High-Temperature Expansions for the Spin-$\frac{1}{2}$ Heisenberg Model*

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We obtain high-temperature power-series-expansion coefficients for the spin-$\frac{1}{2}$ Heisenberg model for the simple cubic, body-centered cubic, and face-centered cubic lattices. The specific heat is carried to 10 terms; the susceptibility series, to 10 terms for the loose-packed lattices and 9 for the close-packed one. The coefficients of the 4th, 6th, and 8th powers of magnetic field are carried to 8 terms. We analyze these series and conclude that the critical points are 0.5972, 0.3963, and 0.2492, respectively, with an error of perhaps 10^{-3}. The critical index for the susceptibility is $\gamma=1.43\pm0.01$ and the gap parameter $2\Delta=3.63\pm0.03$ for all three lattices.

1. INTRODUCTION

THIS paper presents the results of calculations, performed over the past three years, which have aimed at taking the computation of high-temperature expansions for the field-dependent free energy of a Heisenberg model ferromagnet, for spin $\frac{1}{2}$ and with nearest-neighbor interactions only, as far as is practicable with available computers. It confines attention to three-dimensional Bravais lattices: simple cubic (sc), body-centered cubic (bcc) and face-centered cubic (fcc). The series themselves have been analysed, by Padé approximant (PA) and other methods, with a view to determining their behavior as the Curie point is approached (from above); this aspect of the work is described in some detail in order that the weight to be attached to our inferences may be critically assessed. Preliminary reports of most (all but one) of the coefficients and some of the inferences have recently been published elsewhere[1,2]; but no details have yet been given either of the calculations themselves or, more importantly, of the evidence on which our preliminary conclusions were based.

We start with the Hamiltonian

$$\mathcal{H}=-\tfrac{1}{2}J\sum_{\langle ij\rangle}\boldsymbol{\sigma}^{(i)}\cdot\boldsymbol{\sigma}^{(j)}-\mu H\sum_i\sigma_3^{(i)}, \tag{1}$$

where $\boldsymbol{\sigma}^{(i)}$ is the Pauli spin vector at site i of a given crystal lattice, σ_3 is the component of $\boldsymbol{\sigma}$ in the direction of the external magnetic field H, μ is the associated magnetic moment, and J is the exchange coupling constant (positive for ferromagnetic coupling and negative for antiferromagnetic coupling). The first summation in (1) includes, once only, each pair of neighboring sites in the lattice.

Our aim is to find the free energy $F(H, T)$, given by

$$F(H, T)=-\kappa T\ln Z \tag{2}$$

with

$$Z=\mathrm{Tr}\exp(-\mathcal{H}/\kappa T), \tag{3}$$

where κ is Boltzmann's constant and T the temperature. In particular, we wish to express F as a double power series in H and $1/T$. Since F is necessarily an even function of H, it is convenient to write

$$N^{-1}\ln Z=F_0(x)+\sum_{s=1}^{\infty}[(2s)!]^{-1}y^{2s}F_s(x), \tag{4}$$

where $x=J/\kappa T$, $y=\mu H/\kappa T$, and N is the number of lattice sites. The zero-field specific heat $C(0)$ and the zero-field susceptibility $\chi(0)$ derive from $F_0(x)$ and $F_1(x)$, respectively: Explicitly,

$$C(0)=N\kappa x^2(\partial^2/\partial x^2)F_0(x) \tag{5}$$

and

$$\chi(0)\kappa T/N\mu^2=F_1(x). \tag{6}$$

For high-temperature series, we require the expansions of $F_0(x)$, $F_1(x)$, $\cdots$ in powers of x, and shall write

$$F_0(x)=\sum_{n\geq0}(e_nx^n/2^nn!) \tag{7}$$

and

$$F_1(x)=\sum_{n\geq0}(\alpha_nx^n/2^nn!), \tag{8}$$

where e_0 and e_1 are ln2 and 0, respectively [though

* Work supported in part by the U.S. Atomic Energy Commission.
[1] G. A. Baker, Jr., H. E. Gilbert, J. Eve, and G. S. Rushbrooke, Phys. Letters **20**, 146 (1966).
[2] G. A. Baker, Jr., H. E. Gilbert, J. Eve, and G. S. Rushbrooke, Phys. Letters **22**, 269 (1966).

TABLE I. Number of connected, basic, graphs with l lines and m vertices. The last two lines list totals for fixed l and cumulative totals, respectively.

l \ M	1	2	3	4	5	6	7	8	9	10
2	1									
3		1	1							
4			2	2	1	1				
5				3	5	5	4	2	1	1
6					6	13	19	22	20	14
7						11	33	67	107	132
8							23	89	236	486
9								47	240	797
10									106	657
11										235
	1	1	3	5	12	30	79	227	710	2322
		2	5	10	22	52	131	358	1068	3390

these terms do not affect $C(0)$], and $\alpha_0=1$. Since when $x=0$, $Z=(2\cosh y)^N$, it is convenient to write

$$F_2(x)=-2F_2^*(x), \qquad F_3(x)=16F_3^*(x),$$
$$F_4(x)=-272F_4^*(x), \cdots, \tag{9}$$

so that the leading coefficients in $F_2^*(x)$, $F_3^*(x)$, $F_4^*(x)$, $\cdots$ are all unity. In general, for $s\geq 2$, we shall write

$$F_s^*(x)=1+a_{s,1}x+a_{s,2}x^2+\cdots \tag{10}$$

(dropping the first suffix when no confusion can arise). The form for the coefficients in (7) and (8) is dictated partly by tradition (see, for example, Domb and Wood[3]) and partly by computational convenience. The numbers e_n and α_n are, in fact, integers. But for the higher-order series the forms (9) and (10) are more convenient in that they avoid having to tabulate very large numbers.

The method adopted for determining these high-temperature expansions has been the so-called finite cluster method originally suggested by Domb[4] (1960), though at that time a formal proof of its validity was lacking. A formal proof is, however, easily supplied (see, for example, Rushbrooke,[5] and references therein) and it is sufficient here to summarize the necessary procedure. To find the coefficient associated with x^n in the series (7), (8), and (10), we require the following:

(i) Consideration, in detail, of all free connected linear graphs with l lines, where $l\leq n$: These are the so-called basic graphs of Ref. 5, in that there is not more than one direct link (line) between any two vertices. Regarded as a connected array of labelled vertices, these are the finite clusters after which the method is named. We shall denote these basic graphs by (m, l, τ) and the corresponding clusters by $[m, l, \tau]$, where m is the number of points (vertices), and τ a descriptive variable designating the topological type of the graph.

FIG. 1. Two different pictorial representations of graph 1029.

(ii) For any such cluster, to find the logarithm of the corresponding partition function $Q_{[m,l,\tau]}$ based on the Hamiltonian

$$\mathcal{H}_{[m,l,\tau]}=-\tfrac{1}{2}J\sum_{\langle i,j\rangle}\boldsymbol{\sigma}^{(i)}\cdot\boldsymbol{\sigma}^{(j)}-\mu H\sum_i\sigma_3^{(i)},$$

where $1\leq i\leq m$ and the first summation includes only interactions corresponding to the l links in $[m, l, \tau]$:

TABLE II. The number of graphs giving nonvanishing contributions to successive coefficients in high-temperature expansions of $\chi(0)$ and $C(0)$.

	n	1	2	3	4	5	6	7	8	9	10
bcc	$\chi(0)$	1	2	3	6	9	17	30	62	119	271
fcc		1	2	4	8	15	32	75	180	473	
bcc	$C(0)$		1	1	3	3	7	7	21	22	66
fcc			1	2	4	6	13	24	53	120	316

TABLE III. High-temperature expansion coefficients, as defined by Eqs. (7) and (8), for cubic lattices.

	n	e_n	α_n
fcc	1	0	12
	2	18	240
	3	108	6 624
	4	180	234 720
	5	−5 040	10 208 832
	6	162 000	526 810 176
	7	14 565 600	31 434 585 600
	8	563 253 408	2 127 785 025 024
	9	17 544 639 744	161 064 469 168 128
	10	750 651 187 968	
bcc	1	0	8
	2	12	96
	3	−24	1 664
	4	168	36 800
	5	1 440	1 008 768
	6	24 480	32 626 560
	7	−297 024	1 221 399 040
	8	28 017 216	51 734 584 320
	9	−533 681 664	2 459 086 364 672
	10	41 156 316 672	129 082 499 311 616
sc	1	0	6
	2	9	48
	3	−18	528
	4	−162	7 920
	5	2 520	149 856
	6	33 192	3 169 248
	7	−1 019 088	77 046 528
	8	−7 804 944	2 231 209 728
	9	723 961 728	71 938 507 776
	10	2 596 523 904	2 446 325 534 208

[3] C. Domb and D. W. Wood, Phys. Letters **8**, 20 (1964).
[4] C. Domb, Phil. Mag. Suppl. **9**, 149 (1960); see p. 330.
[5] G. S. Rushbrooke, J. Math. Phys. **5**, 1106 (1964).

TABLE IV. Coefficients for the face-centered cubic lattice series.

	n	a_n	p
F_2*	1	2.4	1
	2	3.27	2
	3	3.345	3
	4	2.865 3	4
	5	2.174 797	5
	6	1.512 289 6	6
	7	9.841 725 229 762	6
	8	6.080 849 413 884	7
F_3*	1	5.1	1
	2	1.29	3
	3	2.240 55	4
	4	3.052 05	5
	5	3.500 313 925	6
	6	3.529 118 588 75	7
	7	3.218 580 587 976	8
	8	2.708 643 241 716	9
F_4*	1	8.752 941 176 471	1
	2	3.506 117 647 059	3
	3	9.129 529 411 765	4
	4	1.788 855 132 353	6
	5	2.855 148 846 471	7
	6	3.898 188 506 515	8
	7	4.704 418 456 448	9
	8	5.136 002 987 609	10

$\ln Q_{[m,l,\tau]}$ has then to be expanded as a double power series in H^2 and $1/T$; the coefficient of $y^{2s}x^n$ in this will be denoted $A(s, n)_{[m,l,\tau]}$.

