

siderable care must be used in treating the dispersion relation² $\sigma_{xx}\sigma_{yy} + \sigma_{xy}^2 \approx 0$, because of the cancellation of a factor $D(A_n)$ between numerator and denominator. We obtain the correct dispersion relation using our approximate solution of the 6×6 matrix equation after demonstrating that this cancellation must occur. The full dispersion relation is too complicated to display here, and its long-wavelength limit is of no value because nonlinear terms in A_2 become important for very small X . We can however, make the following statements about the dispersion relation: first, it contains no Fermi-liquid terms lower than fourth order except the term linear in A_2 , and second, in contrast to the other polarization,

there is no shift of ω away from the value ω_c for $X=0$. In this respect the dispersion relation is much closer to the prediction of the free-electron model than the experimental data.¹² The exact numerical results for both polarizations will be presented in a more detailed later publication.

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¹² W. M. Walsh, Jr., has informed us that further experimental studies have shown that the original assignment of the wavelengths of the plasma waves in Ref. 2 was incorrect, and that the correct experimental data does lie much closer to the prediction of the free-electron model.

Free Energy of the Classical Heisenberg Model

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High-temperature power-series expansions for the free energy of a classical Heisenberg ferromagnet in an applied field are given in the form

$$-F/NkT = \sum_{n,l} a_{2n,l} h^{2n} x^l,$$

where $h = g\beta H/kT$ and $x = J/kT$. The coefficients are given for $l \leq 7$ and $4 \leq 2n \leq 10$. Estimates of the critical exponents for the fourth to tenth field derivatives of F are given.

I. INTRODUCTION

IN recent years much work has been done on obtaining high-temperature series expansions of thermodynamic functions for the Heisenberg model and the estimation, from these series, of various critical parameters. For general spin only six terms of the susceptibility expansion and five terms of the specific-heat expansion are known.¹ For the special cases of $S = \frac{1}{2}$ and $S = \infty$ further terms are known. Baker *et al.*² have given the free energy for the $S = \frac{1}{2}$ Heisenberg model to order $1/T^{10}$ [for the bcc and simple cubic (sc) lattices] and $1/T^9$ (for the fcc lattice) and also the field dependence in powers of the applied field H up to $(H/T)^8$.

It is the purpose of the present paper to present the results of a similar calculation for the $S = \infty$ Heisenberg model. Currently, high-temperature expansions for the zero-field susceptibility and specific heat are known to 8 and 9 terms for close-packed lattices and 9 and 10 terms for open lattices, respectively, using this model.³ We shall give the temperature and field dependence to orders $1/T^7$ and $(H/T)^{10}$.

¹ G. S. Rushbrooke and P. J. Wood, *Mol. Phys.* **1**, 257 (1958).

² G. A. Baker, H. E. Gilbert, J. Eve, and G. S. Rushbrooke, *Phys. Letters* **20**, 146 (1966); **22**, 269 (1966); *Phys. Rev.* **164**, 800 (1967).

³ H. A. Brown and J. M. Luttinger, *Phys. Rev.* **100**, 685 (1955); H. E. Stanley and T. A. Kaplan, *Phys. Rev. Letters* **16**, 981 (1966); P. J. Wood and G. S. Rushbrooke, *ibid.* **17**, 307 (1966); G. S. Joyce and R. G. Bowers, *Proc. Phys. Soc. (London)* **88**, 1053 (1966).

In Sec. II we shall describe how the calculation was performed. Section III will be concerned with the susceptibility series, Sec. IV with the high-temperature series proportional to powers of the applied field greater than 2. Finally, in Sec. V we consider some two-dimensional lattices.

II. CALCULATION OF THE FREE ENERGY

We start with the Hamiltonian

$$\mathcal{H} = -2J \sum_{\langle ij \rangle} \mathbf{S}^{(i)} \cdot \mathbf{S}^{(j)} - g\beta H \sum_i S_z^{(i)} = \mathcal{H}_1 + \mathcal{H}_0, \quad (1)$$

where J is the exchange-energy constant for nearest-neighbor interactions, $\mathbf{S}^{(i)}$ the spin vector on lattice site i , g the gyromagnetic ratio, β the Bohr magneton, and H the applied field (taken to be in the z direction). We use the abbreviation $S(S+1) = X$.

