High-temperature series for the susceptibility of the spin-S Ising model

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We have extended the series for the zero-field susceptibility of the spin-S Ising model to eighth order in the reduced temperature K , on the triangular, simple cubic, body-centered-cubic, and face-centered-cubic lattices. The coefficients of these series $h_n(S)$ are expressed as simple polynomials in $X = S(S + 1)$. For the face-centered-cubic lattice, an accurate polynomial fit to the critical point $K_c(S)$ is presented; and the apparent spin dependence of the critical exponent γ is briefly discussed. The series are quite well behaved for all S. However, the large-S series seems to exhibit more rapid apparent convergence.

I. INTRODUCTION

Domb and Sykes' have presented high-temperature series for the zero-field susceptibility of the spin-S Ising model on the face-centered-cubic (fcc) lattice. Their series extend through order six (but contain a minor typographical error in order four²). In this work we report new calculations for this model, in which we extend the series through order eight on the fcc lattice, and also present new series through eighth order on the triangular (TRI), simple cubic (sc), and body-centered-cubic (bcc) lattices. These series are presented in the format chosen by Domb and Sykes, 1 to facilitate compar ison with their results.

We have performed extensive analyses of the fcc series, and find that the apparent critical index γ varies from 1.232 for $S = \infty$ to 1.246 for $S = \frac{1}{2}$. The former value agrees with the analysis of Jasnow and Wortis³ for the Ising limit of the classical ($S = \infty$) anisotropic Heisenberg model. The latter value is changed to 1.²⁴⁸ if the order-twelve series developed by Moore, Jasnow, and Wortis⁴ for the spin- $\frac{1}{2}$ Ising model is employed. In addition, we have obtained an accurate two-parameter fit to the "best" eighth-order estimates of the critical point $K_c(S)$.

The series expansions presented herein have been derived by means of a generalization of the recursive method of Stanley and Kaplan.⁵ This method is, in turn, a variation of the linked-cluster expansions employed by Domb and others. 6 The recursion-relation procedure developed by Stanley and Kaplan makes the calculation of lower-order over $laps⁶$ in the linked-cluster method essentially automatic. Stanley and Kaplan used their procedure on the classical isotropic Heisenberg model, 4-6 for which two significant simplifications are present. Namely, no articulated diagrams^{6} contribute to the expansions, and a decomposition theorem for the computation of overlaps may be developed from the recursion relation.

We have considered the general class of models with Hamiltonians of the form

$$
-\beta \mathcal{C} = \sum_{\vec{\mathbf{r}}} W(Q(\vec{\mathbf{r}})) + \frac{1}{2}K \sum_{\vec{\mathbf{r}}} \sum_{\vec{0}} Q(\vec{\mathbf{r}}) \cdot Q(\vec{\mathbf{r}} + \vec{\delta}), \quad (1.1)
$$

where $\beta = 1/(kT)$, $Q(\vec{r})$ is a classical tensor variable with arbitrary domain, W is an even function of Q , and $Q(\vec{r}) \cdot Q(\vec{r} + \vec{\delta})$ is the inner product of $Q(\vec{r})$ and $Q(\vec{r}+\vec{\delta})$. In general, for this class of models, the simplifications available for the classical isotropic Heisenberg model are not present. That is, articulated diagrams are necessarily included; and the decomposition theorem of Stanley and Kaplan⁵ must be interpreted with care. In general we have found it more useful to employ the recursion relations in their multiplicative form. Series expansions for the susceptibility (and other functions of interest) have been derived through eighth order in K for arbitrary models of the type described by Eq. (1.1) . Details of the method, and other applications, are described elsewhere.⁷