(iii) To find the elements $t_{(m',l',\tau')}{}^{[m,l,\tau]}$ of the matrix T, where $t_{(m',l',\tau')}{}^{[m,l,\tau]}$ is the number of ways a free (unlabeled) basic graph (m', l', τ') can be located on the basic cluster $[m, l, \tau]$.

(iv) To find the quantities $\phi(s, n)_{[m,l,\tau]}$ related to the $A(s, n)_{[m,l,\tau]}$ by the matrix equations

$$A(s, n) = T\phi(s, n), \tag{11}$$

where the elements of the column vector ϕ are labeled $[m, l, \tau]$.

(v) To find, for each lattice under consideration, the occurrence numbers, $N_{(m,l,\tau)}$, specifying the number of times the free basic graph (m, l, τ) can be located among the sites and nearest-neighbor linkages of the given lattice. $N_{(m,l,\tau)}$ is, of course, proportional to N.

(vi) To form the scalar product $\sum_{m,l,\tau} N_{(m,l,\tau)} \phi(s, n)_{[m,l,\tau]}$, which is then equal to the coefficient of $y^{2s}x^n$ in $\ln Z$ for the Hamiltonian (1) and the lattice under consideration. Thus this leads directly to the series (7), (8), and (10).

TABLE V. Coefficients for the body-centered cubic lattice series.

	n	a_n	p
F_2*	1	1.6	1
	2	1.38	2
	3	8.886 666 666 667	2
	4	4.765 333 333 333	3
	5	2.262 98	4
	6	9.844 556 666 667	4
	7	4.010 053 420 635	5
	8	1.551 082 469 345	6
F_3*	1	3.4	1
	2	5.52	2
	3	6.099 666 666 667	3
	4	5.250 333 333 333	4
	5	3.790 254 5	5
	6	2.399 790 291 667	6
	7	1.372 685 800 397	7
	8	7.240 251 275 149	7
F_4*	1	5.835 294 117 647	1
	2	1.509 176 470 588	3
	3	2.516 219 607 843	4
	4	3.136 760 686 275	5
	5	3.170 734 858 824	6
	6	2.732 592 781 667	7
	7	2.076 756 738 407	8
	8	1.425 491 650 982	9

TABLE VI. Coefficients for the simple cubic lattice series.

	n	a_n	p
F_2*	1	1.2	1
	2	7.35	1
	3	3.245	2
	4	1.176	3
	5	3.761 35	3
	6	1.100 224 583 333	4
	7	3.005 826 904 762	4
	8	7.785 024 174 107	4
F_3*	1	2.55	1
	2	2.985	2
	3	2.317 25	3
	4	1.378 5	4
	5	6.809 421 25	4
	6	2.931 814 958 333	5
	7	1.135 642 090 476	6
	8	4.044 279 238 170	6
F_4*	1	4.376 470 588 235	1
	2	8.212 941 176 471	2
	3	9.729 058 823 529	3
	4	8.493 258 088 235	4
	5	5.950 474 970 588	5
	6	3.527 771 238 480	6
	7	1.834 035 935 256	7
	8	8.575 010 300 318	7

This method of attack was chosen because all the steps except (i) are readily computerized. The crux of the matter is (ii), where group theoretic arguments reduce the calculation of the partition function for a given cluster to finding the matrix Γ_k for $\sum_{\text{cluster}}(2P_{ij}-1)$ in appropriate irreducible representations k of the symmetric group. Here P_{ij} is the permutation operator. The basic formula is

$$Z(H, T) = \sum_{n=0}^{\infty} \frac{x^n}{2^n n!} \{ \sum_{k=0}^{[m/2]} \mathrm{Tr}(\Gamma_k{}^n) \sum_{p=k}^{m-k} \exp[(m-2p)y] \}. \tag{12}$$

Equation (12) will not be discussed further here, since to test the feasibility of this approach, which is confined to spin $\frac{1}{2}$, we first tried it out on the linear chain,

FIG. 2. (a) graph 1446; (b) the eight-line graph resulting from the double contraction of 1446.

and we have already published elsewhere[6] details of that calculation, including the derivation of this equation.

We turn now to the details of the present application of this method.

2. COMPUTATION OF THE COEFFICIENTS

On starting the calculation, it is first necessary to get an idea of the magnitude of the problem; in particular, with how many basic graphs shall we be concerned under (i) above. To this end we use the Polya algorithm given by Uhlenbeck and Ford,[7] to count free connected graphs having m vertices and l lines, and produce the data presented in Table I. All graphs $l \leq 9$ have been drawn out explicitly. For $l=10$ we have drawn out only the graphs we needed (except that all were constructed for $m \leq 7$). There is no great difficulty in constructing the graphs systematically, by adding lines to existing graphs (or joining two existing graphs by a line), but any such systematic procedure generates a given graph several times, and it is imperative to be able to recognize distinct graphs unambiguously. Confusion can arise only within a given (m, l) set, but it is perhaps not immediately obvious that, for example, (a) and (b) of Fig. 1 are identical graphs. Since the vast majority of graphs have articulation points (most being simply star graphs with "tails" attached to them), particular care has to be taken to recognize distinct stars (multiply connected graphs): Other duplicates are then easily avoided. And for recognizing stars, as illustrated above, it proves convenient always to present explicitly in outline the largest closed polygon within the graph, i.e., to use (b) rather than (a) in Fig. 1. We also checked for duplicates (which would imply omissions) mechanically, but shall discuss this in the next section (on checking procedures).

Because a single (11, 10) graph was found to require over 20 min IBM Stretch machine time at Los Alamos for the completion of step (ii) above (up to $n=10$), we decided not to go beyond α_{10} in the series (8). In this case we are involved only with the 10-link chain, and not with other 10-link trees (which have more than two free ends, and so do not contribute to the zero-field susceptibility series if this is not taken beyond α_{10}).

TABLE VII. Smallest positive real roots ($\times 10^4$), and corresponding residues ($\times -10^3$), from denominators of PA's to $(d/dx)\ln\chi$ for the fcc lattice.

N \ D	0	1	2	3	4	5	6	7
				Roots				
1	2500	2667	2521	2427	2445	2489	2509	2503
2	2679	2588	2291	2442	2411	2526	2505	
3	2519	2376	2473	2482	2495	2491		
4	2448	2455	2483	a	2492			
5	2456	2444	2498	2493				
6	2482	2541	2491					
7	2501	2502						
8	2502							
				Residues				
1	1500	1707	1442	1238	1287	1430	1512	1487
2	1732	1582	859	1277	1213	1609	1493	
3	1441	1106	1369	1396	1442	1427		
4	1298	1315	1398		1430			
5	1317	1293	1458	1432				
6	1401	1750	1422					
7	1427	1472						
8	1484							

[a] $2443 \pm 149\,i$.

TABLE VIII. Smallest positive real roots ($\times 10^4$), and corresponding residues ($\times -10^3$), from denominators of PA's to $(d/dx)\ln\chi$ for the bcc lattice.

N \ D	2	3	4	5	6
		Roots			
3	3909	3922	4119	3995	3892
4	3926	3960	3953	3971	
5	4144	3953	3958		
6	4003	3970			
7	4074				
		Residues			
3	1324	1343	1940	1483	1182
4	1349	1398	1387	1424	
5	2166	1387	1396		
6	1505	1423			
7	1663				

TABLE IX. Smallest positive real roots ($\times 10^4$), and corresponding residues ($\times -10^3$), from denominators of PA's to $(d/dx)\ln\chi$ for the sc lattice.

N \ D	2	3	4	5	6
		Roots			
3	19 908	5180	6272	5658	6365
4	5 700	5944	5964	5950	
5	6 163	5965	5956		
6	5 828	5948			
7	6 052				
		Residues			
3	5 243	838	1854	1019	2311
4	1 202	1407	1430	1411	
5	1 725	1431	1420		
6	1 242	1407			
7	1 608				

[6] G. A. Baker, Jr., G. S. Rushbrooke, and H. E. Gilbert, Phys. Rev. 135, A1272 (1964).

[7] G. E. Uhlenbeck and G. W. Ford, in *Studies in Statistical Mechanics*, edited by J. de Boer and G. E. Uhlenbeck (North-Holland Publishing Company, Amsterdam, 1962), Vol. I, Part B, Chap. IV, Sec. 4.

TABLE X. γ's for fcc lattice by method (iv). Upper entry for $x_c=0.246$; lower entry for $x_c=0.249$.

D \ N	0	1	2	3	4	5	6
1	1.70_{-1} 1.70_{2}	1.585 1.586	0.96 0.93	1.31_{3} 1.31_{-4}	1.29 1.28	1.70 1.73	1.48_{-1} 1.48_{3}
2	1.46 1.45	0.4 0.3	1.38_{0} 1.38_{-4}	1.39_{1} 1.39_{-2}	1.445 1.445	1.423 1.421	
3	1.27 1.26	1.29 1.28	1.39_{1} 1.39_{-2}	1.37_{4} 1.37_{0}	1.427 1.426		
4	1.29 1.28	1.27 1.26	1.435 1.435	1.426 1.424			
5	1.41_{-2} 1.41_{-4}	1.8_{-3} 1.8_{1}	1.424 1.422				
6	1.50 1.51	1.50_{-3} 1.50_{2}					
7	1.50_{-3} 1.50_{2}						

Having made this decision we are not concerned with any $l=10$ graph with more than two "tails" (nodes of order one). Graphs with $l>10$ make no contribution to coefficients $n\leq 10$. Even this restriction still leaves a formidable program, particularly time consuming at step (v); we therefore decided to take the series (7) and (8) to $n=10$ for open lattices (sc and bcc), but to terminate them at $n=9$ for the close-packed lattice (fcc). This means that for $l=9$ we include all even graphs (i.e., graphs in which closed circuits always involve an even number of vertices) but only those odd graphs (containing closed circuits involving an odd number of vertices) which have no more than two "tails." For $l=10$ we include only even graphs having no more than two tails. This reduces the cumulative totals of Table I for $l=9$ and 10 from 1068 and 3390 to 877 and 1026, respectively, and the problem has manageable proportions. We subsequently decided to include e_{10} in (7) for the fcc lattice, but shall discuss this separately below.