We introduce a new vector $\mathbf{T}^{(i)} = \mathbf{S}^{(i)}/\sqrt{X}$. It is then easily seen that in the limit $S \rightarrow \infty$, $\mathbf{T}^{(i)}$ becomes a unit classical vector. In terms of the vectors $\mathbf{T}^{(i)}$ the Hamiltonian becomes

$$\mathcal{H} = -2JX \sum_{\langle ij \rangle} \mathbf{T}^{(i)} \cdot \mathbf{T}^{(j)} - g\beta H \sqrt{X} \sum_{i=1}^N T_z^{(i)}. \quad (2)$$

In the following we shall write J for JX and H for

$H\sqrt{X}$, whence we obtain

$$\mathcal{H}C = -2J \sum_{\langle ij \rangle} \mathbf{T}^{(i)} \cdot \mathbf{T}^{(j)} - g\beta H \sum_{i=1}^N T_z^{(i)} \quad (3)$$

as the Hamiltonian for the classical Heisenberg model.

Since $\mathcal{H}C_0$ and $\mathcal{H}C_1$ commute we may write the partition function

$$Z = \text{Tr} \exp(-\mathcal{H}C/kT) = Z_0 Z_1, \quad (4)$$

where

$$Z_0 = \text{Tr} \exp\{(g\beta H/kT) \sum_{i=1}^N T_z^{(i)}\} \quad (5)$$

and

$$Z_1 = \langle \exp\{(2J/kT) \sum_{\langle ij \rangle} \mathbf{T}^{(i)} \cdot \mathbf{T}^{(j)}\} \rangle, \quad (6)$$

and for any operator A we define the mean trace as

$$\langle A \rangle = \frac{\text{Tr}\{A \exp(-\mathcal{H}C_0/kT)\}}{\text{Tr} \exp(-\mathcal{H}C_0/kT)}. \quad (7)$$

We can expand the exponential in (6) as

$$\sum_{l=0}^{\infty} (l!)^{-1} (2J/kT)^l \langle (\sum_{\langle ij \rangle} \mathbf{T}^{(i)} \cdot \mathbf{T}^{(j)})^l \rangle \quad (8)$$

and represent

$$\langle (\sum_{\langle ij \rangle} \mathbf{T}^{(i)} \cdot \mathbf{T}^{(j)})^l \rangle$$

by a set of l -line graphs; a line between points i and j of such a graph representing $\mathbf{T}^{(i)} \cdot \mathbf{T}^{(j)}$. With each graph is associated (i) a trace factor and (ii) an occurrence factor. The graphs may be connected or disconnected. We can avoid having to consider the disconnected graphs by forming a graphical expansion of the free energy $F = -kT \ln Z$ rather than Z .⁴ This expansion requires us to use the cumulants of graphs rather than the mean traces. Occurrence factors for connected graphs are tabulated by Baker *et al.*⁵

If we denote the links in an l -line graph by $\alpha, \beta \dots \omega$, the cumulant function by $[\alpha \dots \omega]$, and the mean trace by $\langle \alpha \dots \omega \rangle$, then it can be shown⁴ that

$$\langle \alpha \dots \omega \rangle = \sum_{k=1}^l \sum_{p(l,k)} [\alpha \dots \beta][\gamma \dots \delta] \dots [\epsilon \dots \omega],$$

where $p(l, k)$ refers to a partition of the l symbols $\alpha \dots \omega$ into k groups (with any sequence within a group and any sequence among the groups). This can be rearranged to give

$$[\alpha \dots \omega] = \langle \alpha \dots \omega \rangle - \sum_{k=2}^l \sum_{p(l,k)} [\alpha \dots \beta][\gamma \dots \delta] \dots [\epsilon \dots \omega]. \quad (9)$$

Thus the cumulant of an l -line graph can be evaluated from its mean trace and the cumulants of $1, 2 \dots (l-1)$ -line graphs which have been previously calculated.

