{m-1}})}\right]. \tag{28}$$

A simple example is a second-order diagram containing cumulants $\langle TL_{lm}(\tau_1)L_{np}(\tau_2)\rangle_c$ $\langle TL_{ab}(\tau_1)L_{cd}(\tau_2)\rangle_c$. The contribution of the diagram according to the above rules is

$$\frac{1}{N}\sum_k[J(k)]^2\frac{\beta(A_{21}-A_{12})}{\epsilon_{lm}+\epsilon_{ab}}\delta(\epsilon_{lm}+\epsilon_{np})\delta(\epsilon_{ab}+\epsilon_{cd})\,, \tag{29}$$

and

$$A_{21}-A_{12}=(D_lD_a-D_mD_b)(\delta_{lp}\delta_{nm}-D_n\delta_{lm}\delta_{np}) \times(\delta_{ad}\delta_{bc}-D_c\delta_{ab}\delta_{cd})\,, \tag{30}$$

where

$$D_l=e^{-\beta\epsilon_l}\Big/\sum_n e^{-\beta\epsilon_n}\,. \tag{31}$$

The explicit result of Eq. (28), when one or more factors in the denominator vanish, can be worked out to expedite the computation. For example the result of Eq. (29) becomes, when $\epsilon_{lm}+\epsilon_{ab}=0$,

$$-\frac{1}{N}\sum_K[J(k)]^2\beta^2D_lD_a\,. \tag{32}$$

Equation (28) simplifies the series-expansion calculation tremendously. However, because of a large number of terms involved in the calculation beyond the second order, a computer is needed to handle the numerous, though simple, algebraic operations. In order to find the analytic expression for the coefficients of the series, each quantity in the calculation is represented by a three-dimensional array. If we define $t=\exp(-\beta D)$, then all quantities that enter in the calculation take the form

$$(1+2t)^{-N}\sum a_{lnp}(\beta D)^{-l}t^nh_m^p$$

and each can be specified by giving the value N and the coefficients a_{lnp}. To obtain the susceptibility from the free energy, a_{lnp} with $p\le 2$ will be required; to find the specific heat at zero external field, only terms with $p=0$ will need to be retained.

The mean-field energies ϵ_n and the matrix ele-

TABLE I. Susceptibility series for a fcc lattice. The coefficients a_{lm}^n are listed under $m=0-5$ in rows. d is a common denominator for the numbers in the row. $\chi=\beta\sum a_n[\beta J(0)]^n$, $a_n=(1+2t)^{-(n+1)}\sum a_{lm}^n t^m(\beta D)^l$.

n	l	d	$m=0$	$m=1$	$m=2$	$m=3$	$m=4$	$m=5$
0	1	1	2	−2				
1	2	1	8	−16	8			
2	1	6	0	−6				
2	2	6	0	−4	−34	−16		
2	3	6	177	−510	543	−210		
3	1	36	0	−8	16	−80		
3	2	36	0	−344	294	−188	−128	
3	3	36	0	−186	−1342	1178	620	
3	4	36	3821	−14168	22143	−17336	5540	
4	1	2592	0	−270	1320	1716	−13224	
4	2	2592	0	−6372	11004	−43160	37600	−16640
4	3	2592	0	−152226	256038	−231234	79212	47616
4	4	2592	0	−70572	−507186	838536	−492300	−272568
4	5	2592	979149	−4400886	9018021	−10072614	6303054	−1826724

ments of the spin operators between the mean-field eigenstates are the basic quantitites for the calculations. A computer code has been written to instruct the computer to perform addition and multiplication of two or more quantities in three-dimensional array and return the result in the same form. For each main diagram, the relevant cumulants and the τ-integration factors are calculated first, and a file is created containing these quantities. The subdiagrams are then evaluated by extracting the needed information from this file. The contribution of a main diagram is finally obtained as a linear combination of the subdiagrams. In fourth order, 396 subdiagrams appear. When the main diagrams are summed, 119 subdiagrams cancel leaving 277 subdiagrams to be evaluated. To calculate these 277 subdiagrams, a total of 238 integration factors and 94 cumulants are required.

