Linked-cluster expansion for quantum spin systems and the perpendicular susceptibility of the Ising model

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The Wick reduction theorem is used in a linked-cluster-expansion calculation to facilitate the evaluation of the multi-integrals of the ordered products encountered in the expansion. The method resolves a major problem in the general linked-cluster expansion for quantum spin systems. We apply it to the evaluation of the perpendicular susceptibility of the Ising model. An eighth-order linked-cluster series is obtained for a general lattice. The temperature behavior of the perpendicular susceptibility of the three-dimensional Ising model (fcc lattice) is discussed.

I. INTRODUCTION

One of the most fascinating and challenging many-body problems in physics is magnetic systems. Because of the relative simplicity of their Hamiltonians magnetic models have been the most extensively studied. Many powerful methods have been applied to tackle the problem.[1] Generally, except for a few particular low-dimensional models, exact solutions are not found. However, many calculations for idealized simple models have produced accurate results that are almost exact.[1]

The question of how to apply these powerful methods to models which more realistically represent physical magnetic systems with quantum spins and single-ion anisotropies is nevertheless nontrivial. Many attempts have been made along this line. Notably, the Monte Carlo simulation method[2] and position-space renormalization-group calculations[3] have been applied to quantum spin systems of low dimensions. Series expansions, which normally converge faster for higher-dimension systems, have been utilized to analyze a few three-dimensional systems.[4] All the methods are at various stages of development. The series-expansion method, for example, can only provide a few terms (compared to the series for the simple idealized models) for analysis.

In this paper we shall first discuss the method of linked-cluster expansion for quantum spin systems with *arbitrary* single-ion energy-level schemes. We introduce a novel technique which facilitates the evaluation of the multi-integral of the ordered products, a major difficulty encountered in the general series-expansion method proposed earlier for quantum spin systems with single-ion anisotropies.[5] Thus, much longer series (perhaps of comparable length to those of the simple models) can be found and accurate results for the more realistic physical models can be obtained. It should be noted that the method discussed in this paper and in Refs. 4 and 5 treats the single-ion potentials exactly; thus, the magnitude of the single-ion anisotropy can be of *arbitrary* size and the series provide information on the system both above and below the transition temperature. These valuable features are difficult to achieve with the long-established high-temperature series-expansion methods.[5(b)]

As an illustration of the major concept in the new method we then calculate the perpendicular susceptibility of the Ising model which is an important problem to study on its own. Recently, it has been observed[6] that a prominent cusp appears in the temperature behavior of the electric susceptibility of the uniaxial ferromagnet $LiHoF_4$ which is proportional to the perpendicular susceptibility[4] of the Ising model. This is in contrast with the prediction of the mean-field approximation which gives a temperature-independent value below the critical temperature T_c.

Many years ago, Fisher[7] obtained an exact result for the perpendicular susceptibility $\chi_\perp$ of the two-dimensional Ising model. Fisher[7] showed that as the temperature is lowered the susceptibility reaches a maximum at a temperature above T_c and that $\partial\chi_\perp/\partial T$ displays a singularity similar to the specific-heat anomaly but of relatively smaller magnitude. For three-dimensional lattices, limited results have been obtained. Fischer[7] has given a high-temperature series to fourth order and a low-temperature series up to a term with three overturned spins. Stinchcombe[8] has worked out the $1/z$ (z being the number of nearest neighbors interacting with a spin) correction to the mean-field result. While Stinchcombe's result suggests a cusplike behavior in the perpendicular susceptibility, the approximation is not valid in the vicinity of T_c. (A comparison of Stinchcombe's results for the nearest-neighbor exchange-interaction model and those of the current series-expansion method has now been published.[9]) Very recently the correlated effective-field theory of Lines has been used[10] to calculate the perpendicular susceptibility for $LiHoF_4$. The theory yields a good fit to the available experimental data with a few parameters. The approximation is, however, appropriate for systems with long-range interactions and will only yield the classical (mean-field) critical behavior near T_c.

We have derived an eighth-order linked-cluster series for the perpendicular susceptibility of the Ising model. The series has been derived for a general lattice. We have used the Padé-approximants method[11] to analyze the series for the fcc lattice and the plane square lattice. While the series is not of adequate length for a two-dimensional lattice, the square-lattice series is analyzed

for the sole purpose of making a comparison with the exact result of Fisher,[7] and thus enhances our confidence in the result of the fcc lattice.