⁴ G. S. Rushbrooke, *J. Math. Phys.* **5**, 1106 (1964).

⁵ G. A. Baker, H. E. Gilbert, J. Eve, and G. S. Rushbrooke, Brookhaven National Laboratory Report No. BNL 50053, T-460, 1967 (unpublished).

We must now describe the methods used to evaluate the mean trace of multiline graphs. Let θ_i and φ_i be the polar coordinates of the direction $\mathbf{T}^{(i)}$ (with the z axis as polar axis) and θ_{ij} the angle between $\mathbf{T}^{(i)}$ and $\mathbf{T}^{(j)}$. Then

$$\begin{aligned} \mathbf{T}^{(i)} \cdot \mathbf{T}^{(j)} &= \cos\theta_{ij} \\ &= \cos\theta_i \cos\theta_j + \sin\theta_i \sin\theta_j \cos(\varphi_i - \varphi_j), \end{aligned} \quad (10)$$

$$T_z^{(i)} = \cos\theta_i. \quad (11)$$

Therefore

$$\begin{aligned} Z_0 &= \text{Tr} \exp\{(+g\beta H/kT) \sum_{i=1}^N T_z^{(i)}\} \\ &= (1/4\pi)^N \int \dots \int \exp\{(g\beta H/kT) \sum_{i=1}^N \cos\theta_i\} \\ &\quad \times \prod_{j=1}^N \sin\theta_j d\theta_j d\varphi_j \\ &= \left[(1/4\pi) \int_0^\pi d\theta \int_0^{2\pi} d\varphi \exp\{(g\beta H/kT) \cos\theta\} \sin\theta \right]^N. \end{aligned} \quad (12)$$

This is the denominator in the expression for the mean trace.

Now any term in the expansion of (8) is represented by a multiline graph, each bond of which represents a factor $\cos\theta_{ij}$. The mean trace of such a graph will be

$$\begin{aligned} &\frac{(\text{combinatorial factor})}{Z_0} \int \dots \int (1/4\pi)^N \prod \cos\theta_{ij} \\ &\quad \times \exp\{(g\beta H/kT) \sum_{i=1}^N \cos\theta_i\} \prod_{k=1}^N \sin\theta_k d\theta_k d\varphi_k, \end{aligned} \quad (13)$$

where the product is taken over those bonds $\langle ij \rangle$ which occur in the graph. Clearly, for each lattice point not involved in a graph a factor

$$(1/4\pi) \int_0^\pi d\theta \int_0^{2\pi} d\varphi \exp\{(g\beta H/kT) \cos\theta\} \sin\theta$$

will cancel in numerator and denominator of the mean trace. Each $\cos\theta_{ij}$ may now be replaced by

$$\cos\theta_i \cos\theta_j + \sin\theta_i \sin\theta_j \cos(\varphi_i - \varphi_j)$$

and the numerator broken down into contributions involving the integrals

$$I(m, n) = \int_0^\pi \cos^m\theta \sin^n\theta \exp\{(g\beta H/kT) \cos\theta\} \sin\theta d\theta,$$

$$J(m, n) = \int_0^{2\pi} \cos^m\varphi \sin^n\varphi d\varphi.$$

$I(m, n)$ was evaluated as a power series in $g\beta H/kT$. Thus we see that the numerator and denominator of (13) and hence the mean trace itself can be evaluated

as a power series in $g\beta H/kT$. The manipulations involved in obtaining the mean trace as a power series in $g\beta H/kT$ were performed on a computer and the calculations were carried out to order $(g\beta H/kT)^{10}$. In obtaining the cumulants from the mean traces we used the methods of Sykes *et al.*⁶ to represent graphs in the computer. It is fairly straightforward to see that only even powers of H are involved.