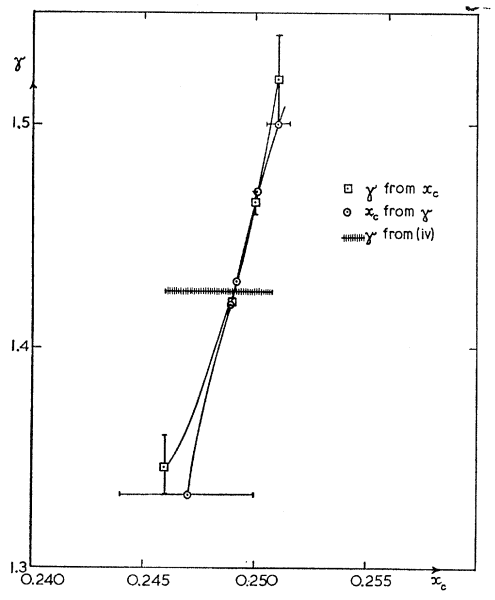

FIG. 3. Locus of points in the (x_c, γ) plane consistent with methods (ii) and (iii).

Not all, of course, of these 1026 graphs make a nonzero contribution to e_{10} or α_{10}. There are, for example, $l=9$ graphs with more than four tails (which make no contribution), but we kept them in in order to check that we did indeed compute vanishing ϕ's. The number of graphs which actually gave nonvanishing contributions to successive coefficients is shown in Table II, from which it is clear that while it would probably not be prohibitively difficult to add e_{11} for open lattices, to extend further the other $\chi(0)$ and $C(0)$ series is barely feasible using the present methods and machines.

Regarding the coefficients $a_{s,n}$, Eqs. (9) and (10), for $s\geq 2$ the situation is a little different. To avoid an excess of machine output in the early stages of the calculation, we arranged that Stretch should print out the Γ's for each basic graph but proceed to find $A(s, n)$ only for $s=0$ and $s=1$. The same Γ's, in conjunction with Eq. (12), could subsequently be used to find $A(s, n)$ for $s=2$, 3, 4, $\cdots$. It later became more convenient to do this remaining part of the calculation on

TABLE XI. fcc lattice; $10^4 x_c$ by method (iii) taking $\gamma=4/3$

D \ N	1	2	3	4	5	6	7	8
1	2353	2446	2467	2463	2461	2464	2469	2472
2		2474	2464	2457	2462	2456	2486	
3	2478	2458	2461	2463	2465	2470		
4	2472	2461	2436	2503	2475			
5	2458	2464	2505	2466				
6	2461	2469	2475					
7		2473						
8	2479							

TABLE XII. fcc lattice; $10^4 x_c$ by method (iii) taking $\gamma=1.43$

D \ N	1	2	3	4	5	6	7	8
1	2440	2510	2514	2499	2490	2489	2491	2493
2		2515	2511	2477	2489	2489	2496	
3	2517	2498	2492	2492	2492	2492		
4	2519	2492	2492	2492	2492			
5	2482	2492	2492	2492				
6	2489	2492	2492					
7	2488	2492						
8	(omitted because of machine overflow)							

the KDF 9 machine at Newcastle, and, for technical reasons, this entailed hand transcription (with consequent careful checking) of the Γ information as input. For this reason we confined attention to the first 358 graphs of Table I. This gave the series $a_{s,n}(s=2, 3, 4)$ for $n\leq 8$, which is more than enough to give us the functions f_n, $0\leq n\leq 10$, in an expansion of $\ln Z(H, T)$ of the form

$$\ln Z(H, T) = \sum_{n=0}^{\infty} f_n \left(\frac{\mu H}{J}\right) x^n. \tag{13}$$

It is convenient next to consider the occurrence numbers $t_{(m',l',\tau')}^{[m,l,\tau]}$ and $N_{(m,l,\tau)}$, the former counting a graph (m', l', τ') on another graph or cluster $[m, l, \tau]$ and the second counting a graph (m, l, τ) on a given infinite lattice: See (iii) and (v) above. $N_{(m,l,\tau)}$ is, of course, proportional to N, the number of lattice sites, and in finding $N_{(m,l,\tau)}$ one point of (m, l, τ) is held fixed. Since a computer program will normally count the occurrences of a labelled graph on a labelled cluster, or lattice, and we require the counts for unlabelled graphs, we need to divide by the symmetry numbers of the basic graphs. These numbers are easily obtained mechanically by counting the occurrences of a graph on itself. The elements of the T matrix, and symmetry numbers, were found at Los Alamos, but the Los Alamos program was slow for finding infinite lattice counts and used to find these counts only for two-dimensional Bravais lattices (plane square and plane triangular) and the simple cubic lattice. A more efficient lattice-counting program was developed at Newcastle and used, on the KDF 9 machine, to find all the three-dimensional lattice counts (sc, bcc, and fcc). This was a master program in the sense that the same program was used

TABLE XIII. fcc lattice; $10^3\gamma$ by method (ii) taking $x_c=0.2492$

D \ N	1	2	3	4	5	6	7
1	1495	1374	1388	1512	1443	1441	1413
2	1382	1412	1424	1431	1429	1430	
3	1394	1425	1435	1430	1430		
4	1543	1432	1430	1430			
5	1442	1429	1430				
6	1437	1430					
7	1478						

TABLE XIV. bcc lattice; $10^4 x_c$ by method (ii) taking $\gamma=4/3$.

D \ N	2	3	4	5	6	7
3	3914	3915	3914	3894	3942	3939
4	3915	3914	3911	3919	3938	
5	3914	3923	2930	3881		
6	3877	3920	3923			
7	3941	3939				
8	3940					

for all graphs, it being necessary to feed in as data only a description of the graph. The program then counted this on all three lattices (except that, to save time, the fcc work was eliminated when that particular count was not required). We believe that this was an efficient counting program for all graphs except closed polygons, for which the earlier program described by Rushbrooke and Eve[8] would have saved machine time. Empirically, the time required to find the count for a given graph is roughly proportional to the final answer (before dividing by the symmetry number). The time thus varied from milliseconds to 2 or 3h (for long chains or polygons), the average time needed to count a graph on all three lattices being a few seconds per graph. It is impracticable, and unnecessary, to present these counts here, but because the results for chains c_l and polygons p_l are of some interest in other connections, we note (after division by symmetry numbers)

$$c_9 \quad \text{(fcc)} = 846886962,$$
$$c_{10} \quad \text{(bcc)} = 118145548,$$
$$p_{10} \quad \text{(fcc)} = 2241420,$$

since these are additional to values listed in Domb's tables.[9] For the simple cubic lattice c_l and p_l are known to $l=16$: See Ref. 8 and Sykes.[10]

The operations (iv) and (vi), namely solving Eqs. (11) and forming the final scalar products, are relatively trivial. We observe only that there is no question of first finding the inverse matrix T^{-1} in order to solve (11): Since T is a triangular matrix we simply solve the equations successively, using the ϕ's for smaller clusters to find those for larger ones. Apart from its

TABLE XV. bcc lattice; $10^4 x_c$ by method (ii) taking $\gamma=1.43$.

D \ N	2	3	4	5	6	7
3	3999	3951	3970	3969	3976	3976
4	3959	3974	3982	3973	3973	
5	3970	3984	3975	3973		
6	3969	3973	3973			
7	3975	3973				
8	3982					

[8] G. S. Rushbrooke and J. Eve, J. Math. Phys. **3**, 185 (1962).
[9] Reference 4, Tables A and B of Appendix III.
[10] M. F. Sykes, J. Chem. Phys. **39**, 410 (1963).

TABLE XVI. bcc lattice; $10^3\gamma$ by method (ii) taking $x_c=0.3923$

D \ N	2	3	4	5	6
3	1345	1345	1344	1332	1286
4	1345	1346	1290	1360	
5	1381	1333	1363		
6	1243	1295			
7	1287				

simplicity, this method has the merit of enabling us to avoid roundoff error—a matter to which we shall return when discussing checking procedures.

The final results are presented in Tables III to VI. Table III gives, for all three lattices, the coefficients e_n and α_n of Eqs. (7) and (8). Tables IV, V, and VI list, for the fcc, bcc, and sc lattices, respectively, the coefficients a_n of Eq. (10), for $s=2$, 3, and 4. The latter coefficients are expressed in the form $a\cdot 10^p$, where $1<a<10$. We believe all entries are free from roundoff and other error except in the case of $a_{4,8}$, where there is no certainty of the absence of roundoff error [in the $\phi(4, 8)$'s for some of the larger clusters]. Even so, we are confident of the $a_{4,8}$ values to six significant figures (all lattices), and suspect that several more digits are in fact reliable.

3. CHECKING PROCEDURES

In a calculation of this magnitude, adequate checking procedures are indispensable, and at least some of them warrant mention. First, we developed a rapid machine check for duplicate diagrams (basic graphs). This was to list for each vertex of a graph the sum of all the shortest distances (defined as the number of links traversed) between it and every other vertex. When the route of shortest distance was not unique, the length of every such route was included in the sum. We thus obtained, for each graph, a set of m numbers which were ordered by their size. This does not provide an unambiguous description of the graph, but the number of false duplicates, i.e., pairs of different graphs yielding the same such description, is very small, and on inspection these are easily distinguished from true duplicates. This check was worthwhile in that it did reveal an error of transcription affecting three graphs. (We later developed a more sophisticated machine check which did not produce false duplicates, but by then the earlier one had served its purpose.)

TABLE XVII. bcc lattice; $10^3\gamma$ by method (ii) taking $x_c=0.3973$.

D \ N	2	3	4	5	6
3	1355	1416	1423	1429	1430
4	1436	1423	1409[a]	1430	
5	1443	1429	1430		
6	1415	1430			
7	1426				

[a] Second real pole in P.A. at $x=0.242$.

TABLE XVIII. γ's for bcc lattice by method (iv). Upper entry for $x_c=0.39$; lower entry for $x_c=0.40$.