In the next section we discuss the major difficulties of applying the linked-cluster-expansion method to general quantum spin systems and introduce the new technique to facilitate the calculation of high-order terms. The perpendicular susceptibility series of the Ising model is calculated in Sec. III to illustrate the concept. The analysis of the series and the discussion of the results for the fcc and the plane square lattices will be presented in Sec. IV.

II. LINKED-CLUSTER EXPANSION AND THE WICK REDUCTION THEOREM

The linked-cluster expansion is essentially a many-body perturbative expansion.[12] Reviews of this have been given by Callen[13] and Wortis.[14] For a many-body system one first divides the Hamiltonian into two parts:

$$H=H_0+H_1 \ . \tag{1}$$

H_0 contains all the single-ion potentials and a "self-consistent-field" term extracted from the two-ion interaction potential. The self-consistent field is characterized by a parameter which can be chosen to minimize the free energy of the system. H_1 contains terms which describe in essence the correlations of the fluctuations of the dynamic variables.

The free energy is then given by

$$F=F_0+\Delta F \ , \tag{2}$$

where

$$-\beta F_0=\ln \mathrm{Tr} e^{-\beta H_0} \tag{3}$$

and

$$-\beta\Delta F=\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\int^{\beta}d\tau_1\int^{\beta}d\tau_2\cdots\int_0^{\beta}d\tau_n\langle T\{H_1(\tau_1)H_1(\tau_2)\cdots H_1(\tau_n)\}\rangle_c \ . \tag{4}$$

In Eq. (4) T is the Dyson τ-ordering operator[12] and $H_1(\tau)$ is the perturbation Hamiltonian in the interaction representation. The angular brackets denote a canonical thermal average over the unperturbed Hamiltonian H_0. The subscript c denotes the cumulant part of the τ-ordered product, or in diagram language, the contribution from the linked clusters only.

For a classical system such as the Ising model or the classical Heisenberg model, $H_1(\tau)$ is τ independent, thus, the multiple integrals are trivial to evaluate. Calculations of the linked clusters of $-\beta\Delta F$ given by Eq. (4) involve only the multiplying of the cumulants in the cluster, the appropriate weight factor, and βJz to the power of the number of interaction lines in the cluster. A recent work[15] on the Blume-Capel model is an example of such a calculation.

The calculation for a general quantum spin system (containing single-ion anisotropies) is more complicated. The operators which appear in the thermal average of Eq. (4) usually do not commute with each other or with H_0. The complications which this produces are (1) the value of the ordered operator product depends on the τ ordering of the operators, (2) the τ dependence of the spin operators can become very complicated, (3) the evaluation of the averages in Eq. (4) can be complicated, and (4) evaluation of the τ integral is a major problem.

Problems (2) and (3) arise, for example, in the presence of a single-ion anisotropy potential in the Hamiltonian but can be solved[5] by introducing the "standard basis operators" defined as

$$L_{mn}\equiv|m\rangle\langle n| \ , \tag{5}$$

where $|m\rangle, |n\rangle$ are energy eigenstates of H_0 with eigenenergies E_m and E_n. The τ dependence of a standard basis operator in the interaction picture is given by the simple relation

$$L_{mn}(\tau)=e^{(E_m-E_n)\tau}L_{mn}(0) \ . \tag{6}$$

Any operator can be expressed as a linear combination of the standard basis operators; thus, a transformation to the standard basis operator can be taken before the evaluation of the thermal averages.

Problem (4) has been a major obstacle in obtaining long series for systems studied.[4,16] Much algebra must be done to evaluate the multiple integrals for the high-order terms. The method we introduce here represents a fundamentally different concept in the evaluation of the multiple integrals. The method is inspired by the Wick theorem used in many-body calculations.[12] To explain the method we first recall that the Wick theorem allows one to express the canonical thermal average of an n operator τ-ordered product as a sum of the averages of $(n-1)$-operator τ-ordered products. This is normally presented for operators of the same site. Yang and Wang[17] have used the Wick reduction theorem for the standard basis operators as a step in the Green's function calculation. Their result can be generalized to accommodate the additional features necessary for the linked-cluster expansion and is an essential step in evaluating the multiple integrals in the simplest way.