II. DETAILS OF THE MODEL

We follow the notation of Domb and Sykes. ' The spin-8 Ising Hamiltonian may be cast in the form

$$
\mathcal{R}(S) = -\frac{J}{S^2} \sum_{\vec{\mathbf{r}}} \sum_{\vec{\mathbf{r}}} S^z(\vec{\mathbf{r}}) S^z(\vec{\mathbf{r}} + \vec{\mathbf{c}}) - \frac{m}{S} \sum_{\vec{\mathbf{r}}} S^z(\vec{\mathbf{r}}) \quad , \quad (2.1)
$$

where J is the exchange energy; H is the magnetic field; m is the magnetic moment; and the variable $S^{Z}(\vec{r})$ takes on values $-S$, $-S+1$, ..., $S-1$, S. Thus, the variable K in the general Hamiltonian described by Eq. (1.1) becomes $K(S) = \beta JS^{-2}$ for the Ising model. In all that follows, the magnetic field is set equal to zero. The zero-field susceptibility is defined as

$$
\chi_0 = \lim_{H \to 0} \frac{\partial}{\partial H} \left(\frac{m}{S} \left\langle S^Z(\vec{0}) \right\rangle \right) \quad . \tag{2.2}
$$

 χ_0 may be obtained either by calculating the Helmholtz free energy $F(K(S), H)$ to at least second order in H and taking the second derivative of F with respect to H at $H = 0$, or by using the zero-field sum rule

$$
\frac{e}{\chi_0} = \frac{\beta m^2}{S^2} \sum_{\vec{r}} G^Z(\vec{r}) \quad . \tag{2.3}
$$

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9

Here $G^{\mathbf{z}}(\overline{\mathbf{R}})$ is the spin correlation function

 $\langle S^{\mathcal{Z}}(\vec{\mathbf{0}}) S^{\mathcal{Z}}(\vec{\mathbf{R}}) \rangle$. It is the latter method that we have actually employed in calculating χ_0 .⁷

Following Domb and Sykes,¹ the zero-field susceptibility is expanded as

$$
\chi_0 = \frac{S(S+1)m^2K(S)}{3J} \sum_{n=0}^{\infty} h_n(S)[K(S)]^n \quad . \tag{2.4}
$$

It turns out that for a given lattice, one may write $h_n(S)$ as a polynomial of degree n in $X = S(S+1)$:

$$
h_n(S) = \sum_{i=1}^{n} \frac{C_i^{(n)} X^i}{D_n} , \qquad (2.5)
$$

where we have explicitly included a common denominator D_n in each polynomial. Note that the coefficient of X^0 is absent from h_n for all n . The coefficients, $C_i^{(n)}$ and common denominator D_n for $n=1, 2, \ldots$, 8 on each lattice are presented in Table I. For each order n , D_n is listed first, followed

TABLE I. Susceptibility series through order eight for spin-S Ising model. For each order the expansion coefficient $h_n(S)$ [see Eq. (2.4)] is given by

$$
D_n h_n(S) = \sum_{l=1}^n C_l^{(n)} X^l
$$

where $X = S(S+1)$ and the coefficients $C_i^{(n)}$ are listed below D_n beginning with $C_i^{(n)}$. For example, on the triangular net, $h_2(S) = \frac{1}{5}(18X^2 - X)$. Note that $h_0(S) = 1$ for all lattices.

by $C_1^{(n)}$, $C_2^{(n)}$, ..., $C_n^{(n)}$. The leading term h_0 is unity for all lattices. The remainder of this work is concerned with the spin dependence of the critical point and susceptibility of the Ising model.

III. ANALYSIS OF fcc SUSCEPTIBILITY SERIES

We have chosen to analyze the series on the fcc lattice because (i) this lattice and topologically equivalent orthorhombic lattices are prevalent in nature and (ii) the series are found in practice to converge more rapidly as the lattice coordination increases. ' Although the results are not discussed herein, somewhat less detailed analyses of the sc and bcc series are in essential agreement with the fcc results. However, the apparent accuracy of the results is lower due to the oscillation of the ratios on loose-packed lattices.

As is well known⁹ the zero-field susceptibility diverges as the critical point is approached. This divergence is characterized by the critical exponent γ , which may be defined by the relationship⁹

$$
\chi_0 = \overline{\chi} \big[1 - K/K_c(S) \big]^{-\gamma}, \quad K \to K_c(S) \quad . \tag{3.1}
$$

We have used the end-shifted-ratio method $^{\rm 9,10}$ to obtain numerical estimates of $K_c(S)$ and $\gamma(S)$ from the series for χ . More than 20 values of S, distributed evenly on a logarithmic scale between $S = \frac{1}{2}$ and $S = \infty$, have been investigated.