IV. RESULTS AND DISCUSSIONS

We have obtained the first five coefficients in the susceptibility series and the specific-heat series

TABLE II. Specific-heat series at zero-external field for an fcc lattice b_{lm}^n are listed under $m=1-6$ in rows. d is a common denominator for the numbers in the row. $c=k_B\sum b_n[\beta J(0)]^n$, $b_n=(\beta D)^2(1+2t)^{-(n+2)}\sum b_{lm}^n t^m/(\beta D)^l$.

n	l	d	$m=1$	$m=2$	$m=3$	$m=4$	$m=5$	$m=6$
0	0	1	2					
2	0	3	1	−4				
2	1	3	−6	−2	2			
2	2	3	6	20	20	8		
3	0	54	4	−40	152	−80		
3	1	54	−12	−210	222	−540		
3	2	54	−63	573	741	174	384	
3	3	54	102	192	−126	−192	24	
4	0	1296	45	−800	462	9960	−4408	0
4	1	1296	−306	92	5880	−8592	−36512	0
4	2	1296	501	−5964	42639	−15756	17124	24960
4	3	1296	−2184	28404	−1188	−37776	14328	2304
4	4	1296	3306	1782	−12090	−30	8784	−1752

$$\chi_c=\beta\frac{\partial^2 F}{\partial(\beta h_m)^2}$$

$$=\beta\sum_n c_n(\beta D)[\beta J(0)]^n\,, \tag{33}$$

$$\chi=\chi_c/[1-2J(0)\chi_c]$$

$$=\beta\sum a_n(\beta D)[\beta J(0)]^n\,, \tag{34}$$

and

$$c_{h=0}=(\beta D)^2\frac{\partial^2(-\beta F)}{\partial(\beta D)^2}$$

$$=k_B\sum b_n(\beta D)[\beta J(0)]^n\,. \tag{35}$$

The coefficients a_n, b_n, and c_n can all be written in the form

$$R_n=\sum_{l,m} R^n_{lm}(\beta D)^{-l}t^m\,. \tag{36}$$

In Appendix A we list the coefficients c^n_{lm} (for χ_c) and b^n_{lm} (for $c_{h=0}$) for a *general* lattice. We present a^n_{lm} (for χ) and b^n_{lm} (for $c_{h=0}$) for an fcc lattice in Tables I and II assuming nearest-neighbor-only interactions. As a check, we took the $D=0$ limit. The series all reduced to the well-known ones found for the isotropic Heisenberg system.[7] It should be noted that D enters in the denominator of every coefficient of the series. Most terms in the coefficients become singular upon taking the zero D limit and intricate cancelations of the singularities yield finite values appropriate for the isotropic Heisenberg Hamiltonian.

As an application of the series found, we have made an estimate of the critical temperature as the value of $D/J(0)$ varies. The calculation has been done for an fcc lattice, assuming the nearest-neighbor-only exchange interaction. The extrapolation scheme of Elliot and Wood[8] has been used. First, the value of βD is fixed and the coefficients a_n calculated. The standard ratio test method[7] is then employed to analyze the series. The critical temperature is obtained by the extrapolation

$$\frac{kT_c}{J(0)}=\left[n\left[\frac{a_n}{a_{n-1}}\right]-m\left[\frac{a_m}{a_{m-1}}\right]\right]\Big/(n-m)\,. \tag{37}$$

The value of $kT_c/J(0)$ found with $n=4$ and $m=3$ is shown in Fig. 2 (solid line). The mean-field result is also plotted (dashed line) for comparison.