We first note that the theorem remains valid if we replace each standard basis operator by an operator which is a product of two or more standard basis operators of different sites but of the same τ variable, i.e., if we define

$$O_1(\tau_1)=O^{i,j,\cdots}_{\alpha_1\beta_1\gamma_1\sigma_1\cdots}(\tau_1)=L^{i}_{\alpha_1\beta_1}(\tau_1)L^{j}_{\gamma_1\sigma_1}(\tau_1)\cdots \ , \tag{7}$$

where $i,j\cdots$ are the labels of the lattice sites. We find

$$\langle T\{O_1(\tau_1)O_2(\tau_2)\cdots O_k(\tau_k)\cdots O_n(\tau_n)\}\rangle = G(\tau_1-\tau_k)\langle T\{[O_1,O_k]_{\tau_1}O_2(\tau_2)\cdots O_n(\tau_n)\}\rangle + G(\tau_2-\tau_k)\langle T\{O_1(\tau_1)[O_2,O_k]_{\tau_2}\cdots O_n(\tau_n)\}\rangle + \cdots + G(\tau_n-\tau_k)\langle T\{O_1(\tau_1)O_2(\tau_2)\cdots [O_n,O]_{\tau_n}\}\rangle \ . \quad (8)$$

The "Green's functions" are defined as

$$G(\tau_i-\tau_k)=\begin{cases} e^{-\epsilon_k(\tau_i-\tau_k)}[1+n(\epsilon_k)], & \tau_i>\tau_k \\ e^{-\epsilon_k(\tau_i-\tau_k)}n(\epsilon_k), & \tau_i<\tau_k \end{cases} \quad (9)$$

where ϵ_k is the "energy" associated with the operator $O_k(\tau_k)$ defined by

$$\epsilon_k=(E_{\alpha_k}-E_{\beta_k})+(E_{\gamma_k}-E_{\sigma_k})+\cdots \ . \quad (10)$$

The boson factor $n(\epsilon)$ is given by

$$n(\epsilon)=1/(e^{\beta\epsilon}-1) \ . \quad (11)$$

We call Eq. (8) the multiple-site Wick reduction (MSWR) theorem.

The essential observation which makes the MSWR theorem useful in the multiple-integral evaluation is that the τ variable of $O_k(\tau_k)$ resides only in the Green's functions. Thus, the integration over τ_k can be easily carried out, independent of the ordered products multiplied to the Green's functions. The integration over τ_k of the Green's functions yields

$$\int_0^\beta G(\tau_i-\tau_k)d\tau_k=\frac{1}{\epsilon_k} \ . \quad (12)$$

We have therefore found the simplest way of evaluating the contributions of the linked clusters. The following equation summarizes the results:

$$\int_0^\beta d\tau_1\cdots\int_0^\beta d\tau_k\cdots\int_0^\beta d\tau_n\langle T\{O_1(\tau_1)\cdots O(\tau_k)\cdots O_n(\tau_n)\}\rangle = \frac{1}{\epsilon_k}\int_0^\beta d\tau_1\cdots\int_0^\beta d\tau_n(\langle T\{[O_1,O_k]_{\tau_1}\cdots O_n(\tau_n)\}\rangle + \langle T\{O_1(\tau_1)[O_2,O_k]_{\tau_2}\cdots O_n(\tau_n)\}\rangle + \cdots + \langle T\{O_1(\tau_1)\cdots [O_n,O_k]_{\tau_n}\}\rangle) \ . \quad (13)$$

An n-fold integral is thus reduced to a sum of $(n-1)$-fold integrals. Using this formula only simple algebra is involved. *It does not require any knowledge about Green's function formalism to use this method.*

The operator $O(\tau)$ represents a product of the standard basis operators of the same τ variable in the diagram, i.e., the operators connected by a single interaction line. In the calculation one selects an interaction line with "energy" $\epsilon\neq 0$ [see Eq. (10) for definition]. The integration over the τ variable of the interaction is then accomplished by applying Eq. (13). Repeating the process reduces the order of the integral further until a trivial single integral appears or no more operators with $\epsilon\neq 0$ can be found. In the latter case the calculation is continued with the evaluation of the integral with τ-independent operators. The value of the integrand will still depend on the order of the operators. This is similar to the situation with an isotropic Heisenberg model. The integral can be simply evaluated by taking a sum of the integrands with all permutations of the operators and multiplying the result by the factor $\beta^n/n!$ (for integrands of n operators). In fact it is possible to use the MSWR method in the case of no operator with $\epsilon\neq 0$. One can add a small quantity δ to the energy of one energy level on a particular site. This will give the corresponding operator an energy $\epsilon=\delta$. One can then apply the MSWR method and at the end take the limit of $\delta\to 0$.