D \ N	1	2	3	4	5
3	1.33	1.35	1.38_2	1.40	1.425
	1.32	1.34	1.38_{-4}	1.39	1.423
4	1.440	3	1.40	1.37	
	1.441	5	1.39	1.36	
5	1.54	1.48	1.424		
	1.55	1.49	1.423		
6	1.427	−0.1			
	1.424	−1.0			
7	1.32				
	1.30				

Regarding the lattice counts, the fact that very different machine programs at Los Alamos and Newcastle, respectively, gave identical counts for all graphs on the simple cubic lattice, and over 400 identical counts on either the body-centered or face-centered lattices (though we did not use the Los Alamos program to complete the counts for these lattices) gives us confidence in both programs. Incidentally, we have agreement with all the counts listed in Domb's tables,[9] excluding c_{10} (triangular) and c_{11} to c_{16} (plane square), which we have not counted.

The main check on the accuracy of the calculation, however, comes from inspection of the ϕ's. Insofar as we can check these we have an indirect check on the elements of the T matrix, as well as on the partition-function side of the calculations. Now $\phi(s, n)$, for the cluster $[m, l, \tau]$, must vanish identically whenever

$$n+2s<l+f, \tag{14}$$

where f is the number of free ends (nodes of order 1) in $[m, l, \tau]$ (and provided $l>1$). This is a consequence of the cumulant character of the ϕ's (see Ref. 5). We deliberately did not discard from the computation many graphs for which (14) holds, even when $n=10$, $s=0$ or 1, in order to retain the benefit of this check on the calculations. Besides the ϕ's which necessarily vanish on account of (14), there are other ϕ's which vanish as a result of two theorems to which we shall refer in the next

TABLE XIX. sc lattice; 10^4x_c by method (ii) taking $\gamma=4/3$.

D \ N	2	3	4	5	6	7
3	5686	5936	5854	5900	5886	5919
4	5502	5863	5879	5889	5896	
5	5750	5885	5892	5864		
6	5933	5891	5883			
7	5865	5903				
8	5987					

TABLE XX. sc lattice; $10^4 x_c$ by method (ii) taking $\gamma=1.43$.

D \ N	2	3	4	5	6	7
3	5781	6118	5944	5975	5945	5978
4	5566	5972	5968	5961	5961	
5	5879	5968	5975	5961		
6	5996	5960	5962			
7	5927	5962				
8	6022					

TABLE XXII. sc lattice; $10^3\gamma$ by method (iii) taking $x_c=0.5963$.

D \ N	2	3	4	5	6
3	1358	1424	1428	1428	1431
4	1455	1429	1428	1428	
5	1409	1428	1428		
6	1445	1432			
7	1427				

section. We confirmed that all ϕ's covered by these theorems were in fact zero.

Even though the calculations are correct in essence, it is still possible to be troubled by roundoff error, due to computers using floating-point arithmetic. Thus the Γ's of Eq. (12) are in fact integers; but they are not necessarily computed as exactly integers. Such roundoff error could produce cumulative trouble, and must certainly be detected before forming the final scalar product under (vi). Provided we can recognize the influence of roundoff error on each new ϕ as this is computed (and remove it), no trouble can arise as we continue to use the elements of the T matrix to compute further ϕ's. We have noticed a remarkable property of the ϕ's which persuades us that the ϕ's we have computed are in fact free of such roundoff error. In one or two cases roundoff error was revealed by this check (and corrected for); its origin was usually easily identifiable. The property relates not to the $\phi(s, n)$'s as defined above, but to the quantities $\phi^*(s, n)$, where

$$\phi^*(s, n) = 2^n n!(2s)!\phi(s, n). \tag{15}$$

It is these quantities $\phi^*(s, n)$ which are actually computed and printed out [see Eqs. (4) and (12)]. We observe (i) that $\phi^*(s, n)$ is always divisible by 2^{2s+n-5}, and (ii) that, after the first five (simplest) clusters, $\phi^*(s, n)$ is divisible by n. We find this last, unexplained, observation most striking, and it gives us confidence in the results. Indeed, we believe that only the quantities $\phi^*(4, 8)$, which are very large numbers, may still be subject to small errors of roundoff origin. An incidental advantage of having to transcribe the input data for computing the $\phi(s, n)$'s, $s>1$, was that it enabled us to eliminate roundoff errors in the Γ's at that stage. We did, of course, repeat the calculation of the $\chi(0)$ coefficients as a check on our transcription.

TABLE XXI. sc lattice; $10^3\gamma$ by method (iii) taking $x_c=0.5883$.

D \ N	2	3	4	5	6
3	1310	1354	1341	1318	1306
4	1368	1343	1401	1234	
5	1306	1317	1251		
6	1319	1310			
7	1292				

The most convincing check on the accuracy of the calculations, however, comes from comparison with completely independent work by other authors. The coefficients $\alpha_1, \cdots, \alpha_6$ and $e_1, \cdots, e_7$ have, of course, been known for a long time, not only for $s=\frac{1}{2}$ but for general spin (see Rushbrooke and Wood,[11] and Domb[4]). During the course of the present calculations, Domb and Wood[12–15] have published the results of very similar calculations which, while not going quite as far, serve in part to confirm our own results. The most complete account of their work is in Ref. 15, where they list $\alpha_1, \cdots, \alpha_9$ and $e_1, \cdots, e_9$ for open lattices and $\alpha_1, \cdots, \alpha_7$ and $e_1, \cdots, e_8$ for close-packed lattices. They give these both as general expressions involving lattice parameters and numerically (as we have done). We find numerical agreement with their results except for e_8 (fcc). This nonagreement led us to infer, from our own work, the general expression for e_8, and we agree with the expression given by Domb and Wood. We believe the numerical discrepancy is due to their having accidentally omitted one (specific) term in this expression when evaluating it.[16]

TABLE XXIII. γ's for sc lattice by method (iv). Upper entry for $x_c=0.59$, lower entry for $x_c=0.60$.

D \ N	2	3	4	5
3	1.03	1.36_4	1.478	1.40_4
	1.01	1.36_{-1}	1.479	1.40_{-1}
4	1.91	1.459	1.439	
	1.94	1.458	1.438	
5	1.0_1	1.433		
	1.0_{-2}	1.431		
6	2.3			
	2.4			

[11] G. S. Rushbrooke and P. J. Wood, Mol. Phys. **1**, 257 (1958).
[12] C. Domb and D. W. Wood, Phys. Letters **8**, 20 (1964).
[13] C. Domb, N. W. Dalton, G. S. Joyce, and D. W. Wood, in *Proceedings of the International Conference on Magnetism, Nottingham, 1964* (The Institute of Physics and The Physical Society, London, 1965), pp. 85–87.
[14] D. W. Wood, Phys. Letters **14**, 191 (1965).
[15] C. Domb and D. W. Wood, Proc. Phys. Soc. (London) **86**, 1 (1965).
[16] More detailed comments are given in a footnote in Ref. 1 The coefficients which we have called α are called j by Domb and Wood. Domb (private communication) has expressed agreement with our comments here.

TABLE XXIV. Neville table for F_4^* (fcc). In constructing the table more digits must be retained than are here displayed.

n	r_n	l_n	q_n					
1	87.53							
2	40.06	−7.417						
3	26.04	−1.996	0.714					
4	19.59	0.260	2.517	3.117				
5	15.96	1.427	3.178	3.618	3.744			
6	13.65	2.115	3.492	3.806	3.899	3.930		
7	12.07	2.558	3.666	3.899	3.968	3.996	4.007	
8	10.92	2.862	3.772	3.948	3.997	4.014	4.020	4.022

No comparable check is possible on our coefficients for the series F_2, F_3, and F_4. However, we have calculated the leading two or three terms in each series by an alternative, direct, method as a check that our computer programs were yielding the information expected from them.

4. CALCULATION OF e_{10} (fcc)

Our decision to compute e_{10} for the face-centered cubic lattice was taken after the calculations described above had been completed. We had, in fact, recorded the contributions to e_{10} (fcc) from all graphs $l\leq 9$ and from $l=10$ even graphs; so we had now to add in the contributions from $l=10$ odd graphs. Fortunately, for $m\leq 7$ these graphs had been processed, as far as the ϕ's, at an earlier stage; so we required only the corresponding lattice counts (which were easily found). But for $l=10$ and $m=8, 9, \cdots$ we had not found the Γ's necessary for computing the partition functions, nor the relevant elements of the T matrix. We nevertheless found it possible to complete the calculation, by deducing the necessary new ϕ's from our previous results.

We must first recognize that for a 10-line graph to contribute to e_{10} it must have no free ends (nodes of order one); thus we are concerned only with closed graphs. This rules out $m=11$ and leaves only the closed polygon (an even graph) for $m=10$. Now, if we were concerned not with the cumulant associated with any such graph but with the corresponding moment, or mean trace, we could appeal to certain theorems formulated by Rushbrooke and Wood,[11,17] in particular the following:

(i) The trace vanishes for any graph which falls into two parts on the removal of a single line [Theorem IV, Ref. 10];

(ii) The trace vanishes for any graph having a sequence of nodes of orders 2, 3, 2 [Theorem IV, Ref. 17].

But it is not difficult to prove that these theorems hold not only for the moments (mean traces) but also for the corresponding cumulants, i.e., the $\phi^*(0, n)$'s where $n=l$. This means that all $l=10$ graphs coming under the descriptions in (i) and (ii) above make no contribution to e_{10}, which greatly reduces the number of graphs still to be considered. In fact we are left with only 17 new (odd-circuit) graphs to consider: 15 for $m=8$ and 2 for $m=9$.

We have still to find the ϕ's for these graphs; but it is not difficult to prove that if $[l]$ is an l-line graph having three consecutive lines $(ij)(jk)(km)$, where the points j and k are not otherwise involved, and $[l-1]$ denotes the corresponding graph with (jk) removed, so making j and k coincide, then, when i and m are distinct points,

$$\phi_{[l]}{}^*(0, l) = l\phi_{[l-1]}{}^*(0, l-1). \qquad (16)$$

Equation (16) is simply the extension to cumulants of the contraction theorem for traces given in Theorem I of Ref. 11. It enables us to infer 16 of the 17 required ϕ's from results already obtained for 9-line graphs. We are left with only one awkward case, namely the graph of Fig. 2(a). But we can build up the ϕ for this if we know the corresponding mean trace, and this is related to the mean trace of the multiline graph of Fig. 2(b) by Theorem I of Ref. 11. Fortunately, the mean trace for this 8-line graph had been found by one of us (J. E., for general spin) in another connection. We were thus able to complete the calculation. Even without knowing this trace, it is possible, by a rather sophisticated argument, based on the cumulant analogs of Theorems I and IV of Ref. 11, to infer the necessary ϕ from earlier (susceptibility series) results.