Since the method of end shifts is not so well known as other series-summation methods, we discuss it briefly herein. Given that a power series has its radius of convergence determined by a singularity on the real axis, we may estimate the radius of convergence (critical point) by forming ratios $R_n = h_n / h_{n-1}$ of succeeding terms in the sequence $\{h_n\}$ of coefficients of the series. By d'Alembert's ratio test, the radius of convergence x_c is determined from

$$
\lim_{n \to \infty} \frac{h_n x_c^n}{h_{n-1} x_c^{n-1}} = 1
$$
\n(3.2)

or

$$
x_c = \lim_{n \to \infty} \frac{1}{R_n} \quad .
$$

Now the approach of R_n to x_c^{-1} may be very slow or nonuniform, in general, so that one cannot really say anything in general about x_c from the first few ratios. However, if we have good reason to believe the function in question has a particular functional form, we may use that information in estimating x_c from the first few R_n . Thus, given Eq. (3.1), we expect that the ratios, $R_n(S) = h_n(S)/h_{n-1}(S)$, for $\chi_0(S)$ will behave as

$$
R_n(S) \approx K_c(S)^{-1} [1 + (\gamma - 1)/n]
$$
 (3.3)

for large enough $n.^9$ Thus, one expects $R_n(S)$ to vary linearly with $1/n$ and to converge rapidly to

 $[K_c(S)]^{-1}$. In practice, the asymptotic behavior of R_n may be partially masked by coincident weaker singularities, or by logarithmic corrections such as $\ln[1 - K/K_c(S)]$. When no singular corrections are present the amplitude functions $[\bar{\chi}]$ in Eq. (3.1) , even though analytic at $K_c(S)$, will introduce curvature in the behavior of $R_n(S)$ at small n. A number of methods of dealing with this curvature have been developed, $3,9$ including the Neville table³ and the method of end shifts 9,10 used herein.

The method of end shifts may be heuristically justified by noting that there is an ambiguity of at least ± 1 in *n* in our definition of the ratios $R_n(S)$. Indeed, according to Eq. (3.3) for large enough n, R_n will become a linear function of $1/(n+\Delta)$ for any (finite) choice of Δ . The idea of end shifts is that the effect of corrections to Eq. (3.1) is largely to make R_n linear as a function of $1/(n+\Delta_0)$, for some choice Δ_0 , rather than as a function of $1/n$. In practice the "best" choice for Δ_0 is determined by forcing linearity in the last three available ratios. That is, the three equations

$$
R_n = R_{\infty}^* + A/(n + \Delta_0) \quad , \tag{3.4a}
$$

$$
R_{n-1} = R_{\infty}^* + A/(n + \Delta_0 - 1) \quad , \tag{3.4b}
$$

and

$$
R_{n=2} = R_{\infty}^* + A/(n + \Delta_0 - 2)
$$
 (3.4c)

TABLE II. Best estimates of the critical point $[K_*(S)]^{-1}$ and the exponent $\gamma(S)$ using eight orders on the fcc lattice. The end shift $\Delta(S)$ employed in the estimate is also listed.

determine the "best" estimate $(R_{{\bullet}}^{*})^{-1}$ for the critical point, the end shift Δ_0 , and the amplitude A, uniquely. The solutions are

$$
\Delta_0 = \frac{2(n-1)R_{n-1} - (n-2)R_{n-2} - nR_n}{R_n - 2R_{n-1} + R_{n-2}}, \qquad (3.5a)
$$

$$
R_{\infty}^{*} = (n + \Delta_{0})R_{n} - (n + \Delta_{0} - 1)R_{n-1} \quad , \tag{3.5b}
$$

and

$$
A = (R_n - R_{\infty}^*) (n + \Delta_0) \quad . \tag{3.5c}
$$

By comparing Eq. (3.3) with $(3.4a)$ we obtain approximants $\gamma_n(\Delta_0)$ for the critical exponent γ :

$$
\gamma_n(\Delta_0) = A/R_{\infty}^* + 1 = (n + \Delta_0)R_n/R_{\infty}^* - (n + \Delta_0 - 1)
$$
 (3.6)

