

## High-Temperature Expansions for the Classical Heisenberg Model. II. Zero-Field Susceptibility\*

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The high-temperature series expansion of the zero-field magnetic susceptibility,  $\chi/\chi_{\text{Curie}}=1+\sum_{l=1}^{\infty} a_l (J/kT)^l$ , is related to the diagrammatic representation of the corresponding high-temperature expansion of the zero-field static spin correlation function  $\langle \mathbf{S}_f \cdot \mathbf{S}_g \rangle_{\beta}$  presented elsewhere. The first nine terms  $a_l$  for loose-packed lattices and the first seven terms for close-packed lattices in the susceptibility series are explicitly obtained in terms of Domb's "general lattice constants"  $p_{l\alpha}$ . The general lattice expressions are then used to evaluate these  $a_l$  numerically for three two-dimensional lattices and for three cubic lattices. Finally, the  $a_l$  are employed to discuss two questions of current interest: (1) Does the critical exponent  $\gamma$ —in the assumed form of the divergence of  $\chi$ ,  $\chi \sim (T-T_c)^{-\gamma}$  as  $T \rightarrow T_c^+$ —have the value  $\frac{3}{2}$  for the fcc, bcc, and sc lattices? (2) Do high-temperature expansions suggest a phase transition ( $T_c \neq 0$ ) for some two-dimensional lattices with nearest-neighbor ferromagnetic interactions? It is argued that extrapolation suggests  $\gamma$  is definitely greater than  $\frac{3}{2}$  for the fcc, bcc, and sc lattices, and that  $T_c$  is appreciably different from zero for the plane square and triangular lattices.

### I. INTRODUCTION

**T**HE high-temperature expansion of the zero-field susceptibility

$$\chi/\chi_{\text{Curie}} = 1 + \sum_{l=1}^{\infty} a_l (J/kT)^l \quad (1)$$

is difficult to extend beyond order  $l=6$  for general spin quantum number  $S$  because of the enormous labor involved.<sup>1</sup> Recently it was shown that order-of-magnitude simplifications occur when one treats the non-commuting quantum-mechanical spin operators occurring in the Heisenberg Hamiltonian as commuting vectors of length  $\bar{S} \equiv [S(S+1)]^{1/2}$ , suggesting that many more terms in the series can be obtained "semi-classically" than "quantum mechanically."<sup>2</sup> Moreover, *useful* results in the critical region ( $T > T_c$ ) can be obtained from this classical Heisenberg model or "infinite-spin approximation," the errors in various critical properties of interest being small and decreasing rapidly with  $S$ .

Elsewhere<sup>3</sup> the simplifications of the classical Heisenberg model were exploited to obtain the diagrammatic representation of the first nine coefficients  $\alpha_l$  for loose-packed lattices and the first eight  $\alpha_l$  for close-packed lattices in a high-temperature series expansion of the

zero-field static spin correlation function

$$\langle \mathbf{S}_f \cdot \mathbf{S}_g \rangle_{\beta} = \sum_{l=0}^{\infty} \frac{(-1)^l}{l!} \alpha_l \beta^l. \quad (2)$$

In Sec. II we utilize these results to calculate the first nine terms  $a_l$  for loose-packed lattices and the first seven terms for the close-packed lattices<sup>4</sup> in the susceptibility series Eq. (1) for the classical Heisenberg model with nearest-neighbor (n.n.) exchange interactions.<sup>5</sup> Following previous practice, we shall first obtain expressions for the susceptibility coefficients  $a_l$  in terms of "general lattice constants,"<sup>6</sup> and then, using the general lattice expressions, we will evaluate the  $a_l$  numerically for three two-dimensional lattices (plane square, triangular, and honeycomb) and for three three-dimensional lattices (fcc, bcc, and sc). Before the present work was finished, Wood and Rushbrooke<sup>7</sup> independently obtained and published eight terms  $a_l$

<sup>4</sup> We do not include the close-packed lattices (e.g., face-centered cubic and plane triangular) in our eighth- and ninth-order calculations. For example, in order  $l=8$  there are roughly four times as many diagrams needed for the close-packed as compared to the loose-packed lattices. Also, there is somewhat less motivation for obtaining additional terms in the series for the close-packed lattices, since the terms are more regular for close-packed than for loose-packed lattices.

<sup>5</sup> Some of the results of this work were presented in November 1966 as parts of two talks at the Twelfth Annual Conference on Magnetism and Magnetic Materials, the proceedings of which will appear in *J. Appl. Phys.* (see Refs. 10 and 13). A preliminary account of this work is also given in H. E. Stanley, M. I. T. Lincoln Laboratory Solid State Research Report No. 4, DDC 647688, 1966, (unpublished). See also *Bull. Am. Phys. Soc.* **12**, 134 (1967); **12**, 334 (1967).

<sup>6</sup> C. Domb, *Advan. Phys.* **9**, 330 (1960), Appendix III; C. Domb and M. F. Sykes, *Phil. Mag.* **2**, 733 (1957).