In this way we obtain

$$F = -NkT \sum_{n=0}^{\infty} h^{2n} F_{2n}(x), \quad (14)$$

where

$$h = g\beta H/kT, \quad x = J/kT \quad (15)$$

and

$$F_{2n}(x) = \sum_{l=0}^{\infty} a_{2n,l} x^l; \quad (16)$$

that is,

$$F = -NkT \sum_{n=0}^{\infty} \sum_{l=0}^{\infty} a_{2n,l} h^{2n} x^l. \quad (17)$$

We have calculated the coefficients $a_{2n,l}$ for $2n \leq 10$ and $l \leq 7$ for the fcc, bcc, sc, plane square, and plane triangular (p.t.) lattices.

The numbers of graphs considered for $l=1,2,\dots,7$ (i.e., multiline connected graphs) are 1, 2, 5, 12, 33, 103, and 333 for the fcc lattice and correspondingly fewer for the other lattices.

In terms of these coefficients the magnetic specific heat and zero-field susceptibility are given by

$$\bar{C} = C/Nk = \sum_{l=2}^{\infty} l(l-1) a_{0,l} x^l \quad (18)$$

and

$$\bar{\chi} = Jx/Ng^2\beta^2 = \sum_{l=0}^{\infty} 2a_{2,l} x^l. \quad (19)$$

These coefficients have been given by several authors³ and are therefore not reproduced here. Our calculations

TABLE I. The Neville table formed from the ratios $a_{2,l-1}/a_{2,l}$ for the fcc lattice.

$l=1$	0.125			
$l=3$	0.14175	0.15013	0.15625	
$l=5$	0.14706	0.15503	0.15707	0.1572
$l=7$	0.14967	0.15619		
$l=2$	0.13636			
$l=4$	0.14494	0.15352	0.15692	
$l=6$	0.14859	0.15579	0.15712	0.1572
$l=8$	0.15053	0.15645		

⁶ M. F. Sykes, J. W. Essam, B. R. Heap, and B. J. Hiley, *J. Math. Phys.* **1**, 1557 (1966).

TABLE II. Neville tables for the estimation of γ assuming different values for x_c .

$x_c=0.1572$			$x_c=0.1573$		
$\gamma_1=1.2576$			$\gamma_1=1.2584$		
	1.3616			1.3643	
$\gamma_3=1.3269$		1.3737	$\gamma_3=1.3290$		1.3787
	1.3713			1.3766	
$\gamma_5=1.3447$		1.3703	$\gamma_5=1.3480$		1.3801
	1.3707			1.3786	
$\gamma_7=1.3521$			$\gamma_7=1.3568$		
$\gamma_2=1.3056$			$\gamma_2=1.3701$		
	1.3708			1.3749	
$\gamma_4=1.3382$		1.3704	$\gamma_4=1.3410$		1.3782
	1.3705			1.3771	
$\gamma_6=1.3490$		1.3702	$\gamma_6=1.3530$		1.3819
	1.3703			1.3795	
$\gamma_8=1.3543$			$\gamma_8=1.3596$		

agree with those of other authors where these overlap. In the Appendix we give the coefficients for $4 \leq 2n \leq 10$, $l \leq 7$.

III. SUSCEPTIBILITY SERIES

We have reanalyzed the extended susceptibility series of Joyce and Bowers³ and have come to essentially the same conclusions as they did. Namely, assuming that

$$\bar{\chi} \sim A/(x_c - x)^\gamma$$

for x near, but less than, x_c , then $x_c \sim 0.1572$, 0.2432, and 0.346 for the fcc, bcc, and sc lattices, respectively. For example, the Neville table² formed from the ratios $a_{2,l-1}/a_{2,l}$ for the fcc is given in Table I.