In the next section we apply the current method to evaluate the multiple integrals occurring in the linked-cluster expansion for the perpendicular susceptibility of the Ising model. It is found that for this particular system only the *single-site* Wick reduction theorem is needed for the evaluation of the integrals. Furthermore, by applying the method of reducing the multiple integral [Eq. (13)] repeatedly a general formula is obtained for the value of the multiple integral.

III. LINKED-CLUSTER EXPANSION OF THE PERPENDICULAR SUSCEPTIBILITY OF THE ISING MODEL

The perpendicular susceptibility of the Ising model has been of much interest recently, especially its behavior near the critical point in a three-dimensional lattice.[6,10,18] In this section we apply the method of linked-cluster expansion introduced above to obtain the linked-cluster series for the perpendicular susceptibility of the Ising model.

The Hamiltonian of the Ising model is given by

$$H_I=-J\sum_{\langle i,j\rangle}\sigma_i^z\sigma_j^z \ , \quad (14)$$

where the summation is over all the nearest-neighbor spin pairs in the lattice. A perpendicular field introduces an additional potential

$$H_f=-g\mu_B h_x\sum_i\sigma_i^x \ . \quad (15)$$

To calculate the perpendicular susceptibility at vanishing external field, one could evaluate the free energy to second order in h_x and take the derivative of the result twice with respect to the field. Alternatively, one could evaluate the "rooted diagrams" directly for the susceptibility. To proceed in the latter way we first separate the Hamiltonian H_I into a single-ion part H_0 and a perturbation H_1 *assuming a ferromagnetic ordering below the critical temperature:*

$$H_0=-JzM\sum_i \sigma_i^z+\tfrac{1}{2}NJzM^2 \tag{16}$$

and

$$H_1=-J\sum_{\langle i,j\rangle}(\sigma_i^z-M)(\sigma_j^z-M)\ , \tag{17}$$

where M is a free parameter chosen to minimize the free energy. It has been shown[14,15] that M determined in this manner is equal to the magnetization (the order parameter) of the system.

The perpendicular susceptibility is then given by

$$\chi_\perp=\frac{1}{\beta}\frac{\partial^2(-\beta F)}{\partial h_x^2}$$

$$=N(g\mu_B)^2\frac{1}{\beta}\int_0^\beta d\tau_l\int_0^\beta d\tau_r\langle T\{\sigma^x(\tau_l)\sigma^x(\tau_r)S(\beta)\}\rangle_c\ , \tag{18}$$

where

$$S(\beta)=\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\int_0^\beta d\tau_1\int_0^\beta d\tau_2\cdots\int_0^\beta d\tau_n T\{H_1(\tau_1)H_1(\tau_2)\cdots H_1(\tau_n)\} \tag{19}$$

and all operators are in the interaction representation.

The susceptibility diagrams are therefore "rooted diagrams" with two operators σ^x placed together on one of the sites of the free-energy diagrams of the Ising model. The contribution of a diagram is equal to the product of the cumulants in the diagram, the weight factor, and the lattice constants. All cumulants containing only σ^z operators are well known and easily generated. They are

$$C_n=\langle(\sigma^z)^n\rangle_c=\frac{\partial^n}{\partial(\beta h)^n}\ln \mathrm{Tr}\, e^{-\beta H_0-\beta h\sigma^z}\ . \tag{20}$$