This completes our account of how the coefficients of Tables III–VI were obtained. We now turn to the analysis of the resulting series, Eqs. (7), (8), and (10), by Padé approximant and other methods.

5. ANALYSIS OF THE SERIES

We are concerned with series of the general form

$$f(x) = 1 + a_1x + a_2x^2 + \cdots + a_nx^n + \cdots, \qquad (17)$$

of which we know only the first n coefficients. We expect the function $f(x)$ to possess certain singularities, those on the real x axis having physical significance. In particular, if the singularity closest to the origin on the positive x axis lies at x_c, then, since $x=J/\kappa T$, x_c will correspond to the Curie temperature T_c of the ferromagnetic problem ($J>0$). Similarly, the singularity x_N closest to the origin on the negative x axis will correspond to the Néel temperature of the corresponding antiferromagnetic problem ($J<0$).

[17] G. S. Rushbrooke and P. J. Wood, Mol. Phys. 6, 409 (1963).

TABLE XXV. Neville tables for γ_2. More digits were retained in computing these than are here displayed.

fcc $x_c=0.2492$				bcc $x_c=0.3973$				sc $x_c=0.5962$		
n	$\gamma_2(n)$	l_n	q_n	n	$\gamma_2(n)$	l_n	q_n	n	$\gamma_2(n)$	l_n
1	5.981			1	6.357			1	7.154	
2	5.791			3	5.675	5.335		2	6.303	5.453
3	5.647			5	5.434	5.071		3	5.897	5.083
4	5.538			7	5.328	5.066	5.062	4	5.643	4.881
5	5.457	5.133		2	5.853			5	5.535	5.102
6	5.397	5.097	5.025	4	5.522	5.190		6	5.464	5.109
7	5.352	5.082	5.046	6	5.370	5.067		7	5.402	5.031
8	5.318	5.076	5.058	8	5.294	5.066	5.064	8	5.353	5.013

To locate the singularities of $f(x)$ we have principally employed the method of Padé approximants (see Baker[18] for a recent review incorporating references to earlier work). We write

$$f(x)=\frac{1+\alpha_1 x+\cdots+\alpha_N x^N}{1+\beta_1 x+\cdots+\beta_D x^D}, \tag{18}$$

and with $N+D=n$ the coefficients $\alpha_1, \cdots, \alpha_N, \beta_1, \cdots, \beta_D$ are uniquely fixed by the requirement that the series expansion of (18) shall coincide with that of (17) through the known coefficients $a_1, \cdots, a_n$. We refer to (18) as the $[D, N]$ Padé approximant (PA) to (17). If we choose $D+N=m(<n)$ then we require that the expansion of (18) shall match the coefficients $a_1, a_2, \cdots, a_m$ in (17), i.e., we consider the PA to a shorter series expansion of $f(x)$.

We are interested not only in the location of x_c or x_N, but in the behavior of $f(x)$ at this singularity. At x_c, with which we are primarily concerned, we shall normally assume that, as x tends to x_c from below,

$$f(x)\sim[A/(x_c-x)^p], \tag{19}$$

where $\sim$ stands for "is asymptotically proportional to"; and we seek to find the so-called critical index p (which we do not expect to be integral). We may then observe the following:

(i) If (19) holds near x_c, then

$$(d/dx)\ \ln f(x)\sim -p/(x_c-x), \tag{20}$$

i.e., the logarithmic derivative of $f(x)$ will have a simple pole at x_c with residue $-p$. Such a function is particularly suitable for representation by Padé approximants, the $[D, N]$ PA having D poles and N zeros. We shall therefore form PA's to the derived series $(d/dx)\ \ln f(x)$, finding the smallest positive real roots of their denominators (as estimates of x_c) and the values of the residues at these roots (as estimates of $-p$).

(ii) If we knew x_c, then since

$$(x-x_c)(d/dx)\ \ln f(x)\sim p, \tag{21}$$

PA's to $(x-x_c)(d/dx)\ \ln f(x)$ evaluated at x_c would give estimates of p. To use this method we take a trial value of x_c, in a range suggested by (i), and evaluate at x_c PA's to the series expansion of the left-hand side of (21).

(iii) If we knew p, then since

$$f(x)^{1/p}\sim A^{1/p}/(x_c-x), \tag{22}$$

i.e., has a simple pole at x_c, representations of the series expansions of $f(x)^{1/p}$ by PA's would enable us to find both x_c and A. To use this method we take a trial value of p, again in a range suggested by (i).

(iv) The function

$$\frac{d}{dx}\ln\frac{df}{dx}\Big/\frac{d}{dx}\ln f(x) \tag{23}$$

has the value $(p+1)/p$ at x_c, and so PA's to the series expansion of (23) evaluated at x_c should provide estimates of p, which we may hope to be relatively insensitive to the precise choice of x_c.

Except for (iv), these methods of determining x_c and p from (17) are not new: They were used, for example, by Baker,[19] in an early paper on the application of Padé approximants to the Ising model. But we have used them perhaps rather more systematically than hitherto: In particular, we have taken a range of different choices for x_c in using method (ii) and a range of different choices of p in using method (iii). Moreover, for any series such as (17) we have always computed a full Padé table, forming all $[D, N]$ PA's where $D+N\leq n$, $D\geq 1$ and $N\geq 0$, displaying the results in tableau form, where N labels the columns and D the rows.[20] In such a Padé table, all entries along a diagonal $D+N=m$ make use of the same number of coefficients, m, in the original series, whereas entries in adjacent diagonals bring in successively one extra term of the original series. Since we do not wish to attach too much significance to any particular PA, and since we hope that the series are long enough for reliable values of x_c and p to be inferred from them (without leaning too heavily on the last calculated coefficient) we shall incline to be most satisfied when several PA's, say $[4, 5]$, $[5, 4]$, $[4, 4]$, $[5, 3]$, $[3, 5]$, $[4, 3]$, and $[3, 4]$, all lead to the same predictions. It is in such circum-

[18] G. A. Baker, Jr., in *Advances in Theoretical Physics*, edited by K. A. Brueckner (Academic Press Inc., New York, 1965), Vol. 1, p. 1.

[19] G. A. Baker, Jr., Phys. Rev. **124**, 768 (1961).

[20] For arithmetic reasons, connected with machine overflow, the $N=0$ column was sometimes omitted, but this is of little importance.

stances that we shall say that the Padé table has converged. Naturally, too, we shall be satisfied only if we have consistency between the four methods, (i) to (iv), listed above.

Two quite valid arguments may be leveled against this attitude. The first, that we should look for trends rather than convergence in the sense in which we have defined it; the second, that both by concentrating on "central" Padé's (D approximately equal to N) and by use of the logarithmic derivative, we are always influenced by early coefficients in the original series (and these may incorporate random elements, which are meaningless as far as the asymptotic behavior of these coefficients is concerned). As an excuse for the first criticism, we can say only that there is no known reliable method of extrapolating predictions from successive Padé approximants and, in any case, we have failed to observe systematic trends. On the second score, if x_c were the only singularity of $f(x)$, then the well-known ratio method, using only successive coefficients in the series expansion of $f(x)$, and incorporating a final extrapolation, might well be preferable to use of Padé approximants. Unfortunately, as we shall see, x_c is never the only singularity of $f(x)$. Nevertheless, we have in fact also explored ratio and related methods and, in particular, we have used the equation of Domb and Sykes,[21]

$$n[x_c(a_n/a_{n-1})-1]\rightarrow p-1, \qquad \text{as} \quad n\rightarrow\infty \qquad (24)$$

as a way of estimating p from the series (17) when x_c is supposed known. In practice, we find agreement with our previous conclusions from Padé approximants.

Any numerical uncertainties that we may attach to our estimates must always be understood against the background of the above philosophy. They certainly have no absolute significance, for from even ten terms of an infinite series no firm conclusions can possibly be drawn. Ultimately, we must regard the analysis of these series as a kind of experimental mathematics conducted in the spirit of previous explorations in this field.

6. THE SUSCEPTIBILITY SERIES

For susceptibility series, the critical index p, above, is customarily denoted by γ. Previous work,[22–24] based on $a_1, \cdots, a_6$ only, had suggested $\gamma=\frac{4}{3}$ for all three lattices (fcc, bcc, sc) though the evidence was, admittedly, not very strong. The values of x_c were estimated to be approximately 0.246, 0.392, and 0.588 for the fcc, bcc, and sc lattices, respectively.

Using our longer series, we have first, following method (i), computed Padé tables for $(d/dx)\ \ln F_1(x)$, finding the smallest positive real roots of the Padé denominators and the residues at these roots. The results are shown in Tables VII, VIII, and IX. For the fcc lattice, Table VII, we present the results in full. For the bcc and sc lattices, Tables VIII and IX, we give only the central parts of the Padé tables (to save space, and because for the sc lattice the entries in the rows for $D=1$ and 2 are much too erratic to be meaningful). It is clear that convergence is best for the fcc lattice, and we shall first discuss this case in some detail.

For the fcc lattice, we next followed methods (ii) and (iii) above, choosing $x_c=0.246$, 0.249, 0.250, and 0.251 in method (ii) and $\gamma=\frac{4}{3}$, 1.42, 1.43, 1.47, and 1.5 in method (iii). We find that there is a very strong correlation between the conclusions of these two methods, as illustrated in Fig. 3. Over a line in the (x_c, γ) plane from about (0.248, 1.38) to about (0.250, 1.47), reasonably good, mutually consistent, sense can be made of the Padé tables—which becomes increasingly impossible outside this range. We therefore turn next to method (iv), evaluating PA's to the function (23) [where $f(x)$ now stands for $F_1(x)$] over the range $0\leq x\leq 0.27$. We present the results only for $x=0.246$ and $x=0.249$ in Table X, where we list the inferred values of γ. We observe that the [2, 4], [4, 2], [2, 5], [3, 4], [4, 3], and [5, 2] PA's all give $\gamma=1.43\pm0.01$ and, moreover, that for these Padé's the results are relatively insensitive to the precise choice of x_c. Finally, we look back at Table VII and observe that what are probably the three best Padé's, namely [4, 4], [5, 3], and [3, 5], were already suggesting this value of γ.