<sup>7</sup> P. J. Wood and G. S. Rushbrooke, *Phys. Rev. Letters* **17**, 307 (1966). For a discussion of the relation between their method and ours, see Appendix A of Ref. 3. See also G. S. Joyce and R. G. Bowers [*Proc. Phys. Soc. (London)* **88**, 1053 (1966)], who have described an alternative procedure of extending Eq. (1) classically.

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<sup>1</sup> Recently additional terms have been obtained for  $S=\frac{1}{2}$  by methods practicable only for  $S=\frac{1}{2}$ . See C. Domb and D. W. Wood, *Proc. Phys. Soc. (London)* **86**, 1 (1965); G. A. Baker, H. E. Gilbert, J. Eve, and G. S. Rushbrooke, *Phys. Letters* **20**, 146 (1966).

<sup>2</sup> H. E. Stanley and T. A. Kaplan, *Phys. Rev. Letters* **16**, 981 (1966).

<sup>3</sup> H. E. Stanley, preceding paper, *Phys. Rev.* **158**, 537 (1967).

TABLE I. The susceptibility coefficients  $a_l$  (notation as in Ref. 6).

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$$\begin{aligned}
a_1 &= \left(\frac{2}{3}\right) (\sigma+1) \\
a_2 &= \left(\frac{2}{3}\right)^2 \sigma (\sigma+1) \\
a_3 &= \left[\frac{2}{3}\right]^3 [1/5] [(5\sigma^2-3)(\sigma+1) - 30p_3] \\
a_4 &= \left[\frac{2}{3}\right]^4 [1/5] [(5\sigma^3-6\sigma)(\sigma+1) - 12(5\sigma+2)p_3 - 40p_4] \\
a_5 &= \left[\frac{2}{3}\right]^5 [1/25] [5(5\sigma^4-9\sigma^2+18/7)(\sigma+1) - 6(75\sigma^2+40\sigma-78)p_3 - 80(5\sigma+2)p_4 - 250p_5 + 120p_{6a}] \\
a_6 &= \left[\frac{2}{3}\right]^6 [1/175] [(175\sigma^5-420\sigma^3+243\sigma)(\sigma+1) - 6(700\sigma^3+420\sigma^2-1302\sigma-891)p_3 - 56(75\sigma^2+40\sigma-93)p_4 - 700(5\sigma+2)p_5 \\
&\quad + 84(20\sigma+89)p_{6a} - 2100p_6 + 840(p_{6a}+p_{6b}) + 1400p_{6c}] \\
a_7 &= \left[\frac{2}{3}\right]^7 [1/875] [5(175\sigma^6-525\sigma^4+459\sigma^2-81)(\sigma+1) - 30(875\sigma^4+560\sigma^3-2268\sigma^2-1950\sigma+804)p_3 \\
&\quad - 32(875\sigma^3+525\sigma^2-1890\sigma-657)p_4 - 350(75\sigma^2+40\sigma-108)p_5 + 12(1050\sigma^2+6230\sigma+7527)p_{6a} + 70\{-60(5\sigma+2)p_6 \\
&\quad + 24(5\sigma+9)p_{6a} + 3(40\sigma+193)p_{6b} + 40(5\sigma+9)p_{6c} + 259.2p_{6d} - 175p_{7a} + 60(p_{7a}+p_{7b}+p_{7c}) + 132p_{7e} \\
&\quad + 100(p_{7d}+p_{7e}) + 990p_{7f}\}] \\
a_8 &= \left[\frac{2}{3}\right]^8 [1/875] [5(175\sigma^7-630\sigma^5+738\sigma^3-270\sigma)(\sigma+1) - 8(4375\sigma^4+2800\sigma^3-12915\sigma^2-6096\sigma+5637)p_4 \\
&\quad + 70\{-6(75\sigma^2+40\sigma-123)p_6 + 7.2(25\sigma^2+60\sigma+213)p_{6a} + 12(10\sigma+52)p_{7a} - 200p_8 + 60p_{8c} + 100p_{8k} + 1080p_{8r}\}] \\
a_9 &= \left[\frac{2}{3}\right]^9 [1/875] [(875\sigma^8-3675\sigma^6+5400\sigma^4-3024\sigma^2+4050/11)(\sigma+1) - 8(5250\sigma^5+3500\sigma^4-19320\sigma^3-10404\sigma^2+16080\sigma+4380)p_4 \\
&\quad + 70\{-24(25\sigma^3+15\sigma^2-69\sigma-867/35)p_6 + 24(10\sigma^3+27\sigma^2+124.8\sigma+159/7)p_{6a} + 6(30\sigma^2+208\sigma+2368/35)p_{7a} \\
&\quad - 80(5\sigma+2)p_8 + 8(5\sigma+9)(3p_{8c}+5p_{8k}) + 144(15\sigma+13)p_{8r} + 172.8p_{8t} + 100p_{9j} + 60(p_{9k}+p_{9i}) + 132p_{9m}\}]
\end{aligned}$$


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for the fcc, bcc, and sc lattices. Although their “moment expansion” of the partition function differs from our use of the spin correlation function, we obtain the same numerical values of the coefficients  $a_l$  when we specialize to the cubic lattices they treated.