The cumulants containing $\sigma^x(\tau_1)\sigma^x(\tau_2)$ can be found by the method introduced in the preceding section. To proceed, we first make a transformation to avoid the need to deal with the complicated τ dependence of σ^x. We introduce

$$\sigma^+=|+1\rangle\langle -1|\ , \tag{21a}$$

$$\sigma^-=|-1\rangle\langle +1|\ , \tag{21b}$$

where $|\pm1\rangle$ are the eigenstates of σ^z and H_0, the τ dependence of $\sigma^\pm$, is of the simplest form

$$\sigma^\pm(\tau)=e^{\mp\epsilon\tau_{\sigma^\pm}}(0) \tag{22}$$

with

$$\epsilon=2JzM\ . \tag{23}$$

The operator σ^x is given by the linear combination $\sigma^++\sigma^-$. Thus, the perpendicular susceptibility can be written as

$$\chi_\perp=(g\mu_B)^2\frac{2N}{\beta}\int_0^\beta d\tau_+\int_0^\beta d\tau_-\langle T\sigma^+(\tau_+)\sigma^-(\tau_-)S(\beta)\rangle_c. \tag{24}$$

In the expansion of Eq. (24), each linked cluster contains cumulants of operators σ^z only, except one cumulant in which $\sigma^+\sigma^-$ are also present. We therefore need to calculate the integrals,

$$\beta^{n+2}I_n=\int_0^\beta d\tau_+\int_0^\beta d\tau_-\int_0^\beta d\tau_1\cdots\int_0^\beta d\tau_n\langle T\sigma^+(\tau_+)\sigma^-(\tau_-)\sigma^z(\tau_1)\cdots\sigma^z(\tau_n)\rangle_c\ . \tag{25}$$

Applying Eq. (13) in the preceding section and noting that

$$[\sigma^+,\sigma^-]=\sigma^z\ , \tag{26a}$$

$$[\sigma^z,\sigma^-]=-2\sigma^-\ , \tag{26b}$$

we find that

$$I_n=\frac{1}{\beta\epsilon}[C_{n+1}-2nI_{n-1}]\ . \tag{27}$$

Solving Eq. (27) or applying Eq. (13) repeatedly we obtain

$$I_n=\frac{1}{\beta\epsilon}\sum_{m=0}^{n}\left[\frac{-2}{\beta\epsilon}\right]^{n-m}\frac{n!}{m!}C_{m+1}\ . \tag{28}$$

The calculation of the perpendicular susceptibility can therefore be simply done by using the free-energy diagrams of the Ising model. One can first write down a free-energy term which is a product of the cumulants of σ^z operators, the weight factor, and the lattice constant, then replace one of the cumulants C_n by I_n (n being the number of σ^z operators in the cumulant) successively, and sum up the terms so produced. A term in the perpendicular susceptibility is then obtained.

IV. THE PERPENDICULAR SUSCEPTIBILITY OF THE ISING MODEL

We have obtained the linked-cluster series for the perpendicular susceptibility of the Ising model to the eighth order. The series reduces to the high-temperature series in the paramagnetic phase when M and ϵ vanish. For a general lattice above the critical point,

$$\chi_\perp = \frac{(g\mu_B)^2}{k_B T} \sum_{n=0}^{\infty} a_n (\beta J)^n , \tag{29}$$

where

$$a_0 = 1 , \tag{30a}$$

$$a_1 = 0 , \tag{30b}$$

$$a_2 = -\tfrac{1}{3} z , \tag{30c}$$

$$a_3 = -\tfrac{1}{3} r_3 , \tag{30d}$$

$$a_4 = \tfrac{1}{15} z(-4+11z) - \tfrac{1}{3} r_4 ,$$

$$a_5 = \tfrac{1}{45}(-58+81z) r_3 - \tfrac{1}{3} r_5 , \tag{30e}$$

$$a_6 = \tfrac{2}{315} z(-136+493z-411z^2) + \tfrac{4}{5} r_3 + \frac{1}{15z}(-34+16z) r_3^2 + \tfrac{4}{45}(-17+24z) r_4 - \tfrac{1}{3} r_6 , \tag{30f}$$

$$a_7 = \tfrac{1}{105}(-1144+2068z-1081z^2) r_3 + \frac{1}{15z}(-78+37z) r_3 r_4 + \frac{82}{15z} r_3^2 - \frac{26}{15z^2} r_3^3 + \tfrac{1}{15}(-26+37z) r_5 - \tfrac{1}{3} r_7 , \tag{30g}$$