Using these values of x_c we may use the method of Domb and Sykes⁷ to estimate γ , namely

$$l[x_c(a_{2,l}/a_{2,l-1}) - 1] = \gamma_l - 1; \quad \gamma_l \rightarrow \gamma \text{ as } l \rightarrow \infty.$$

This procedure leads to the estimates 1.37, 1.38, and 1.39 for γ for the fcc, bcc, and sc lattices, respectively. It should, however, be noted that the precise value of γ depends very critically on the value assumed for x_c . For example, we can draw up the Neville tables given in Table II for the estimation of γ for the fcc according as we assume $x_c=0.1572$ or 0.1573.

One sees from Table II that a change of 0.0001 in x_c can lead to a change of 0.01 in γ . On this basis we would hesitate at being able to point to any dependence of γ on the lattice structure.

Analysis of $\bar{\chi}$ by Padé approximants gives the same story. For the open lattices, however, there is evidence of a much weaker singularity at approximately $-x_c$. This point represents the Néel point of the antiferromagnetic problem. Previous work by Rushbrooke and Wood⁸ would suggest that, for infinite spin, the singularity occurs at exactly $-x_c$. There was no evidence of a similar singularity for the fcc lattice, supporting the

⁷ C. Domb and M. F. Sykes, *J. Math. Phys.* **2**, 63 (1961).

⁸ G. S. Rushbrooke and P. J. Wood, *Mol. Phys.* **6**, 409 (1963).

TABLE III. Root of the denominator in the Padé approximant to $d[\ln F_{10}(x)]/dx$.

$\frac{N}{D}$	0	1	2	3	4	5
1	-0.0797	-0.0156	-0.0211	-0.0202	-0.0202	-0.0202
2	0.0502	0.1866	0.1173	0.2804	0.6644	
3	-0.0247	0.1353	0.1567	0.1560		
4	0.0408	-0.1610	0.1561			
5	-0.0215	0.1301				
6	0.0373					

belief that for the fcc lattice, nearest-neighbor interactions alone cannot produce antiferromagnetic ordering.

For the open lattices an attempt was made to subtract out the ferromagnetic singularity and to sharpen the antiferromagnetic singularity by considering Padé approximants to (i)

$$(d/dx) \{ (d/dx) \ln \bar{\chi} - [\gamma/(x_c - x)] \}$$

and (ii)

$$(x - x_c) (d/dx) \ln \bar{\chi}.$$

In both cases a range of x_c 's was taken and in the former a range of γ 's. However, in no case was there a consistent Padé table, although indications persisted of the presence of a singularity at approximately $-x_c$.

IV. HIGHER-ORDER SERIES

We must next consider the series $F_{2n}(x)$ $n=2, 3, 4, 5$. We assume that these series behave like

$$A_{2n}/(x_c^{(2n)} - n)\gamma^{(2n)}$$

for x near, but less than, x_c . No firm conclusions can be drawn as to the values of $x_c^{(2n)}$ and $\gamma^{(2n)}$ by using the method of Padé approximants, since it turns out that the series vanish for small negative values of x , and consequently the Padé approximants are in some cases rather erratic. This does not happen to the susceptibility series. For example, the Padé table for $F_{10}(x)$ for the fcc (i.e., the root of the denominator in the Padé approximant to $d[\ln F_{10}(x)]/dx$) is given in Table III.

One can see in Table III the influence of the singularity at $x \sim -0.0202$, which is due to the vanishing of $F_{10}(x)$ at this value.

The ratio method is unaffected by these zeros and its

TABLE IV. Values of x_c and $x_c^{(2n)}$ for the three-dimensional lattices.

	x_c	$x_c^{(4)}$	$x_c^{(6)}$	$x_c^{(8)}$	$x_c^{(10)}$
fcc	0.1572	0.1566	0.1552	0.1558	0.1566
bcc	0.2432	0.2435	0.2410	0.2422	0.2424
sc	0.346	0.344	0.345	0.345	0.345

use leads to values of $x_c^{(2n)}$ which are very close to x_c . The values obtained are as given in Table IV.

It would seem very likely, therefore, that $x_c^{(2n)} = x_c$ for all n (recall that the estimates $x_c^{(2n)}$ are made on the basis of fewer series terms than those of x_c). We shall make this hypothesis in the remainder of this paper.