This estimate for γ is not independent of R_{∞}^{*} , the estimate for $[K_c(S)]^{-1}$. One might hope to obtain an "unbiased" estimate for γ by use of the approximants $\gamma_n^{(u)}(\Delta)$ defined by

$$
\gamma_n^{(u)}(\Delta) = \frac{R_n(n+\Delta)}{(n+\Delta)R_n - (n+\Delta-1)R_{n-1}} - (n+\Delta-1),
$$
\n(3.7)

since R_{∞}^{*} is not specified as it is in Eq. (3.6). However, the use of Δ -and particularly its choice according to the criterion that last two available estimates $\gamma_{n=1}^{(u)}(\Delta)$ and $\gamma_{n}^{(u)}(\Delta)$ to be equal to one another-forces the equality $\gamma_n^{(u)} = \gamma_n$. That is, the same solutions for the end shift Δ_0 and exponent γ are obtained in both cases. Thus, unlike other ratio methods, the method of end shifts does not produce independent estimates for γ . (Compare with the work of Hunter and Baker. 11)

On this point, however, note that the end-shift estimate for γ is not biased in the sense that the word is used in Ref. 11. That is, one obtains a biased estimate¹¹ for γ by supplying an accurate estimate for K_c (say from logarithmic-derivative series^{9,11}) and forcing the ratios to reproduce this value of K_c by adjustment of γ . The estimates for γ obtained from Eq. (3.6) appear to be biased in that they apparently depend on the estimate R^*_{\bullet} for K_c^{-1} . However, R_{∞}^{*} and γ are *both* fixed once the "best" value for Δ is chosen- γ and R^* are actually treated on equal footing. Biased estimates for γ can easily be obtained within the end shift method; and we have employed such estimates to check the results for γ described below.

The method of end shifts is by no means a cure all for series analysis; it suffers from many of the same failings as other ratio variants. (For a discussion of the applicability of various series, summation methods, consult Ref. 11.) However, it is less "rigid" than the Neville table³ as an extrapolation method. In addition, it can be extended to sequences which have a more general functional dependence on n than $1/n$; for example, Fisher and Camp^{10} have used this method to extrapolate sequences which behave as $n^{-\nu}$ for large n.¹²

TABLE III. Critical-parameter estimates obtained using N terms for $S = \frac{1}{2}$ (N = 5, 6, ..., 13) and $S = \infty (N = 5$, ..., 9) on the fcc lattice.

\boldsymbol{N}	$[K_{c}(\frac{1}{2})]^{-1}$	$\gamma(\frac{1}{2})$	$\Delta(\frac{1}{2})$	$[K_{c}(\infty)]^{-1}$	$\gamma(\infty)$	$\Delta(\infty)$
5	9.7667	1.269	0.13	3.48310	1.300	1.30
6	9.7776	1.261	0.08	3.50527	1.241	0.82
$\overline{7}$	9.8019	1.238	-0.12	3.50825	1.232	0.72
8	9.8047	1.235	-0.15	3.50779	1.233	0.74
9	9.796 06	1.246	0.0	3.50814	1.232	0.72
10	9.79398	1.247	0.06			
11	9.79467	1.248	0.04			
12	9.79547	1.247	0.01			
13	9.79496	1.248	0.04			

The end-shift analysis has been checked throughout against Neville-table results.^{3,11} The estimates for K_c and γ obtained from the two methods agree closely, and the choice of end shifts over Neville tables reflects personal preference.

The estimates for $[K_c(S)]^{-1}$ exhibit a very smooth behavior as a function of S. In fact the variation with S is very close to that predicted by molecularfield theory.¹³ Namely,

$$
[K_c(S)]^{-1} \propto (S+1)/S \quad . \tag{3.8}
$$

In fact, we have constructed a two-parameter least-squares fit

$$
S^{2}K_{c}(S)^{-1} = S(S+1)K_{c}(\infty)^{-1} + K_{0} + K_{1}/S \quad , \quad (3.9)
$$

where $K_0 = -0.20949$ and $K_1 = 0.01370$ -which reproduces the results of Table II for $[K_c(S)]^{-1}$ to within 0. 002% for all values listed. The variation of $K_c(S)$ with S when S is not too small is thus very well accounted for by molecular-field theory. It is gratifying, also, that the estimates for $K_c(S)$ are sufficiently self-consistent that a two-parameter fit is accurate to more than four places.