That the evidence for $\gamma=1.43$ is stronger than was that for the former conclusion $\gamma=1.33$ is rather clearly shown by comparison of Tables XI and XII, which give the smallest positive real roots of PA's to $F_1^{1/1.43}$ and $F_1^{3/4}$, respectively. With $\gamma=1.43$, we infer $x_c=0.2492$. Choosing $x_c=0.2492$ in method (ii) leads to the estimates of γ shown in Table XIII, and if we are looking for convergence and mutual consistency it is hard to improve on this. We have not listed the residues at the roots in Tables XI and XII, but those appropriate to $F_1^{1/1.43}$ are very well converged to the value 0.262. Thus our conclusion for the fcc lattice is

$$\frac{\chi(0)\kappa T}{N\mu^2}\sim\left(\frac{0.262}{0.2492-x}\right)^{1.43}=\frac{1.07}{(1-T_c/T)^{1.43}}.$$

We have followed a similar procedure for the other lattices, bcc and sc. For brevity, we present simply the central parts of the most relevant Padé tables. For the bcc lattice, Tables XIV and XV show x_c as estimated, method (iii), from $F_1^{3/4}$ and $F_1^{1/1.43}$, respectively. There is not a great deal to choose between the choices ($\gamma=\frac{4}{3}$, $x_c=0.3923$) and ($\gamma=1.43$, $x_c=0.3973$). On the other hand, comparison of Tables XVI and XVII, showing estimates of γ obtained following method (ii) for $x_c=0.3923$ and $x_c=0.3973$, respectively, certainly favors the latter value, and thus the higher value of γ. So, we

[21] C. Domb and M. F. Sykes, J. Math. Phys. **2**, 63 (1961).
[22] C. Domb and M. F. Sykes, Phys. Rev. **128**, 168 (1962).
[23] J. Gammel, W. Marshall, and L. Morgan, Proc. Roy. Soc. (London) **A275**, 257 (1963).
[24] G. A. Baker, Jr., Phys. Rev. **136**, A1376 (1964).

TABLE XXVI. Neville tables for γ_3. More digits were retained in computing these than are here displayed.

	fcc $x_c=0.2492$			bcc $x_c=0.3973$				sc $x_c=0.5962$			
n	$\gamma_3(n)$	l_n	n	n	$\gamma_3(n)$	l_n	q_n	n	$\gamma_3(n)$	l_n	q_n
1	12.709			1	13.508			1	15.203		
2	11.607	10.504		2	11.900	10.293		2	12.958	10.713	
3	10.985	9.741		3	11.171	9.711		3	11.885	9.738	
4	10.578	9.359		4	10.679	9.205		4	11.187	9.093	
5	10.290	9.137		5	10.341	8.987		5	10.725	8.879	
6	10.075	9.000	8.726	6	10.093	8.855	8.590	6	10.402	8.784	8.593
7	9.909	8.913	8.695	7	9.908	8.797	8.655	7	10.166	8.750	8.664
8	9.777	8.856	8.686	8	9.764	8.760	8.649	8	9.986	8.725	8.653

feel, does Table XVIII, giving the estimates of γ from method (iv), and the higher value of x_c is itself suggested by Table VIII. Finding the residues associated with the roots displayed in Table XV leads to (bcc lattice)

$$\frac{\chi(0)\kappa T}{N\mu^2}\sim\left(\frac{0.422}{0.3973-x}\right)^{1/1.43}=\frac{1.04}{(1-T_c/T)^{1.43}}.$$

Similarly, for the sc lattice, Tables XIX and XX show x_c as estimated, method (iii), from $F_1^{3/4}$ and $F_1^{1/1.43}$, respectively: Again perhaps there is little to choose between the choices ($\gamma=\frac{4}{3}$, $x_c=0.5883$) and ($\gamma=1.43$, $x_c=0.5962$). But comparison of Tables XXI and XXII, showing estimates of γ obtained following method (ii) for $x_c=0.5883$ and $x_c=0.5962$, respectively, certainly favors the latter value, and thus the higher value of γ. So does Table XXIII, giving the estimates of γ from method (iv), and the higher value of x_c is itself suggested by Table IX. Finding the residues associated with the roots displayed in Table XX leads to (sc lattice)

$$\frac{\chi(0)\kappa T}{N\mu^2}\sim\left(\frac{0.679}{0.5962-x}\right)^{1/1.43}=\frac{1.10}{(1-T_c/T)^{1.43}}.$$

Finally, with these choices of x_c, we look at the ratio method of Domb and Sykes expressed in Eq. (24). For the sc lattice the estimates of γ so obtained vary erratically between 1.2 and 1.8 and no inference can be drawn from them; but for the fcc lattice, with $x_c=0.2492$, $n=3, 4, \cdots, 9$ lead to the estimates 1.439, 1.415, 1.419, 1.430, 1.435, 1.434, and 1.432 for γ; and for the bcc lattice, with $x_c=0.3973$, $n=3, 4, \cdots, 10$ lead to γ values 1.443, 1.393, 1.445, 1.425, 1.437, 1.414, 1.442, and 1.428.

We believe that, subject to our basic procedural assumptions, the evidence that $\gamma=1.43\pm0.01$ for all three lattices is rather strong (and does not rest on the unsupported values of our last computed coefficients). It is, perhaps, relevant that, on the evidence of six terms only, Gammel, Marshall, and Morgan[23] commented that with increasing spin value γ appeared to decrease smoothly from about 1.4 for $s=1$ to 1.33 for $s=\infty$. At that time the case $s=\frac{1}{2}$ was exceptional. The new value removes the anomaly. Recent estimates of γ for $s=\infty$ by Wood and Rushbrooke[25] (1.36) and Joyce and Bowers[26] (1.38) suggest a limiting value rather higher than 1.33, but still lower than our $s=\frac{1}{2}$ value of 1.43.

7. ANTIFERROMAGNETIC SINGULARITIES

Each susceptibility series $F_1(x)$ exhibits, as we have seen, a singularity for a positive real value of x, x_c, corresponding to the ferromagnetic Curie point. We next ask whether there are other values of x for which $F_1(x)$ is singular. To this end we have looked at all the zeros of the denominators of all the PA's to $(d/dx)\ \ln F_1(x)$ and also to $(d/dx)\ \ln F_1(x)-1.43/(x_c-x)$. When these are plotted in the complex x plane it is evident that in no case is x_c the only singularity of the series $F_1(x)$.

For the fcc lattice, besides the singularity at $x=0.2492$ there is a pair of singularities at approximately $x=0.2\pm0.4i$. We have not succeeded in locating this pair of singularities very precisely, and suspect that the singularities concerned are weak in comparison with the ferromagnetic singularity. Attempts to remove this complex pair have not produced a significant change in our estimate of x_c. There is no evidence of a singularity in $F_1(x)$ on the negative real axis, supporting the belief that nearest-neighbor interactions only cannot produce antiferromagnetic ordering in a face-centered cubic lattice.

For the open lattices, bcc and sc, the situation is otherwise: For both lattices there is evidence of a singularity at x approximately equal to $-x_c$. For the bcc lattice, this is the only other singularity of which we find unambiguous evidence (though there may be a number of weak singularities for which $0.25<|x|<0.35$). But for the sc lattice there is quite certainly a complex pair of singularities at approximately $x=-0.075\pm0.504i$. It is possible to locate this complex pair more sharply than in the fcc case, but again there seems to be little interference between this and the Curie point singularity at x_c.

Although the complex singularities to which we refer

[25] P. J. Wood and G. S. Rushbrooke, Phys. Rev. Letters **17**, 307 (1966).

[26] G. S. Joyce and R. G. Bowers, Proc. Phys. Soc. (London) **89**, 776 (1966).

TABLE XXVII. Neville tables for γ_4. More digits were retained in computing these than are here displayed.

	fcc $x_c=0.2492$					bcc $x_c=0.3973$					sc $x_c=0.5962$			
n	$\gamma_4(n)$	l_n	q_n	c_n	n	$\gamma_4(n)$	l_n	q_n	c_n	n	$\gamma_4(n)$	l_n	q_n	c_n
1	21.812				1	23.184				1	26.093			
2	18.964	16.116			2	19.551	15.918			2	21.377	16.661		
3	17.467	14.472			3	17.872	14.516			3	19.188	14.810		
4	16.531	13.726			4	16.811	13.628			4	17.819	13.712		
5	15.887	13.310	12.685		5	16.080	13.156	12.447		5	16.885	13.151	12.310	
6	15.414	13.050	12.531	12.377	6	15.544	12.863	12.278	12.109	6	16.208	12.819	12.156	12.001
7	15.052	12.877	12.445	12.330	7	15.136	12.690	12.255	12.225	7	15.697	12.632	12.165	12.177
8	14.765	12.757	12.397	12.317	8	14.817	12.580	12.250	12.240	8	15.300	12.524	12.199	12.255

would not seem to have any direct physical significance, nevertheless the presence of these singularities invalidates the conclusions from a Stieltjesising procedure previously[24] used by one of us to assign bounds to γ and x_c. We no longer support these bounds.[27]

For the open lattices, the root at $x=x_N\doteq -x_c$ does have physical significance, for it represents the Néel point of the antiferromagnetic problem, $J<0$. Gammel, Marshall, and Morgan[23] attempted to find x_N from the first six coefficients in $F_1(x)$, using a method close to but not identical with the one we ourselves adopt, but had too few terms to display any form of convergence. Their work supported the existence of an antiferromagnetic singularity, but hardly located it. With longer series we may hope to do better.

Of course, perhaps the most powerful method of locating an antiferromagnetic singularity is through use of the series expansion, not of the physical susceptibility $\chi(0)$ but of the so-called staggered susceptibility. Work of Rushbrooke and Wood[17] along these lines had suggested that (for equal $|J|$):

(i) bcc lattice, $T_N=1.09T_c$, i.e., if $x_c=0.397$, then $x_N=-0.364$;

(ii) sc lattice, $T_N=1.13T_c$, i.e., if $x_c=0.596$, then $x_N=-0.527$,

and very similar results are predicted by internal field theories (see Ref. 17). We may hope to find confirmation of this from the physical susceptibility series, and to get some indication of the behavior of $\chi(0)$ near x_N.