The critical temperature is seen substantially reduced. The critical value of D, beyond which there is no ordering even at $T=0$, is reduced from the mean-field value $4J(0)$ to $3.43J(0)$. The accuracy of the estimated critical temperature is difficult to access because of the shortness of the series. At $D=0$, the long series estimate is available.[7] For an fcc lattice $T_c/J(0)=1.0026$. Our result is 0.991 which deviates from this almost exact result by only 1%. Near D_c, however, the uncertainty in T_c becomes greater. This is evidenced by the fact that in the plot of a_n/a_{n-1} vs $1/n$, the points of $n=2,3,4$ are scattered further away from a straight line for D near D_c than for small D. Nevertheless, the value of D_c should be rather accurate because of the sharp drop of the critical temperature near D_c.

The current extrapolation scheme approaches the phase boundary radially in the (T,D) plane and is perhaps more reliable than the other schemes of the same category. It, however, does not find the behavior of T_c near D_c correctly. Similar to the Ising model in a transverse field,[8,9] a soft mode occurs at the phase transition for the easy-plane ferromagnet. Thus, it is expected that near D_c,

$$T_c\sim(D_c-D)^{\psi}\,. \tag{38}$$

Indeed, in the random-phase approximation (RPA), it can be shown that $\psi=\frac{1}{3}$. Contrary to the power-law behavior, we find the inverse logarithmic dependence of T_c on D_c-D as in the mean-field

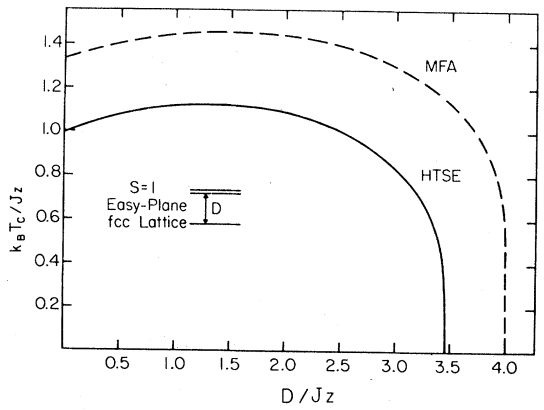

FIG. 2. Critical temperature vs easy-plane anisotropy. The critical temperature estimated from the high-temperature series (HTSE) is plotted as a function of the easy-plane anisotropy for a fcc lattice. The exchange interaction is assumed to extend to the nearest neighbors only. For comparison, the mean-field result (MFA) is also shown (in dashed line).

theory. The persistence of the mean-field behavior in the series analysis is first surprising and thought to owe its origin to the shortness of the series. A closer examination of the coefficients, however, shows that this behavior would always exist if the series has a finite number of terms and if the current extrapolation scheme is used. Nevertheless the longer the series is, the closer D becomes to D_c before the inverse logarithmic behavior sets in. It should be mentioned that the same difficulty is associated with the analysis of the series of the Ising model in a transverse field.[8,9] An entirely different method of analyzing the series should probably be designed for this type of series.

At $T=0$, if we define $K=J(0)/D$, the susceptibility series reduces to

$$\chi=\frac{2}{D}\left(1+4K+\tfrac{59}{4}K^2+\tfrac{3821}{72}K^3+\tfrac{326383}{72}K^4+\cdots\right) \tag{39}$$

for an fcc lattice and to

$$\chi=\frac{2}{D}\left(1+4K+\tfrac{27}{2}K^2+\tfrac{769}{18}K^3+\tfrac{3161}{24}K^4+\cdots\right) \tag{40}$$

for a triangular lattice. The critical value of $D/J(0)$ can be estimated by using Eq. (37) with k_BT replaced by D. Taking $n=4$ and $m=3$, we find $D_c/J(0)$ to be 3.43 for the fcc lattice and 2.84 for the triangular lattice. While the series is too short to give an accurate estimate of the critical exponent, it is interesting to note that the values of γ found are consistent with those expected from a general theory of Hertz.[10] Again, employing the ratio test method,[7] the value of γ can be found by