In Sec. III we analyze the extended series (1) by Padé approximants and “slope methods” and consider two questions of current interest: (1) Does the critical exponent  $\gamma$ —in the assumed form of the divergence of  $\chi$ ,  $\chi \sim (T-T_c)^{-\gamma}$  as  $T \rightarrow T_c^+$ —have the value  $\frac{4}{3}$  for the fcc, bcc, and sc lattices? (2) Do high-temperature expansions suggest a phase transition ( $T_c \neq 0$ ) for some two-dimensional lattices with nearest-neighbor ferromagnetic interactions? We argue that  $\gamma$  is definitely greater than  $\frac{4}{3}$  for the fcc, bcc, and sc lattices, and that extrapolation to  $T_c=0$  for the plane square and triangular lattices is much less reasonable than extrapolation to nonzero  $T_c$ .

## II. CALCULATION OF THE SUSCEPTIBILITY COEFFICIENTS

For a Heisenberg Hamiltonian

$$\mathcal{H} \equiv -2J \sum_{f,g} \mathbf{S}_f \cdot \mathbf{S}_g - g\mu_B H \sum_f S_{fz} \quad (3)$$

with nearest-neighbor exchange parameter  $J$ , the zero-field susceptibility per spin  $\chi$  and the zero-field spin correlation function  $\langle \mathbf{S}_f \cdot \mathbf{S}_g \rangle_\beta$  are related by

$$\chi = (g^2 \mu_B^2 \beta / 3N) \sum_{f,g} \langle \mathbf{S}_f \cdot \mathbf{S}_g \rangle_\beta, \quad (4)$$

as may be readily verified upon differentiating the partition function with respect to the magnetic field. Hence the susceptibility coefficients  $a_l$  in Eq. (1) may be obtained directly from the  $\alpha_l$  in the high-temperature series (2) for  $\langle \mathbf{S}_f \cdot \mathbf{S}_g \rangle_\beta$  by means of the formula

$$a_l = [N S(S+1) (-J)^l l!]^{-1} \sum_{f,g} \alpha_l. \quad (5)$$

In the preceding paper a diagrammatic representation  $\alpha_l = \sum_{\vec{d}} \bar{\alpha}_l(\vec{d})$  was developed for the coefficients  $\alpha_l$  in

(5). Now all diagrams  $\vec{d}$  of the same “topological type”  $\tau$  contribute equally. Thus the summation  $\sum_{f,g} \sum_{\vec{d}} \bar{\alpha}_l(\vec{d})$  may be replaced by  $2 \sum_{\tau} \alpha_l(\tau) \Lambda(\tau)$ , where  $\Lambda(\tau)$  denotes the number of occurrences on a given lattice of the diagram of topological type  $\tau$ . (For example, the number of four-sided polygons which can be placed on a square lattice is  $N$ ; the number of six-sided polygons is  $2N$ .)

The above is of general validity; henceforth we specialize to the classical Heisenberg model, for which the nonzero  $\alpha_l(\tau)$  are given in Figs. 1–5 of the preceding paper. Hence to find the coefficients  $a_l$  we need only calculate the lattice factors  $\Lambda(\tau)$ . We first express the  $\Lambda(\tau)$  in terms of Domb’s “general lattice constants,”<sup>6</sup> in order to obtain expressions for the  $a_l$  valid for any lattice of equivalent spins. For example, we write  $Np_n$  for the number of  $n$ -sided polygons and  $N[z\sigma^2/2 - 3p_3]$  for the number of three-step chains, where  $\sigma \equiv z-1$  and  $z$  is the lattice coordination number. The “general lattice” expressions thereby obtained are given in Table I. The lattice constants  $p_{lx}$  have been tabulated for common lattices by Domb,<sup>6</sup> so that it is a simple task to compute numerical values for  $a_l$  from Table I. In Table II we list the  $a_l$  for the fcc, bcc, and sc three-dimensional lattices and for the triangular, square, and honeycomb two-dimensional lattices.

## III. APPLICATION TO CRITICAL PHENOMENA

We now utilize the extended series in Eq. (1) to discuss two questions of current interest:

(1) *The divergence of  $\chi$  as  $T \rightarrow T_c^+$  is assumed to be of the form  $\chi \sim (T-T_c)^{-\gamma}$ . Does the critical exponent  $\gamma$  have the value  $\frac{4}{3}$  for the fcc, bcc, and sc lattices?*

Previous arguments<sup>8,9</sup> for  $\gamma = \frac{4}{3}$  have been based upon the assumption that the more classical the model, the more rapidly the terms of the high-temperature series settle into a smooth behavior. This assumption, coupled

<sup>8</sup> C. Domb and M. F. Sykes, Phys. Rev. **128**, 168 (1962).

<sup>9</sup> J. Gammel, W. Marshall, and L. Morgan, Proc. Roy. Soc. (London) **A275**, 257 (1963).