Since we expect $\chi(0)$ to remain finite at the Néel point, we are concerned with a singularity at x_N much weaker than the ferromagnetic singularity and must first subtract this out, i.e., form

$$(d/dx)\ \ln F_1(s)-1.43/(0.3973-x). \qquad (25)$$

To sharpen the singularity we now differentiate (25), thus following the Ising-model procedure of Fisher and Sykes[28] in that we look for a logarithmic singularity in (25). We find

$$\begin{aligned} d/dx\{(d/dx)\ \ln F_1(x)-1.43/(0.3973-x)\} \\ =-1.0594+2.3948x-14.1825x^2+38.8224x^3 \\ -67.4595x^4+166.8834x^5-798.8519x^6 \\ +2500.8160x^7-3976.857x^8+\cdots. \end{aligned} \qquad (26)$$

The Padé table to (26) settles down only for $D\geq 3$, $N\geq 3$, but this part of the table exhibits quite good convergence, and to our surprise we find that the [4, 4] and [3, 5] Padé's both give $x_N=-0.364$. (The [4, 3] and [3, 4] estimates are -0.354 and -0.365, respectively.) This is much better than we have any right to expect, and doubtless is largely coincidence. But it does show that $\chi(0)$ reflects the antiferromagnetic singularity, and that there is room for the conclusion $T_N\doteq 1.09T_c$ within our present results.

If, further, we look at the residues for the above [4, 4] and [3, 5] Padé's, in both cases we find -0.56. Putting $-x\equiv y=-J/\kappa T$, $=|J|/\kappa T$ in the antiferromagnetic problem, we have

$$(d\ \ln F_1)/dy\sim 0.56\ \ln(0.364-y),$$

which implies the same kind of singularity as Fisher and Sykes found for the Ising problem; i.e., χ as a function of T has infinite positive gradient at T_N.[29]

Attempts to follow the same procedure for the sc lattice seem to be frustrated by the presence of the

[27] An additional point made in passing in Ref. 24, but not sufficiently emphasized therein, is that the lower bounds ($[N, N-1]$) depend, for their validity, on the hypothesis that $\chi=(x_c-x)^{-\gamma}A(x)+B(x)$ with $B(x)$ zero. Otherwise, there will be a right-hand cut starting at x_c and only the $[N, N]$ Padé approximants can be valid bounds. Consequently, on the basis of the weaker hypothesis that $B(x)$ is non-negative near x_c, we can obtain only the bounds (taking into account the restricted region of analyticity mentioned above by the use of flattened circular regions)

fcc $0<x_c<0.2557$,

bcc $0<x_c<0.4123$,

sc $0<x_c<0.6548$,

which encompass by a wide margin our best estimates. Without this hypothesis on $B(x)$ (or, more precisely, on the sign of the imaginary part across the right-hand cut), in addition to the analyticity assumptions, we can say nothing rigorously.

[28] M. E. Fisher and M. F. Sykes, Physica **28**, 939 (1962).

[29] If one insists on fitting a Fisher-Sykes form to the data, then we conclude that the series expansions are not inconsistent with

$$F_1\sim 0.29-0.06(1-x/x_N)\ \ln(1-x/x_N), \quad \text{bcc}$$

$$F_1\sim 0.25-0.03(1-x/x_N)\ \ln(1-x/x_N), \quad \text{sc}$$

near the Néel points, $x_N=-0.364$ (bcc) and -0.527 (sc), respectively. We would emphasize that these results are not so much derived as merely fitted to the data available.

complex roots to which we have referred: There is clearly an antiferromagnetic singularity, but we have not located it at all sharply.

8. ANALYSIS OF F_2, F_3, and F_4 SERIES

We turn now to an analysis of the higher-order series F_2, F_3, and F_4 or, more accurately, F_2^*, F_3^*, and F_4^* [see Eq. (9)]. We naturally start by looking, for all three lattices, at Padé approximants to $(d/dx)\ln F_s^*(x)$, $s=2$, 3, 4. On determining the smallest positive real roots of the denominators of these PA's it is clear that the critical values of x at which the functions themselves diverge are certainly close to the values of x_c found from analysis of the $F_1(x)$ series. On the other hand, good estimates of x_c are not provided by these Padé tables, which are by no means well converged. This is doubtless partly because the present series are comparatively short (only seven terms after differentiating), but there would also seem some evidence that the functions with which we are concerned are not particularly well suited to this form of Padé analysis. The reason is that, for all three lattices, F_3 and F_4 vanish for small negative values of x, these zeros being reflected in the logarithmic derivative as poles with residue minus one close to the origin. F_1 (the susceptibility) is thermodynamically constrained to be positive, and so this trouble does not arise with it. F_2 seems also to vanish for negative real x. Estimates of the positions of these roots (both from poles in the logarithmic derivatives and from the zeros of PA's to the functions themselves) are that for the fcc, bcc, and sc lattices, respectively, $F_2(x)$ vanishes at -0.43, -0.23, and -0.29, $F_3(x)$ vanishes at -0.0800, -0.0926, and -0.1133, and $F_4(x)$ vanishes at -0.0353, -0.0464, and -0.0578. We would expect a direct use of the familiar ratio method to be unaffected by the presence of these zeros.

Appeal to the ratio test does indeed provide more convincing answers. The sequences of coefficients in these series are rather exceptionally smooth, especially for the fcc lattice. By way of illustration we tabulate in Table XXIV the ratios a_n/a_{n-1} for the F_4^* (fcc) series, and follow these with their linear, quadratic, etc., extrapolants when plotted against $1/n$, according to the procedure of constructing a Neville table.[30] Here, if a_n/a_{n-1} is called r_n, the "linear" extrapolants l_n are given by $nr_n-(n-1)r_{n-1}$, the "quadratic" extrapolants q_n are given by $\frac{1}{2}[nl_n-(n-2)l_{n-1}]$, the "cubic" extrapolants by $\frac{1}{3}[nq_n-(n-3)q_{n-1}]$, and so on. F_4^* (fcc) provides a rather extreme example in that all sequences of successive extrapolants remain monatonic, but the table shows signs of convergence, and the final estimate (calling on all the coefficients) yields $x_c=1/4.022=0.2486$, very close to our previous value, from the susceptibility series, $x_c=0.2492$. With the F_2^* (fcc) and F_3^* (fcc) series we must stop the extrapolation when successive estimates cease to progress monotonically, but if we take the entry opposite $n=8$ in the first column that ceases to be monotonic, we infer $x_c=1/4.024=0.2485$ from F_2^* and $x_c=1/4.029=0.2482$ from F_3^*. There can really be no doubt that all the series diverge at the same value of x, which we might estimate to be 0.249 ± 0.001. For the open lattices the sequences are less regular, and we can infer only that x_c (bcc)$\approx$0.4 and x_c (sc)$\approx$0.6. Even so, it is clear that these series for F_2^*, F_3^*, and F_4^* diverge when $x=x_c$, where x_c corresponds to our previous estimate from the $F_1(x)$ expansions.

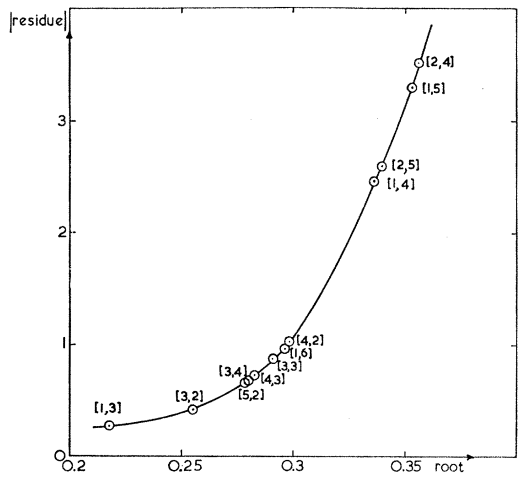

FIG. 4. Plot of the position of the smallest positive real root versus the absolute value of the residue at the corresponding pole in the Padé approximant.

In analyzing $F_2^*(x)$, $F_3^*(x)$, and $F_4^*(x)$ further, to find their critical indices, we have used the values of x_c found from the susceptibility series (see Sec. 6 above). We shall denote the critical index for the series $F_s(x)$ by γ_s (in which notation γ of Sec. 6 becomes γ_1). As a first approach we may use method (ii) of Sec. 5, taking $x_c=0.2492$, 0.3973, and 0.5962 for the fcc, bcc, and sc lattices, respectively. The Padé tables so obtained are again not particularly well converged, but the mean values of the [3, 3], [4, 3], and [3, 4] estimates of γ_2 are 5.06, 5.07, and 5.09 for the three lattices concerned (always taken in the sequence fcc, bcc, and sc). Similarly for γ_3 we find 8.69, 8.73, and 8.75 and for γ_4 the estimates are 12.47 (where we have used the [5, 2] PA instead of the [4, 3], which is anomalous), 12.29, and 12.25. It seems that the γ's are independent of lattice structure, but we can hardly draw conclusions better than $\gamma_2=5.07\pm0.05$, $\gamma_3=8.72\pm0.1$, and $\gamma_4=12.3\pm0.2$.

When, however, we turn to Eq. (24), and use the Domb-Sykes method to find successive estimates of γ_s, we obtain sequences of approximations which behave very smoothly. Denoting by $\gamma_s(n)$ the approximation to γ_s obtained from the ratio a_n/a_{n-1} in (24), Tables XXV–XXVII give, for γ_2, γ_3, and γ_4, respectively, the Neville table extrapolants for all three lattices.

[30] See D. R. Hartree, *Numerical Analysis* (Oxford University Press, Oxford, England, 1952), pp. 84–86.