$$\gamma^{(n)}=\frac{U_m-U_n}{U_n/m-U_m/n}+1\ . \tag{41}$$

Letting $m=n-1$, we find for $n=2,3,4$, $\gamma^{(n)}$ equal to 1.19, 1.16, 1.14 for the fcc lattice and 1.45, 1.46, 1.35 for the triangular lattice. According to the theory of Hertz,[10] the critical exponents of the present system at $T=0$ should be the same as the corresponding ones at finite T for a lattice of one higher dimensionality. Since the symmetry of the present model is XY-like, the value of $\gamma^{(n)}$ should approach 1.0 and 1.34 for the fcc and the triangular lattices, respectively. Our results, while not definitive, are consistent with the theory.[10] It is obvious that higher-order terms are desirable for an in-depth study of this system. It is hoped that an improvement of the present method can be made to allow calculations of more terms in the series.

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APPENDIX A

1. Susceptibility

The susceptibility series for a general lattice with arbitrary range of interaction is given here to the fourth order. We recall

$$\chi=\beta\sum_n a_n[\beta J(0)]^n \tag{A1}$$

and

$$\chi_c=\beta\sum_n c_n[\beta J(0)]^n\ . \tag{A2}$$

The coefficients a_n are calculated from c_n as follows:

$$a_0=c_0\ , \tag{A3}$$

$$a_1=2c_0^2\ , \tag{A4}$$

$$a_2=4c_0^3+c_2\ , \tag{A5}$$

$$a_3=8c_0^4+4c_0c_2+c_3\ , \tag{A6}$$

$$a_4=16c_0^5+12c_0^2c_2+4c_0c_3+c_4\ . \tag{A7}$$

The coefficients c_n take the form

$$c_n=(1+2t)^{-(n+1)}\times\sum I_q^n c_{qlm}^n t^m/(\beta D)^l\ . \tag{A8}$$

If we define

$$\gamma(K)=J(K)/J(0)\ , \tag{A9}$$

we find

$$I_1^0=1\ , \tag{A10}$$

$$I_1^2=\frac{1}{N}\sum\gamma(K)^2\ , \tag{A11}$$

$$I_1^3=\frac{1}{N}\sum\gamma(K)^3\ , \tag{A12}$$

$$I_2^3=\frac{1}{N^2}\sum\gamma(K_1)\gamma(K_2)\gamma(K_1+K_2)\,, \tag{A13}$$

$$I_1^4=\frac{1}{N}\sum\gamma(K)^4\,, \tag{A14}$$

$$I_2^4=\frac{1}{N^2}\sum\gamma(K_1)\gamma(K_2)\gamma(K_1+K_2)^2\,, \tag{A15}$$

$$I_3^4=\frac{1}{N^3}\sum\gamma(K_1)\gamma(K_2)\gamma(K_3)\gamma(K_1+K_2+K_3)\,, \tag{A16}$$

$$I_4^4=(I_1^2)^2\,. \tag{A17}$$

The coefficients c_{qlm}^n are listed in Table III under $m=1-5$ in rows.

2. Specific heat

For a general lattice, the specific-heat series at zero-external field in the paramagnetic phase can be written as

$$c_{h=0}=k_B\sum b_n[\beta J(0)]^n\,, \tag{A18}$$

where

TABLE III. Coefficients c_{qlm}^n in Eq. (A8).