$$\begin{aligned} a_8 = {} & \tfrac{1}{2835} z(-16864+71544z-84900z^2+33303z^3) + \tfrac{2}{105}(904-661z) r_3 + \frac{92}{15z} r_3 r_4 \\ & + \frac{2}{15z}(-44+21z) r_3 r_5 + \tfrac{1}{945}(-47328+45708z-12375z^2) r_3^2 - \frac{88}{15z^2} r_3^2 r_4 + \frac{184}{15z^2} r_3^3 \\ & + \tfrac{1}{945}(-12956+22854z-12375z^2) r_4 + \frac{1}{15z}(-44+21z) r_4^2 + \frac{2}{45}(-44+63z) r_6 - \tfrac{1}{3} r_8 - \tfrac{16}{5} r_a + \tfrac{46}{15} r_b - \tfrac{22}{45} r_c . \end{aligned} \tag{30h}$$

In the linked-cluster-expansion calculation the "free embedding lattice constants" (free multiplicities) are used instead of the "weak embedding lattice constants" used in the conventional high-temperature series calculation. The two sets of lattice constants are, however, related.[19] Here in the series coefficients r_n is for the n-size polygon and is equal to $(z^n/N)\sum_k \gamma_k^n$, where

$$\gamma_k = \frac{1}{z} \sum_{\delta} e^{i\mathbf{k}\cdot\delta} . \tag{31}$$

δ is a vector pointing from a site to its nearest-neighbor site. The numerical values of r_n have been tabulated.[20] The graphs of r_a, r_b, and r_c are the ones corresponding to p_{6d}, p_{6a}, and p_{8r} (Ref. 20). However, in the evaluation of r_a, r_b, and r_c, the lattice sites of the graph are allowed to coincide. For the convenience of the reader, we have collected the numerical values of r_n and r_a, r_b, and r_c for some simple lattices and presented them in Table I. It should be noted that in the disordered phase only diagrams with all cumulants containing an even number of σ^z contribute to the perpendicular susceptibility.

In the ordered phase, the linked-cluster series for a general lattice is too long to be presented here. We will show only the series for the fcc lattice. The series is of the form

$$\chi_\perp = \frac{N(g\mu_B)^2}{k_B T} \sum_n b_n(p) [\beta J]^n , \tag{32}$$

where $b_n(p)$ are polynomials in p,

$$p = \tanh\left[\frac{\epsilon}{2}\right] \tag{33}$$

and

$$\epsilon = 2\beta J z M . \tag{34}$$

In fact the coefficients $b_n(p)$ can be written as

$$b_n(p) = \sum_{m=\text{odd}} \alpha_{mk}^n p^{2k+1}/\epsilon^m + \sum_{m=\text{even}} \alpha_{mk}^n p^{2k}/\epsilon^m . \tag{35}$$

The first term ($n=0$) is simply the mean-field result

$$b_0(p) = \frac{2p}{\epsilon} . \tag{36}$$

The second term ($n=1$) is zero. For $n \geq 2$, the values of α_{mk}^n for the fcc lattice are given in Table II. We note that as T tends to zero the coefficients of the correction terms

TABLE I. Lattice constants involved in the high-temperature perpendicular susceptibility series of the Ising model. (sq denotes square and tr denotes triangular.)

	sq	tr	sc	bcc	fcc
r_3	0	12	0	0	48
r_4	36	90	90	216	540
r_5	0	360	0	0	4320
r_6	400	2040	1860	8000	42 240
r_7	0	10 080	0	0	403 200
r_8	4900	54 810	44 730	343 000	4 038 300
r_a	0	0	0	0	48
r_b	100	318	318	1000	3084
r_c	324	1494	1494	5832	25 740

in the series approach zero exponentially in βJ; thus, the mean-field result is recovered at zero temperature.

We have employed the Padé-approximants method to obtain an estimate of the perpendicular susceptibility for the fcc lattice as a function of temperature. In the paramagnetic phase Eq. (29) is used. In the ferromagnetic phase the value of the magnetization M is required for the calculation. We have used the values of M found by the low-temperature series, since they are perhaps the most accurate values known for the model. In Fig. 1 we plot the estimated perpendicular susceptibility of the fcc lattice as a function of temperature. The error bar is used to indicate the apparent convergence of the Padé approximants. The absolute accuracy of the estimate is difficult to obtain. (See comments in the concluding remark below.) As expected, the accuracy deteriorates, in the vicinity of the critical point, as evidenced by the wide spread in the values of the Padé approximants.