TABLE II. The susceptibility coefficients  $a_l$ .

$l$	Honeycomb net	Square	Triangular	Simple cubic	Body-centered cubic	Face-centered cubic
1	2.0000	2.6667	4.0000	4.0000	5.3333	8.0000
2	2.6667	5.3333	13.3333	13.3333	24.8889	58.6667
3	3.0222	9.9556	39.8222	43.3778	114.7259	413.8667
4	3.3185	16.9086	110.6963	136.2963	509.7877	2 855.3481
5	3.6797	27.2404	292.3096	424.5446	2 249.9706	19 415.8527
6	3.5759	42.2122	741.8552	1 301.5034	9 779.9445	130 694.4263
7	2.8846	63.0670	1822.0514	3 967.8674	42 335.1558	873 209.9634
8	2.6796	91.6638		11 998.0391	181 758.3614	5 800 796.3979 <sup>a</sup>
9	3.2328	129.4967		36 150.6748	778 141.1626	

<sup>a</sup> From Ref. 7.

with the observation from the first six terms that  $\gamma(S=\infty)=\frac{4}{3}$ , has led to the proposal<sup>8,9</sup> that  $\gamma(S)=\frac{4}{3}$  independent of spin and lattice.<sup>10</sup> Here we consider the effect of additional terms  $a_l$  upon  $\gamma(\infty)$ . We find  $\gamma(\infty)$  to be several percent larger than  $\frac{4}{3}$  by means of extrapolations based upon both the method of Padé approximants and the simpler "slope method." The former method is well known<sup>9</sup>; we shall concentrate our discussion on the slope method. If  $\chi$  diverges as  $T \rightarrow T_c^+$  with a power law, then for large  $l$

$$\rho_l \equiv (a_l/a_{l-1}) \rightarrow t_c [1 + (\gamma - 1)/l], \quad (6)$$

so that the limiting slope of a plot of ratios of successive coefficients against  $1/l$  will be proportional to  $\gamma - 1$ . Here  $t_c \equiv T_c/T_M$ , and  $T_M$  is the critical temperature predicted by the molecular-field approximation.

The ratios  $\rho_l$  for the fcc, bcc, and sc lattices are listed in Table III and plotted against  $1/l$  in Fig. 1. The straight lines shown were chosen in such a way as to weight the last few  $\rho_l$  more heavily than the early  $\rho_l$ . They correspond to  $\gamma \cong 1.33$  for the fcc and bcc lattices, and  $\gamma \cong 1.37$  for the sc lattice.

Contrary to the appearance of the top curve in Fig. 1, even the last few  $\rho_l$  for the fcc lattice do *not* lie on a straight line—rather, they possess a *small but steady downward curvature*. A more refined method of estimating the limiting slope (as  $l \rightarrow \infty$ ) could be to determine the slopes of successive "straight-line extrapolations" (SLE's) given 6, 7, 8, ... terms in the series, and then to extrapolate the slopes of these successive SLE's to  $l = \infty$ . But this "second-order" extrapolation would require a subjective choice of the best SLE for each order. A more precise procedure is to choose successive straight lines passing through  $\rho_l$  and  $\rho_{l-1}$ , and to calculate numerically the corresponding functions

$$t_{l,l-1} \equiv \rho_l + (l-1)(\rho_l - \rho_{l-1}), \quad (7)$$

$$\gamma_{l,l-1} \equiv 1 - l[(t_{l,l-1} - \rho_l)/t_{l,l-1}], \quad (8)$$

<sup>10</sup> Recently Stanley and Kaplan suggested (essentially on the basis of the first six terms) that there exists a slow but nevertheless clear variation of  $\gamma$  with  $S$  for fcc, bcc, and sc lattices, and that for the *spinel* lattice with n.n. interactions between the B sites, the value of  $\gamma$  predicted by extrapolations ( $\gamma \cong 1$ ) may differ from  $\frac{4}{3}$  by as much as 50%. See H. E. Stanley and T. A. Kaplan *J. Appl. Phys.* **38**, 977 (1967).

which approach  $t_c$  and  $\gamma$ , respectively, in the  $l \rightarrow \infty$  limit. These new sequences  $t_{l,l-1}$  and  $\gamma_{l,l-1}$  determined from the successive "two-point" SLE's for the fcc lattice are plotted against  $1/l$  in Fig. 2; we see that the  $t_{l,l-1}$  and  $\gamma_{l,l-1}$  are, respectively, monotonically decreasing and increasing. Because of this unambiguous "downward curvature" in the plot of  $\rho_l$  versus  $1/l$ , the SLE chosen in Fig. 1 would seem to be in error. The fact that the last four  $\rho_l$  lie very nearly on a straight line motivates the SLE to  $l = \infty$ , and the identification of this intercept, 1.38, with the value of  $\gamma$ ; reasonable extrapolation of the plot of  $t_l$  suggests that  $t_c \equiv T_c/T_M \cong 0.792$ . We obtain the same limiting values for  $\gamma$  and  $t_c$