n	q	l	$m=0$	$m=1$	$m=2$	$m=3$	$m=4$	$m=5$
0	1	1	2	−2				
2	1	1	0	−12				
2	1	2	0	−8	−68	−32		
2	1	3	−30	132	−66	−36		
3	1	1	0	−8	16	−80		
3	1	2	0	−56	48	−176	−128	
3	1	3	0	−68	−112	308	−128	
3	1	4	−88	616	−888	280	80	
3	2	2	0	0	−168	−48		
3	2	3	0	296	840	24	−80	
3	2	4	84	−960	540	384	−48	
4	1	1	0	−4	−8	52	−376	
4	1	2	0	$-\frac{136}{3}$	16	−120	$-\frac{1040}{3}$	−512
4	1	3	0	−244	232	−220	744	−512
4	1	4	0	−236	−360	1428	−832	
4	1	5	−298	2816	−6232	4780	−638	−428
4	2	1	0	0	−64	−64	128	
4	2	2	0	0	$-\frac{1504}{3}$	$\frac{1328}{3}$	$-\frac{1696}{3}$	
4	2	3	0	312	−1728	3816	3120	−192
4	2	4	0	3808	4176	−8960	10272	2944
4	2	5	616	−11248	17528	−10576	−1760	5440
4	3	1	0	0	−40	116	−280	
4	3	2	0	0	$-\frac{56}{3}$	−568	−80	$-\frac{1024}{3}$
4	3	3	0	−120	2524	560	992	256
4	3	4	0	−2508	−1860	18540	12408	3120
4	3	5	−464	7196	−19002	−4768	10378	6660
4	4	1	0	0	128	−88	656	
4	4	2	0	72	−48	1024	1024	1024
4	4	3	0	1068	−2088	−220	−1432	512
4	4	4	0	320	−1056	−19536	−11600	−2688
4	4	5	1044	−8032	26320	−3768	−9956	−5608

TABLE IV. Coefficients b^n_{qlm} in Eq. (A19).

n	q	l	$m=1$	$m=2$	$m=3$	$m=4$	$m=5$	$m=6$
0	1	0	2					
2	1	0	4	−16				
2	1	1	−24	−8	8			
2	1	2	24	80	80	32		
3	1	0	$\frac{8}{3}$	$-\frac{80}{3}$	$\frac{304}{3}$	$-\frac{160}{3}$		
3	1	1	−8	−144	144	−352		
3	1	2	−44	392	540	152	256	
3	1	3	72	144	−72	−144		
3	2	1	0	16	16	−32		
3	2	2	8	−40	−184	−144		
3	2	3	−16	−64	−48	64	64	
4	1	0	$\frac{4}{3}$	$-\frac{16}{3}$	−68	$\frac{1712}{3}$	−752	
4	1	1	$-\frac{8}{3}$	$-\frac{608}{3}$	312	$-\frac{1696}{3}$	$-\frac{6112}{3}$	
4	1	2	−12	−240	2916	−144	1488	1536
4	1	3	−132	1872	324	−2352	288	
4	1	4	240	240	−720	−240	480	
4	2	0	0	$\frac{128}{3}$	$-\frac{192}{3}$	$-\frac{768}{3}$	$\frac{256}{3}$	
4	2	1	0	$-\frac{320}{3}$	$-\frac{1392}{3}$	$-\frac{576}{3}$	$\frac{1856}{3}$	
4	2	2	−8	96	−24	−160	672	
4	2	3	80	−192	−816	640	2112	768
4	2	4	−112	−480	−464	352	576	128
4	3	0	0	$\frac{80}{3}$	−196	528	$-\frac{560}{3}$	
4	3	1	0	$-\frac{560}{3}$	648	−608	$-\frac{4384}{3}$	
4	3	2	40	−416	1616	−1024	992	1024
4	3	3	−268	1632	636	−2000		
4	3	4	296	408	−776	−632	480	224
4	4	0	0	$-\frac{256}{3}$	344	−992	$\frac{1312}{3}$	
4	4	1	−24	$\frac{2464}{3}$	−416	1280	$\frac{10496}{3}$	
4	4	2	100	240	−6324	−1072	−3984	−3072
4	4	3	248	−3936	−1128	4576	−192	
4	4	4	−520	−576	1576	832	−1056	−256

$$b_n=(1+2t)^{-(n+2)}(\beta D)^2 \times \sum I_q^n b_{qlm}^n t^m/(\beta D)^l . \quad \text{(A19)}$$

The lattice sums I_q^n have been given in Eqs. (A10) to (A17). The coefficients b^n_{qlm} are listed in Table IV under $m=1-6$ in rows.

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