Estimates of $\gamma^{(2n)}$ can now be made using the method of Domb and Sykes as in the previous section. We find the values given in Table V (we include the values of γ given in Sec. III).

It is evident that relation between $\gamma^{(2n)}$ and n is remarkably linear. A least-squares calculation for each lattice gives

$$\gamma^{(2n)} = 3.44n - 2.07, \quad \text{fcc}$$

$$\gamma^{(2n)} = 3.45n - 2.06, \quad \text{bcc}$$

$$\gamma^{(2n)} = 3.50n - 2.11, \quad \text{sc.}$$

Thus not only is the relation very nearly linear but it is also almost lattice-independent. Indeed, the uncertainties in the values of x_c and the γ 's are such as to make one conjecture that $\gamma^{(2n)} = mn + c$, where $m \sim 3.45$ and $c \sim -2.07$.

Very similar results were found for the case $S = \frac{1}{2}$ by Baker *et al.*² These authors found a value of m equal to 3.63. It would therefore appear that m is spin-dependent.

A number of scaling arguments have recently been put forward⁹ which suggest that all the critical indices can be expressed in terms of just two of them. If α_s is the index of the singular point of the specific heat, β the degree of the magnetic phase boundary, δ the degree

TABLE V. Values of γ and $\gamma^{(2n)}$ for the three-dimensional lattices.

	fcc	bcc	sc
γ	1.37	1.38	1.39
$\gamma^{(4)}$	4.83	4.85	4.90
$\gamma^{(6)}$	8.26	8.29	8.41
$\gamma^{(8)}$	11.69	11.74	11.91
$\gamma^{(10)}$	15.12	15.19	15.41

⁹ M. E. Fisher, Rept. Progr. Phys. **30**, 615 (1967), and references therein.

of the critical isotherm, γ the index of the susceptibility, and 2Δ the gap parameter, then on the basis of scaling arguments

$$\alpha_s = 2 - 2\Delta + \gamma,$$

$$\beta = \Delta - \gamma,$$

$$\delta = \Delta / (\Delta - \gamma).$$

Using our values (i.e., $\gamma = 1.38$ and $2\Delta = 3.45$) the scaling laws give

$$\alpha_s = -0.07,$$

$$\beta = +0.345,$$

$$\delta = +5.$$

The spin- $\frac{1}{2}$ values² are, for comparison, $\alpha_s = -0.2$, $\beta = +0.38$, and $\delta = 4.73$.

V. TWO-DIMENSIONAL LATTICES

In this final section we consider two two-dimensional lattices—the plane triangular (p.t.) and the plane square (p.s.) and attempt to perform a similar analysis on the series $F_{2n}(x)$. Stanley¹⁰ has already given the first coefficients of $F_2(x)$ for these lattices. We give the series $F_{2n}(x)$ $n = 2, 3, 4, 5$ in the Appendix.

Recently, Mermin and Wagner¹¹ have argued that it is impossible for one- or two-dimensional isotropic Heisenberg lattices to exhibit ferro- or antiferromagnetism as the spontaneous magnetization is zero.

TABLE VI. Neville tables for the ratios $a_{2n,l-1}/a_{2n,l}$ for the p.t. lattice for $n = 2$ and 3.

$n = 2$			
$l = 1$	0.0625		
$l = 2$	0.1115	0.1605	
$l = 3$	0.1503	0.2280	0.3224
$l = 4$	0.1816	0.2752	0.3631
$l = 5$	0.2073	0.3104	0.3865
$l = 6$	0.2287	0.3357	0.4148
$l = 7$	0.2472	0.3582	
$n = 3$			
$l = 1$	0.0309		
$l = 2$	0.0620	0.0932	
$l = 3$	0.0904	0.1472	
$l = 4$	0.1155	0.1910	0.280
$l = 5$	0.1377	0.2264	0.314
$l = 6$	0.1574	0.2557	0.339
$l = 7$	0.1748	0.2795	

¹⁰ H. E. Stanley, Phys. Rev. **158**, 546 (1967).