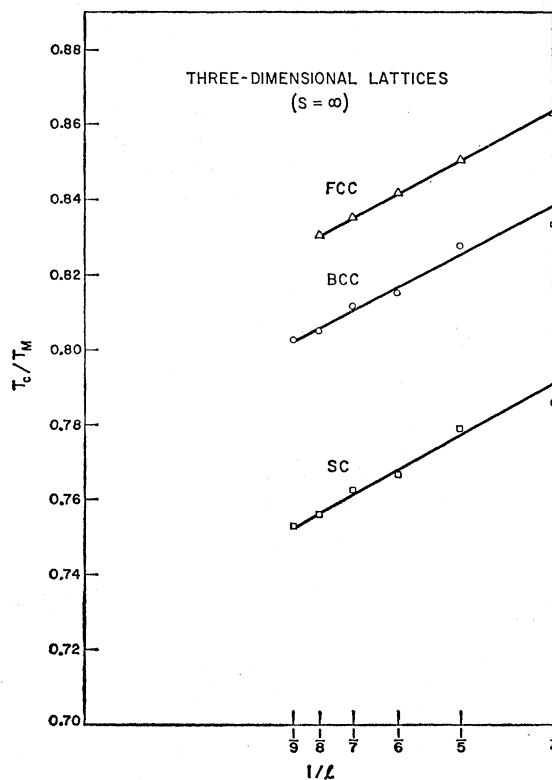


Fig. 1. The ratios  $\rho_l \equiv a_l/a_{l-1}$  of successive terms in the susceptibility series (1) for the face-centered cubic (fcc) body-centered cubic (bcc), and simple cubic (sc) lattices.

TABLE III. The ratios  $\rho_l \equiv a_l/a_1 a_{l-1}$ .

$l$	Honeycomb net	Square	Triangular	Simple cubic	Body-centered cubic	Face-centered cubic
1	1.00000000	1.00000000	1.00000000	1.00000000	1.00000000	1.00000000
2	0.66666667	0.75000000	0.83333333	0.83333333	0.87500000	0.91666667
3	0.56666667	0.70000000	0.74666667	0.81333333	0.86428571	0.88181818
4	0.54901968	0.63690476	0.69494047	0.78551912	0.83316115	0.86239977
5	0.55442176	0.60413885	0.66016110	0.77871635	0.82753963	0.84997746
6	0.48588957	0.58110497	0.63447736	0.76641142	0.81500602	0.84141570
7	0.40333895	0.56026812	0.61401854	0.76216996	0.81164486	0.83516373
8	0.46446376	0.54503830		0.75595011	0.80499745	0.83038396
9	0.60323157	0.52977551		0.75326214	0.80272217	

when we plot against  $1/l$  the residues and roots of the Padé approximants  $P_l^l$  and extrapolate to  $l = \infty$ ; higher-order Padé approximants are not inconsistent with  $\gamma \cong 1.38$  and  $t_c \cong 0.792$  for the fcc lattice.

Direct extrapolation is unrealistic for the bcc and sc lattices since the ratios  $\rho_l$  oscillate from term to term. Improved results *can* be obtained by extrapolating the functions  $t_{l,l-2}$  and  $\gamma_{l,l-2}$  given by successive straight lines passing through  $\rho_l$  and  $\rho_{l-2}$ . However, a more satisfactory procedure is as follows: If  $\chi \sim (T - T_c)^{-\gamma}$  as  $T \rightarrow T_c^+$ , then for large  $l$

$$\rho_l' \equiv \frac{1}{a_1} \left[ \frac{a_l}{a_{l-2}} \right]^{1/2} \rightarrow t_c \left[ 1 + \frac{\gamma-1}{l} + \mathcal{O}\left(\frac{1}{l^2}\right) \right]. \quad (9)$$

Thus a plot of  $\rho_l'$  against  $1/l$  should also approach the critical temperature  $t_c$  with limiting slope proportional to  $\gamma-1$ . Such plots of  $\rho_l'$  were constructed and were

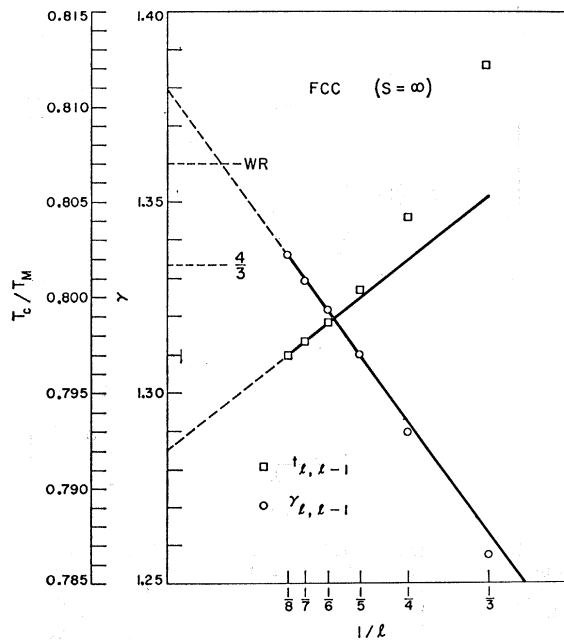


FIG. 2. The sequences  $t_{l,l-1}$  and  $\gamma_{l,l-1}$ , defined in Eqs. (7) and (8), which should approach  $t_c \equiv T_c/T_M$  and  $\gamma$ , respectively, if  $\chi$  diverges with a power law as  $T \rightarrow T_c^+$ . The extrapolations indicated by the dashed lines suggest  $t_c \cong 0.792$  and  $\gamma \cong 1.38$  for the face-centered cubic lattice.