An important fact to be noted about Table II is the difference between the estimates $\gamma(\frac{1}{2}) \approx 1.246$ and $\gamma(\infty) \approx 1.232$. Furthermore, this difference is evident between $\gamma(\frac{1}{2})$ and $\gamma(S)$, which for all S greater than $S = 3$ are unchanged from $\gamma(\infty)$ (to within quoted apparent accuracies). Such a marked difference is confounding in the face of the universality hypothesis^{3,4,9,14} which states, in particular, that γ does not depend on such things as kinematics. This hypothesis has recently been put on a firmer basis in the context of Wilson's renormalizationbasis in the context of Wilson's renormalizatio
group theory (RGT).¹⁵ According to this theory the spin-S Ising models all correspond to the same fixed point of the renormalization group, and must therefore have the same value of γ .

If we are thus not to believe the differences in γ to be real, we must face the question of which value of γ to accept, $\gamma \approx 1.246$ (S = $\frac{1}{2}$) or $\gamma \approx 1.232$ (S = ∞), or neither? Scaling theory⁹ and RGT¹⁵ both make the choice $\gamma = \frac{5}{4}$ attractive: the scaling relations are beautifully satisfied with $\gamma = \gamma' = \frac{5}{4}$, $\beta = \frac{5}{16}$, and $\alpha = \alpha' = \frac{1}{8}$. We note that RGT predicts, via the ϵ ex-

—
pansion, ¹⁵ that γ ≈ 1. 244; this result is obtained by keeping all terms through second order in $\epsilon = 4-d$, keeping all terms through second order in $\epsilon = 4 - d$,
where d , the dimensionality, is equal to 3.¹⁵ How ever, there is good evidence from series that $\gamma' \approx 1.29 - 1.31 \neq \gamma$ and that $\alpha' \approx \frac{1}{16} \neq \alpha$, ⁹ so that scaling arguments may not be valid in three dimensions for the Ising model. In addition, the ϵ expansion is probably asymptotic, at best¹⁵; so, while $\frac{1}{4}$ is favored, the question cannot be settled by RGT and scaling theory. Rather, the small, but readily apparent, spin dependence we have found must be considered, along with evidence that $\alpha \neq \alpha'$ and $\gamma \neq \gamma'$, as evidence against scaling $^{\mathsf{9}}$ and universality $^{\mathsf{14}}$ in the three-dimensional Ising model.

We have made end-shift estimates for $[K_c(\mathcal{S})]^{-1}$ and $\gamma(S)$ with $S=\frac{1}{2}$ and $S=\infty$, using 5-9 terms for $S = \infty$, and 5-13 terms for $S = \frac{1}{2}$. The longer series for $S = \frac{1}{2}$ was taken from Ref. 4. The results are presented in Table III. Note that the $S = \infty$ results, to eighth order, have apparently converged at γ =1.232, whereas the S = $\frac{1}{2}$ results are still changing significantly at eighth order. This apparent convergence of the $S = \infty$ series could be due to a defect, 16 and thus disappear in higher orders. The result for $\gamma(\frac{1}{2})$ using 13 terms is $\gamma(\frac{1}{2}) \approx 1.248 \approx \frac{5}{4}$. (Our result for K_c^1 based on the longer series is 9.7950 which differs by 1 part in $10⁴$ from the value 9.7940 obtained for the same series in Ref. 4.)