The general behavior of the perpendicular susceptibility is found to be consistent with Fisher's speculation. However, the precise behavior at the critical point is not conclusive in the present analysis. The susceptibility shows a maximum which is about 12% higher than that at zero temperature. The temperature at which the maximum occurs lies extremely close to or almost coinciding with the critical temperature. With regard to this it is of interest to compare it with the similar behavior of the parallel antiferromagnetic susceptibility (of the Ising model). For a (two-dimensional) plane square lattice[7] the temperature $T_{\max}$ at which the parallel antiferromagnetic susceptibility reaches its maximum lies about 54% above the critical temperature T_c, while $T_{\max}$ for the perpendicular susceptibility lies only 9% above T_c. For a three-dimensional lattice it has been shown[21] that for a body-centered cubic lattice $T_{\max}$ for the parallel antiferromagnetic susceptibility is only 6.5% higher than T_c; $T_{\max}$ for the perpendicular susceptibility is thus expected to lie very close to T_c.

The curve of the perpendicular susceptibility shows a positive curvature at high temperature but turns negative as T_c is approached. Just below T_c (in the ordered phase) the susceptibility decreases rapidly with an infinite slope at T_c. A prominent "cusp" is observed. The mean-field result is also plotted in Fig. 1 for comparison. It is seen that the mean-field approximation fails to predict correctly even the qualitative behavior of the perpendicular susceptibility.

Based on the results of series analysis for other physical quantities of the Ising models, the eighth-order linked-cluster series may very well have produced quite reliable

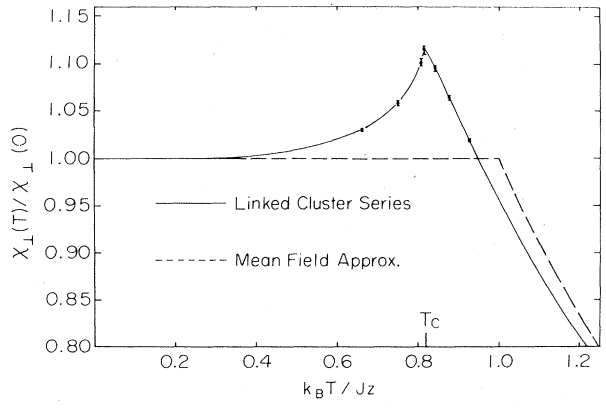

FIG. 1. The temperature behavior of the perpendicular susceptibility of the Ising model on an fcc lattice. The solid curve shows the results of the linked-cluster series analysis. The error bar shows the apparent convergence of the Padé approximants. The mean-field result is shown by the dashed line.

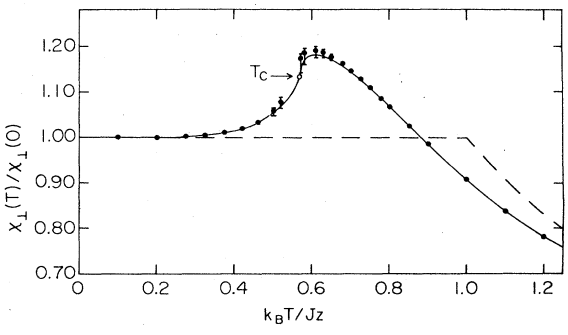

FIG. 2. The temperature behavior of the perpendicular susceptibility of the Ising model on a plane square lattice. Fisher's exact result is drawn in the solid line. The results of the series analysis are shown by dots. The error bar shows the apparent convergence of the Padé approximants. The mean-field result is shown by the dashed line for comparison.

TABLE II. Coefficients α_{mk}^{n} of Eq. (35) for the perpendicular susceptibility linked-cluster series of the Ising model on an fcc lattice.