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

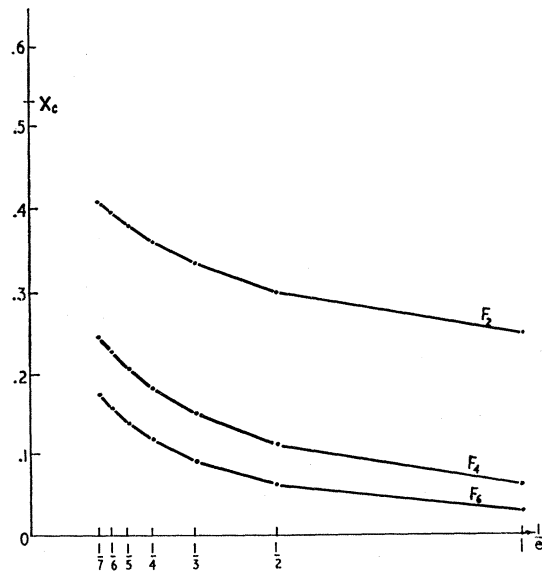


FIG. 1. A plot of the ratios $a_{2n,l-1}/a_{2n,l}$ for the plane triangular lattice against $1/l$ for $n = 1, 2, 3$.

However, Stanley and Kaplan¹² found a nonzero x_c on analyzing the susceptibility series for the p.t. and p.s. lattices. They suggested that this represented a transition to a low-temperature state with zero spontaneous magnetization but with an infinite zero-field susceptibility at the transition point—a possibility not ruled out by Mermin and Wagner.

We have analyzed the series $F_{2n}(x)$ for the p.t. and p.s. lattices by both Padé approximants and by the ratio method. Padé approximants to the susceptibility series, $F_2(x)$, for the p.t. lattice would suggest the existence of a second singularity at $x \sim 0.79$. They may account for the slow convergence. The Padé method is unsatisfactory for $n > 1$ for the same reasons as in Sec. III. It would seem to us quite likely that quantities $x_c^{(2n)}$ exist as in Sec. III, but it is difficult to give values with any precision. For example, the Neville tables of the ratios $a_{2n,l-1}/a_{2n,l}$ for the p.t. lattice for $n = 2$ and 3 are given in Table VI.

A plot of the ratios against $1/l$ is also given. It would seem quite plausible from Fig. 1 that these series have a singularity at about the same value as that given by Stanley from an analysis of the susceptibility series, i.e., $x_c \sim 0.53$, but the Neville tables suggest that the convergence of the ratios to this value is extremely slow. Many more terms in the series are required before we can be confident about the behavior of the two-dimensional lattice series.

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

APPENDIX

Coefficients of the series $F_{2n}(x) = \sum a_{2n,i} x^i$. Numbers in parentheses give appropriate powers of 10.

(i) fcc lattice:

l/n	2	3	4	5
0	-5.555 555 556(-3)	3.527 336 860(-4)	-2.645 502 639(-5)	2.137 779 930(-6)
1	-1.777 777 778(-1)	2.285 714 286(-2)	-2.821 869 488(-3)	3.376 470 677(-4)
2	-3.371 851 852	7.714 991 182(-1)	-1.457 750 903(-1)	2.454 545 963(-2)
3	-4.952 493 827(1)	1.847 696 358(1)	-5.073 789 423	1.159 538 211
4	-6.226 039 647(2)	3.554 099 865(2)	-1.363 369 402(2)	4.112 088 256(1)
5	-7.042 328 331(3)	5.859 822 439(3)	-3.042 838 684(3)	1.184 008 759(3)
6	-7.377 886 756(4)	8.611 300 682(4)	-5.899 074 826(4)	2.905 723 422(4)
7	-7.290 935 637(5)	1.157 201 971(6)	-1.023 453 635(6)	6.279 512 493(5)