- *Work supported by the U. S. Atomic Energy Commission. ¹C. Domb and M. F. Sykes, Phys. Rev. 128, 168 (1962).
- ²Namely, 2322 X should replace 2331 X in the coefficient h_4 of Appendix I of Ref. 1.
- ${}^{3}D.$ Jasnow and M. Wortis, Phys. Rev. 176, 739 (1968).
- ⁴M. A. Moore, D. Jasnow, and M. Wortis, Phys. Rev. Lett. 22, 940 (1969).
- ⁵H. E. Stanley and T. A. Kaplan, Phys. Rev. Lett. 16, 981 (1966); H. E. Stanley, Phys. Rev. 158, 537 (1967).
- 6 C. Domb [Adv. Phys. $9, 149$ (1960)] presents a thorough review of linked-cluster expansions, and extensive references to other series work before 1960.
- 7 J. P. Van Dyke and W. J. Camp, AIP Conf. Proc. (to be published); and W. J. Camp and J. P. Van Dyke (unpublished). Actually, we have derived series for the more general class of Hamiltonians for which the term $Q(\vec{r}) \cdot Q(\vec{r} + \vec{\delta})$ is replaced by an arbitrary two-body interaction function, $F(Q(\overline{r}); Q(\overline{r}+\delta))$.
- 8 From a series point of view, this has two causes: (i) the close-packed lattices lack the alternation caused by the antiferromagnetic singularity of the loose-packed lattices; and (ii) the higher the lattice coordination, the more complex the graphs entering into a given orderthus series display their asymptotic character sooner on such lattices.
- 9 For a review of the behavior of systems near critical points, and, in particular, for a definition of the various critical exponents, consult M. E. Fisher, Rept. Prog. Phys. 30, 615 (1967).
- 10 M. E. Fisher and W. J. Camp, Phys. Rev. B $_5$, 3730 (1972).
- 11 D. L. Hunter and G. A. Baker, Jr., Phys. Rev. B $\frac{7}{1}$,

Unfortunately, while the eighth-order results are apparently well converged, they are not sufficient evidence to settle the question of the spin dependence. If we accept the universality hypothesis, ¹⁴ then based on the four additional terms in the $S=\frac{1}{2}$ series we would tentatively conclude $\gamma = \frac{5}{4}$ for all S, although the contradictory evidence for $S \gtrsim 4$ cannot be ignored.¹⁷

Another viewpoint in analyzing these series, and Another viewpoint in analyzing these series, and
one adopted by Wortis, Saul, Moore, and Jasnow, ¹⁸ is-accepting universality and scaling-to force γ to equal $\frac{5}{4}$ for all S. This may be done by allowing for weaker confluent singularities in χ . Within the spirit of universality one would expect the exponent of the weaker singularity to also be independent of S, while its amplitude would decrease with decreasing S and perhaps become identically zero at $S=\frac{1}{2}$. Such an analysis is very interesting and does yield, if the nature of the confluent singularity is found to be reasonable, a plausible explanation for the apparent spin dependence we have found in our estimates for γ .

Note added in proof. We have extended the series through order ten on the two- and threedimensional lattices. The apparent convergence of γ (S) to 1.232–for large S–persists when the two additional terms are included, the change in $K_{\alpha}(\infty)$ being less than 3 parts in 10.

3346 (1973).

- 12 In this context, we note that the method can be successfully employed to predict logarithmic corrections of the form $[-\ln(1-K/K_c)]^{\Omega}/(1-K/K_c)^{\gamma}$. We have used this fact to estimate and remove the logarithmic corrections to renormalization group theory on the close-packed hypercubic four-dimensional lattice which has 24 nearest neighbors. This work will be reported elsewhere.
- 13 H. E. Stanley, Introduction to Phase Transitions and Critical Phenomena (Clarendon, Oxford, England, 1971), p. 90.
- 14 L. P. Kadanoff, in Proceedings of the International L. P. Kadanoff, in Proceedings of the International
School of Physics "Enrico Fermi," Course 51, Critica Phenomena (Academic, New York, 1971); R. B. Griffiths, Phys. Rev. Lett. 24, 1479 (1970).
- 15 For a review of this theory, and extensive references, consult K. Wilson and J. Kogut, Phys. Reports (to be published}.
- See Ref. 11 for a discussion of series defects.
- 17 In this context we have examined how the series for $\chi(\infty)$ and $\chi(\frac{1}{2})$ differ. The most striking differences between them is that the series for $\chi(\infty)$ includes contributions from all two-point diagrams, while only nonarticulated diagrams contribute to $\chi(\frac{1}{2})$. Therefore, we have formed the series, $\chi_{NA}(\infty)$, obtained by neglecting articulated diagrams in $\chi(\infty)$. This series has a critical point $(K_c^*)^{-1} \approx 3.32675$, and critical exponent $\gamma^* \approx 1.245$. The exponent agrees much better with the $S=\frac{1}{2}$ value than does that estimated from the full series. However, since $(K_c^*)^{-1}$ disagrees with $(K_c)^{-1}$, χ_{NA} cannot fully represent the dominant singularity in $\chi(\infty)$.
- 18 D. Jasnow (private communication).