b_2

m \ k	0	1	2
1	-24	48	-24
2	-48	96	-48
3	96	-96	

b_3

m \ k	0	1	2	3
1	-80	208	-176	48
2	-192	480	-384	96
3	192	-384	192	
4	0	384	-384	

b_4

m \ k	0	1	2	3	4
1	-56	-1136	3712	-3792	1272
2	-1040	448	4768	-6720	2544
3	-2400	9888	-12576	5088	
4	-6528	23424	-27264	10368	
5	13056	-24576	11520		

b_5

m \ k	0	1	2	3	4	5
1	496/5	-54896/5	194464/5	-259104/5	30384	-6576
2	-6400	-992	54400	-93376	59520	-13152
3	-20032	89984	-146176	102528	-26304	
4	-49152	179328	-226176	110976	-14976	
5	12288	3072	-43008	27648		
6	0	172032	-337920	165888		

b_6

m \ k	0	1	2	3	4	5	6
1	-39616/15	-194368/15	-241216/15	238592	-450112	329408	-86208
2	-212672/5	158464/5	467968/5	126720	-620736	583680	-172416
3	-114176	254336	270464	-1192064	1126272	-344832	
4	-367616	772096	813568	-3374592	3058176	-901632	
5	-1019904	494132	-8587776	6431232	-1764864		
6	-1394688	7305216	-13191168	10045440	-2764800		
7	2789376	-6660096	4976640	-1105920			

b_7

m \ k	0	1	2	3	4	5	6	7
1	-3412384/105	21665696/105	-28125664/15	241389408/35	-414385056/35	10475488	-4654944	823392
2	-4527488/15	6824768/15	-18253312/15	119084224/15	-90923648/5	93015104/5	-8940288	1646784
3	-3635584/5	-210688/5	55766144/5	-146131968/5	160454016/5	-16541952	3293568	
4	-2670592	3182848	19684096	-55856128	57716736	-26492160	4435200	
5	-11926528	54935552	-96243712	78538752	-28455936	3151872		
6	-14794752	62994432	-87595008	33626112	17528832	-11759616		
7	-8503296	72302592	-162889728	142884864	-43794432			
8	0	76185600	-213319680	198180864	-61046784			

b_8

m \ k	0	1	2	3	4	5	6	7	8
1	-26588696/105	26759984/21	-919073072/105	131300336/5	-142150368/5	-21285488/5	161887728/5	-23939568	5721144
2	-47306192/21	425419136/105	-857689792/105	206187136/5	-370560992/5	158432384/5	188788288/5	-41642112	11442288
3	-81409312/15	36392416/15	820841056/15	-1663306912/15	192949984/5	79907936	-82216992	22884576	
4	-97292672/5	20667776	573346432/5	-990002304/5	-418201728/5	1954307712/5	-299943552	74844288	
5	-101822720	342577664	-150999808	-771341312	1321742592	-827414016	187257600		
6	-133222400	292569088	646057984	-2788319232	3562401792	-2007588864	428101632		
7	-533225472	2969714688	-6313893888	6462234624	-3195518976	610689024			
8	-392429568	2601517056	-5852725248	5897945088	-2681634816	427327488			
9	784859136	-1742733312	648216576	792723456	-483065856				

results for the fcc lattice, except in the vicinity of the critical point. The series is certainly not of adequate length to treat the two-dimensional lattices. However, it is of interest to make a comparison between the results of the eighth-order series analysis and the exact results of the plane square lattice obtained by Fisher.[7] We have carried out the same Padé-approximants analysis for the plane square lattice. In the ferromagnetic phase we have substituted the exact values of the magnetization for M in the coefficients of the series. In Fig. 2 we have plotted Fisher's exact results with the solid line. The results of the eighth-order series analysis are shown with dots. The error bar again indicates only the apparent convergence of the Padé approximants. For temperatures within the range 15% above and below the critical temperature ($k_B T_c/Jz = 0.5673$) the approximants show a general decrease of values as the order of the approximant increases. We therefore have chosen the lowest value of the approximants and made an estimate of the uncertainty by comparing it with the values of lower-order approximants. The Padé approximants fail to indicate any convergence for temperatures ($k_B T/Jz$) from 0.55 to the critical point. Outside the vicinity of the critical point (15% above and below T_c) the Padé approximants show definite convergence and the results agree with the exact values, with uncertainties smaller than the size of the dots.

It is quite encouraging to find that the linked-cluster series yields accurate results up to the vicinity of the critical point for a two-dimensional model. While it is difficult to estimate the absolute accuracy for the three-dimensional model, it is generally true that the series converges much faster for the higher-dimensional lattices. We can therefore conclude that the results for the fcc lattice should be reliable apart from the uncertainties indicated by the error bars. The precise critical behavior is, however, not deducible with confidence in the present work. Much longer series can be obtained using the current method. Work on a longer series is in progress to improve the results in the critical region.

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