(ii) bcc lattice:

l/n	2	3	4	5
0	-5.555 555 556(-3)	3.527 336 860(-4)	-2.645 502 639(-5)	2.137 779 930(-6)
1	-1.185 185 185(-1)	1.523 809 524(-2)	-1.881 246 325(-3)	2.250 980 451(-4)
2	-1.457 777 778	3.552 380 952(-1)	-6.347 145 936(-2)	1.069 720 638(-2)
3	-1.390 617 284(1)	5.222 416 244	-1.438 719 857	3.293 503 715(-1)
4	-1.133 088 709(2)	6.523 792 458(1)	-2.513 924 961(1)	7.601 635 042
5	-8.306 291 483(2)	6.980 163 485(2)	-3.645 339 399(2)	1.423 323 174(2)
6	-5.636 158 072(3)	6.652 931 194(3)	-4.588 634 589(3)	2.270 002 680(3)
7	-3.607 009 325(4)	5.796 075 955(4)	-5.166 498 105(4)	3.186 375 899(4)

(iii) sc lattice:

l/n	2	3	4	5
0	-5.555 555 556(-3)	3.527 336 860(-4)	-2.645 502 639(-5)	2.137 779 930(-6)
1	-8.888 888 889(-2)	1.142 857 143(-2)	-1.410 934 744(-3)	1.688 235 339(-4)
2	-7.970 370 370(-1)	1.842 680 776(-1)	-3.496 161 921(-2)	5.897 992 268(-3)
3	-5.467 654 321	2.079 010 106	-5.758 835 419(-1)	1.321 951 847(-1)
4	-3.184 216 343(1)	1.868 617 250(1)	-7.267 319 593	2.208 518 725
5	-1.662 401 693(2)	1.432 601 857(2)	-7.579 961 209(1)	2.981 837 219(1)
6	-8.014 814 154(2)	9.755 989 869(2)	-6.843 223 142(2)	3.419 715 193(2)
7	-3.638 134 855(3)	6.059 812 113(3)	-5.513 840 224(3)	3.444 319 109(3)

(iv) Plane triangular lattice:

l/n	2	3	4	5
0	-5.555 555 556(-3)	3.527 336 860(-4)	-2.645 502 639(-5)	2.137 779 930(-6)
1	-8.888 888 889(-2)	1.142 857 143(-2)	-1.410 934 744(-3)	1.688 235 339(-4)
2	-7.970 370 370(-1)	1.842 680 776(-1)	-3.496 161 921(-2)	5.897 992 268(-3)
3	-5.301 728 395	2.038 174 519	-5.668 750 595(-1)	1.303 799 585(-1)
4	-2.920 209 759(1)	1.763 932 521(1)	-6.939 691 767	2.121 100 202
5	-1.408 567 886(2)	1.280 824 232(2)	-6.929 378 695(1)	2.757 294 611(1)
6	-6.158 465 898(2)	8.138 316 808(2)	-5.917 693 739(2)	3.013 806 446(2)
7	-2.490 927 715(3)	4.655 213 109(3)	-4.461 330 608(3)	2.866 353 936(3)

(v) Plane square lattice:

l/n	2	3	4	5
0	-5.555 555 556(-3)	3.527 336 860(-4)	-2.645 502 639(-5)	2.137 779 930(-6)
1	-5.925 925 926(-2)	7.619 047 618(-3)	-9.406 231 627(-4)	1.125 490 226(-4)
2	-3.338 271 605(-1)	7.807 172 252(-2)	-1.487 976 260(-2)	2.515 386 501(-3)
3	-1.390 617 284	5.447 468 249(-1)	-1.528 312 571(-1)	3.530 763 642(-2)
4	-4.766 501 273	2.957 467 335	-1.179 346 075	3.631 697 407(-1)
5	-1.425 733 882(1)	1.341 754 664(1)	-7.395 259 394	2.974 953 154
6	-3.851 066 745(1)	5.311 188 013(1)	-3.954 239 701(1)	2.043 364 848(1)
7	-9.603 808 236(1)	1.887 377 106(2)	-1.861 866 922(2)	1.218 311 653(2)