found to be almost straight lines; this suggests we apply the same idea of successive two-point SLE's used above for the ratios  $\rho_l$ , defining new functions  $t_{l,l-1}'$  and  $\gamma_{l,l-1}'$  by equations analogous to Eqs. (7) and (8). Successive values of  $t_{l,l-1}'$  and  $\gamma_{l,l-1}'$  for the bcc and sc lattices are plotted against  $1/l$  in Figs. 3 and 4, respectively. For the bcc lattice, these sequences are seen to oscillate with "amplitudes" that seem to be decreasing with larger and larger  $l$ , suggesting the "extrapolation envelopes" shown on Figs. 3 and 4, which converge to  $t_c \cong 0.77$  and  $\gamma \cong 1.38$ . For the sc lattice, the sequences are less regular and reliable extrapolation appears impossible, although the plausible extrapolation envelopes indicated in Figs. 3 and 4 suggest the values  $t_c \cong 0.72$  and  $\gamma \cong 1.42$ . Extrapolations from sequences of Padé approximants are consistent with our conclusions for the bcc lattice. For the sc lattice, neither the Padé approximant sequences nor the sequences  $t_{l,l-2}$  and  $\gamma_{l,l-2}$  converge any better than the sequences  $t_{l,l-1}'$  and  $\gamma_{l,l-1}'$  plotted. However, the "plausible" values of  $t_c$  and  $\gamma$  suggested by all three extrapolation methods appear to agree.

In summary, then, our analysis suggests that  $\gamma$  does *not* have the value  $\frac{4}{3}$  for the fcc, bcc, and sc lattices. In fact, our extrapolated values of  $\gamma$  are slightly larger than the value  $\gamma = 1.36$  proposed by Wood and Rushbrooke for all three lattices on the basis of eight terms (and indicated by WR in Figs. 2-4).<sup>7</sup> Although we predict  $\gamma \cong 1.38$  for the bcc and fcc lattices and  $\gamma \cong 1.42$  for the sc lattice, the series for the sc is unfortunately not smooth enough to say with confidence that  $\gamma$  is indeed lattice-dependent.<sup>10</sup>

(2) *Do high-temperature expansions suggest a possible phase transition ( $T_c \neq 0$ ) for some two-dimensional lattices with n.n. ferromagnetic interactions?*

For two-dimensional Heisenberg lattices with short-range interactions, the spontaneous magnetization or "order parameter" is zero<sup>11</sup> and it is commonly believed that no phase transition can occur. However, there is the possibility—previously pointed out—of a phase transition to a low-temperature state with zero spontaneous magnetization but with an infinite zero-field

<sup>11</sup> N. D. Mermin and H. Wagner, Phys. Rev. Letters **17**, 1133 (1966).

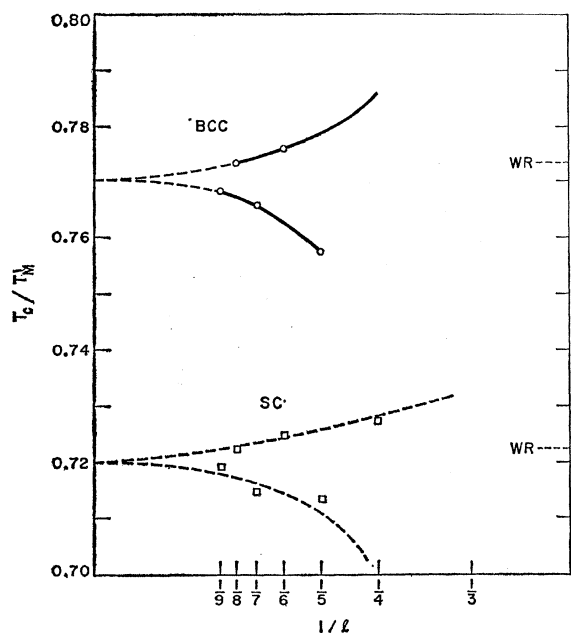


FIG. 3. The sequence  $t'_{l,l-1}$ , defined by Eq. (7) with primes on all quantities, should approach  $t_c$  as  $l \rightarrow \infty$ . The "extrapolation envelope" indicated for the body-centered cubic lattice indicates  $t_c \cong 0.770$ . For the simple cubic lattice, the sequence plotted (as well as the sequence  $t_{l,l-2}$  and the various sequences of Padé approximants) is too irregular to afford reliable extrapolation. However, if one imagines the numbers  $t_{l,l-1}'$  to be approaching the "extrapolation envelope" indicated by the dashed line, then one would expect  $t_c \cong 0.720$  for the sc lattice.

susceptibility.<sup>12-14</sup> To our knowledge, not even a plausibility argument has been presented against the existence of such a phase transition. However, Stanley and Kaplan have argued that for some two-dimensional lattices extrapolations to nonzero  $T_c$  are as reasonable as for three-dimensional lattices.<sup>12,13</sup> Their extrapolations were based upon the first six terms in the high-temperature series (1) which are available for all  $S$ . The effect of additional terms for any spin value would certainly be useful in connection with this question,<sup>15</sup> and consequently we have computed  $a_7$  for the triangular (close-packed) lattice and  $a_7 - a_9$  for the plane square and honeycomb (loose-packed) lattices (see Table II).

In Fig. 5 we plot  $\rho_l$  for the triangular lattice and  $\rho_{l+1}'$  for the square lattice. The downward curvature, although greater than for the three-dimensional lattices discussed above, is not sufficient to suggest an extrapolation to  $T_c = 0$ .

However, our present more careful method of taking into account the downward curvature does give appreciably lower values of  $t_c$  (even on the basis of only six terms) than reported previously.<sup>12</sup> In Fig. 6 are plotted the successive  $t_{l,l-1}$  (corresponding to straight-line extrapolations through  $\rho_l$  and  $\rho_{l-1}$ ) for both square and triangular lattices together with  $t_{l,l-1}'$  for the square net. It again appears that extrapolated values of  $t_c = 0$  are unreasonable: The regularity of the sequence  $t_{l,l-1}$  for the triangular lattice suggests  $t_c \cong 0.4$ , and consideration of  $t_{l,l-1}$  and  $t_{l,l-1}'$  together for the square net suggests  $t_c \cong 0.3$ . Moreover, the roots of Padé approximants extrapolate near the suggested values of  $t_c$ . Of course, extrapolation from a finite number of terms of an infinite series never constitutes a rigorous proof; however, our analysis of the extended series for the square and triangular lattices supports the original suggestion that high-temperature series expansions indicate  $\chi$  diverges at a nonzero  $T_c$  for some two-dimensional lattices.

The ratios  $\rho_l$  for the non-Bravais honeycomb lattice listed in Table III are seen to be quite irregular. This, of course, does not mean that the critical temperature is zero for the honeycomb net, but means only that

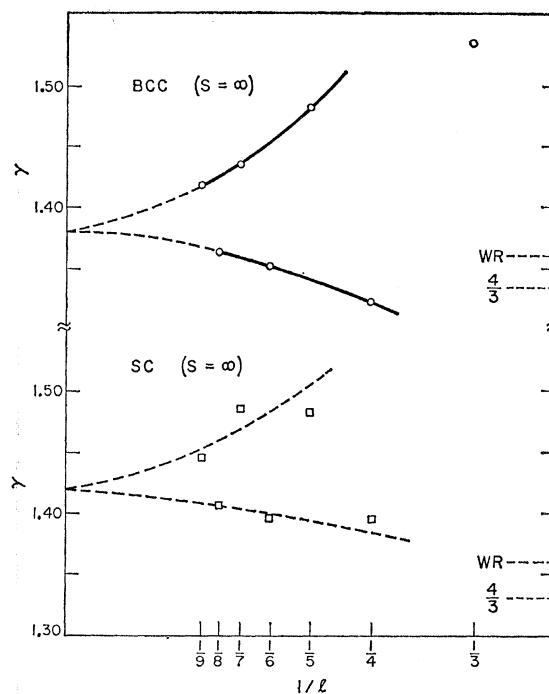


FIG. 4. The sequence  $\gamma_{l,l-1}'$  defined by Eq. (8) with primes on all quantities. The same statements made in the caption to Fig. 3 apply here: The sequence  $\gamma_{l,l-1}'$  seems to approach  $\gamma \cong 1.38$  for the bcc, and if one imagines the corresponding numbers for the sc lattice to be approaching the "extrapolation envelope" indicated by the dashed line, then one expects  $\gamma \cong 1.42$  for the sc lattice. The latter conclusion, if made, would contradict the common belief that the critical indices (in particular  $\gamma$ ) are identical for all three-dimensional lattices. WR indicates the Wood-Rushbrooke extrapolations (Ref. 7).

<sup>12</sup> H. E. Stanley and T. A. Kaplan, Phys. Rev. Letters **17**, 913 (1966).

<sup>13</sup> H. E. Stanley and T. A. Kaplan, J. Appl. Phys. **38**, 975 (1967).

<sup>14</sup> For example, if at large  $R$  the spin correlation function  $\langle S_0 \cdot S_R \rangle \sim R^{-\gamma}$ , then  $\chi \propto \sum_R \langle S_0 \cdot S_R \rangle \rightarrow \infty$  for  $\gamma < 2$ , but the spontaneous magnetization is zero (see Ref. 13).

<sup>15</sup> For  $S = \frac{3}{2}$ ,  $a_7$  is negative for the square and honeycomb nets. [H. E. Stanley (to be published)].

there is no clear evidence one way or the other. (Even if  $T_c$  were zero for the honeycomb lattice, this would certainly *not* imply  $T_c=0$  for all two-dimensional lattices.) An analogous situation occurs in the Ising model: The ratios  $\rho_l$  are regular for the plane square and triangular lattices and irregular for the honeycomb lattice, despite the fact that all three lattices undergo phase transitions.

IV. SUMMARY

In summary, then, we have obtained expressions—in terms of Domb’s lattice constants  $p_{lx}$ —for the first nine terms  $a_l$  for loose-packed lattices and the first seven terms for close-packed lattices in the high-temperature series (1) for the zero-field magnetic susceptibility. These “general lattice expressions” were used to compute numerical values of the coefficients  $a_l$  for the fcc, bcc, and sc (three-dimensional) lattices, and for the plane square, triangular, and honeycomb (two-dimensional) lattices.

Two questions of current interest were then discussed with the aid of the coefficients. (1) It was argued, on the basis of extrapolations from both Padé approximants and from the simpler “slope method,” that  $\gamma=4/3$  is far less plausible than  $\gamma \cong 1.38$  for the bcc and

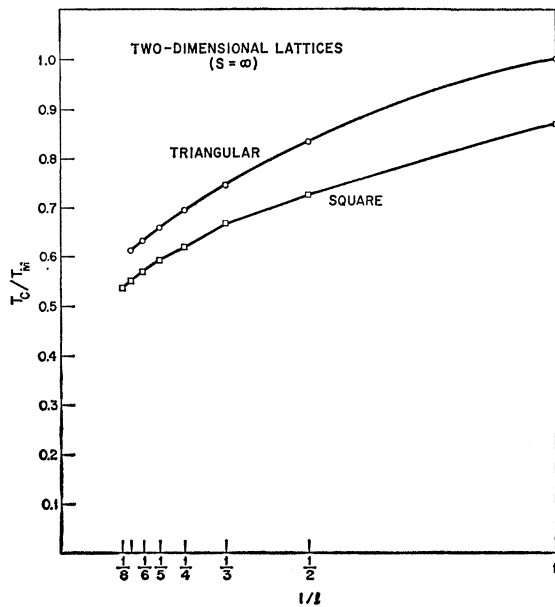


FIG. 5. The sequence  $\rho_l \equiv a_l/a_{l-1}$  for the triangular lattice and the sequence  $\rho_{l+1} \equiv (a_{l+1}/a_{l-1})^{1/2}/a_l$  for the square lattice. If these sequences tend to limiting values, these values are  $T_c/T_M$ .

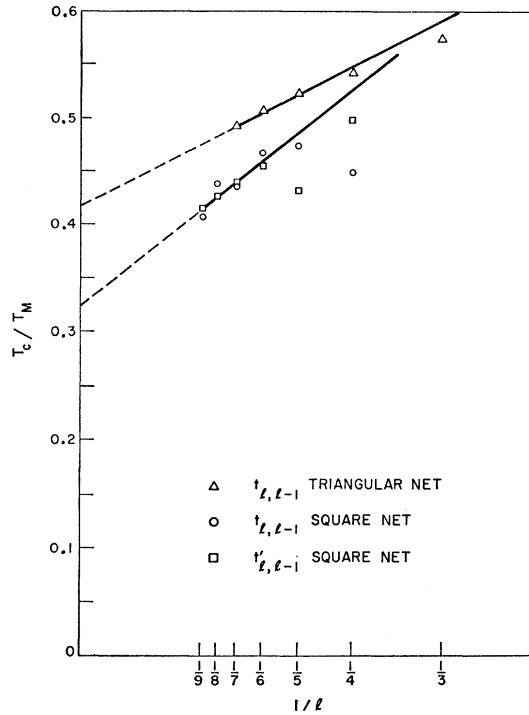


FIG. 6. The functions  $t_{l,l-1}$  for both square and triangular lattices and the function  $t_{l,l-1}'$  for the square lattice. The extrapolations indicated by the dashed lines suggest  $t_c \cong 0.4$  for the triangular net and  $t_c \cong 0.3$  for the square net.

fcc lattices, and  $\gamma \cong 1.4$  (perhaps 1.42) for the sc lattice. Unfortunately, the series for the sc lattice is not sufficiently smooth to say reliably that  $\gamma$  is indeed lattice-dependent within the class of fcc, bcc, and sc lattices.<sup>10</sup> (2) The same extrapolation methods were applied to the question of whether or not  $T_c=0$  in two-dimensional lattices for the classical Heisenberg model. It was argued that the extrapolations to  $T_c/T_M \cong 0.3$  and 0.4, respectively, for the plane square and triangular lattices are more convincing than the extrapolation to  $T_c=0$ .

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