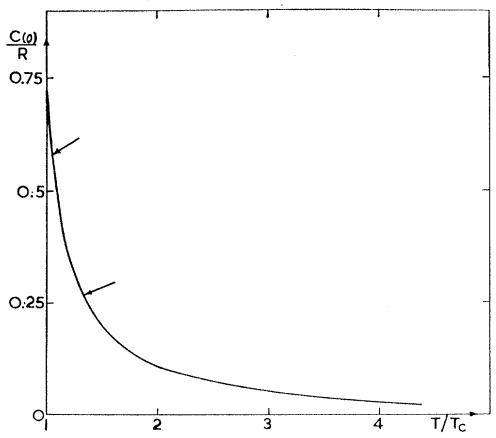

FIG. 5. $C(0)$ versus temperature for the bcc lattice. The portion between the arrows is covered by (35).

We have again taken the values of x_c suggested by analysis of the susceptibility series, and we present only those parts of the Neville tables which seem to us to have diagnostic value.

Looking first at Table XXV, for the fcc lattice the linear and quadratic extrapolants combine to suggest that γ_2 lies in the range 5.06 to 5.07. An identical conclusion follows from the bcc estimates when we consider separately the sequences $n=1, 3, 5, 7$ and $n=2, 4, 6, 8$ (such alternating behavior, easily revealed graphically, is familiar from Ising-model sequences for open lattices). Unfortunately we can draw no conclusions for the sc lattice since, as plotting reveals, the estimates show a wavelike oscillation about a monotonically decreasing smooth curve.

Turning next to Table XXVI, for the fcc lattice we infer that γ_3 is close to 8.69. The data for open lattices suggest a slightly lower value close to 8.65.

With γ_4, Table XXVII, the extrapolations are lengthy, but the sequences are smooth and it has seemed legitimate to go as far as the cubic extrapolants, c_n. For the fcc lattice we infer γ_4 close to 12.32; for the open lattices values closer to 12.25 seem indicated.

Because we believe that, for a given number of terms, series for the close-packed lattice (fcc) will best reflect true thermodynamic behavior, and believing that it is for this lattice that our estimate of x_c is most reliable, we are inclined to put the most weight on the fcc conclusions, namely

$$\gamma_1=1.43, \qquad \gamma_2=5.06,$$
$$\gamma_3=8.69, \qquad \gamma_4=12.32,$$

for which we observe, further, that

$$\gamma_4-\gamma_3=\gamma_3-\gamma_2=\gamma_2-\gamma_1=3.63. \tag{27}$$

But we must allow that there is some uncertainty in these values, not only because the open lattice estimates of γ_3 and γ_4 are a little lower, but also because the fcc tables have really only converged moderately well. As we have emphasized, uncertainty limits are necessarily subjective, but the conclusions

$$\gamma_1=1.43\pm0.01, \qquad \gamma_2=5.06\pm0.02,$$
$$\gamma_3=8.69\pm0.04, \qquad \gamma_4=12.32\pm0.08,$$

do not seem unreasonable. If so,

$$\gamma_s-\gamma_{s-1}=3.63\pm0.03, \qquad s=2, 3, 4. \tag{28}$$

We shall follow the recent example of Fisher,[31] and denote this "gap parameter" by 2Δ.

9. ANALYSIS OF THE SPECIFIC HEAT

We turn, finally, to an analysis of the series $F_0(x)$. More precisely, we write

$$C(0)=\tfrac{1}{4}N\kappa e_2 x^2 c(x) \tag{29}$$

[see Eqs. (5) and (8)], and analyze the series $c(x)$, which will show the same critical behavior as does $C(0)$.

Specific-heat series are notoriously difficult to analyze, and the present ones are no exception. Our first aim must be to transform a presumably weak singularity into a simple pole. To this end we have considered PA's to both $(d/dx)c(x)$ and $(d/dx)\ \ln c(x)$. The former transformation would be appropriate for a logarithmic singularity in $C(0)$; the latter for one of type (19), in which case the critical index is customarily denoted by α.

In both cases we have drawn up Padé tables of the smallest positive real roots of the denominators of these approximants. The tables appropriate to a logarithmic singularity in $C(0)$ show exceptionally poor convergence; thus for the fcc lattice the central entries, $D+N\geq5$, range from 0.12 to 0.34 with no particular pattern and no indication that x_c is close to 0.25. The situation for the open lattices is equally unsatisfactory. The tables based on $(d/dx)\ \ln c(x)$ show better convergence, particularly for the fcc lattice. Here the [3, 2], [3, 3], [3, 4], [4, 2], [4, 3], and [5, 2] roots are all in the range 0.255 to 0.298. Instead of reproducing this table, we present in Fig. 4 a plot of the position of the smallest positive real root (when this exists) against the absolute value of the residue of the corresponding pole in the Padé approximant (estimate of α), and we observe that they are smoothly correlated. We conclude, from this plot, that if $C(0)$ has an infinity at the susceptibility Curie point, $x_c\sim0.25$, then $\alpha\sim0.4$, but it is noticeable that what we would expect to be the better PA's prefer to place this infinity at a rather higher value of x, i.e., at a somewhat lower temperature. Although for the sc lattice the tables are

[31] M. E. Fisher, Rept. Progr. Phys. (to be published).

too erratic for this plot to be made, exactly the same position obtains if we make the corresponding plot for the bcc lattice. Again there is a smooth correlation as in Fig. 4, and the Curie point, $x_c \sim 0.4$, correlates with $\alpha \sim 0.4$; but again the higher-order PA's prefer to place this infinity at a value of x somewhat greater than x_c, and to make it rather stronger.

Following the procedures of Sec. 5, we next use method (ii), evaluating at x_c Padé approximants to $(x-x_c)(d/dx)\ \ln c(x)$. We choose for x_c the values we have found from an analysis of the susceptibility series. For the fcc lattice all PA's with $D \geq 2$ and $N \geq 2$ give α values in the range 0.3 to 0.4 except for [2, 5], [3, 4], and [4, 3], which give estimates in the range 0.2 to 0.3. In particular, the [2, 2] and [3, 3] entries are 0.38 and 0.39, respectively. For the bcc lattice also, the story is similar. We appear to need $D \geq 3$ before the table shows any convergence, but the [3, 2], [3, 3], [4, 2], and [4, 3] values are all within the range 0.36 to 0.37. For the sc lattice, however, the Padé table shows no convergence, and only the [4, 3] and [3, 4] estimates lie in the range 0.4 ± 0.1. Finally we turn to method (iii) of Sec. 5, and examine the Padé approximants to $c(x)^{1/\alpha}$. We have taken $\alpha = 0.2, 0.3, \cdots, 0.6$, and constructed Padé tables of estimates of x_c from the denominators of the approximants. For the fcc lattice the tables show moderately good convergence, and we might infer that a value of $\alpha \sim 0.34$ would lead to $x_c \sim 0.25$. Again, for the bcc lattice we might conclude $\alpha \sim 0.32$ would correspond to $x_c \sim 0.4$. For the sc lattice we seem to need $D \geq 6$ before the tables show any convergence, and no conclusions can be drawn.

Despite the unsatisfactory features of this analysis, if we insist on looking for a specific-heat infinity of the type defined in Eq. (19), with critical index α, then we must conclude that α is probably greater than 0.3 and may well lie in the range 0.4 ± 0.1. But the analysis is indeed unsatisfactory, and we cannot have the same confidence in this conclusion as in our earlier estimates of γ_s, $s = 1, 2, \cdots, 4$.

An explanation of the difficulty in determining α is afforded by the possibility that the specific-heat anomaly is not of the type defined in Eq. (19) and is thus not converted into a simple pole by taking the logarithmic derivative of the series concerned. Indeed, Eq. (27), together with our value of γ_1, tempts us to write

$$\gamma_1 - \gamma_0 = 3.63, \qquad \text{i.e., } \gamma_0 = 1.43 - 3.63 = -2.20, \quad (30)$$

as if the singular part of $F_0(x)$ were proportional to $(x_c-x)^{2.20}$ near x_c. If this is so, then the singular part of $c(x)$ will be proportional to $(x_c-x)^{0.20}$, i.e., $c(x)$ may be expected to have the form

$$c(x) \sim A - B(x_c-x)^{0.20} \quad (31)$$

for x near x_c, and the logarithmic derivative of (31) is certainly not a simple pole.

To test this hypothesis, we have first evaluated $c(x)$ numerically and have then examined the extent to which the values are reproduced by an expression of the form (31). To find $c(x)$ numerically we form all PA's to the series $c(x)$ and evaluate these at x, drawing up the full Padé table. For small x this table shows extremely good convergence, and $c(x)$ can be estimated accurately. For x near x_c the entries show more scatter, but we must emphasize that even at $x = x_c$ there is no sign of any infinity. Thus, for the fcc lattice, for $x = 0.15$ we estimate $c(x) = 1.499$ with certainly no more ambiguity than ± 0.001; for $x = 0.23$ the [3, 4], [3, 5], [4, 3], [4, 4], and [5, 3] estimates are 2.247, 2.213, 2.313, 2.199, and 2.230, and we take their mean, 2.240, as the best estimate of $c(x)$ available. At $x = x_c = 0.2492$, these same PA's are 2.883, 2.755, 3.171, 2.698, and 2.822, and again we have taken their mean, 2.866, as the best PA estimate of $c(x_c)$. We then plot $c(x)$ against $(1-x/x_c)^{0.20}$ and look for linearity. For the fcc lattice we find this linearity over the range $x = 0.17$ to $x = 0.244$, to within 1% in $c(x)$.

Numerically, and in terms of T rather than x, we find that the expression

$$C(0)/R = (T_c/T)^2[1.206 - 0.966(1-T_c/T)^{0.20}] \quad (32)$$

covers the Padé-approximant estimates of $C(0)$ to within 1% over the temperature range $0.70 \leq T_c/T \leq 0.96$. At lower temperatures the expression (32) underestimates $C(0)$, while in the range $0.96 \leq T_c/T \leq 1.00$ the Padé estimates fall below those given by (32). This is because whereas (32) gives $C(0)$ a vertical cusp of height 1.206 R at T_c, with infinite gradient, the Padé estimates do not give $C(0)$ an infinite gradient at T_c and so make the height only $0.801R$.

The success of (32) in reproducing the specific-heat curve, as well as it is known, over a significant range of temperature should not, however, be viewed as strong independent support for the index 0.20. The expression

$$C(0)/R = (T_c/T)^2[1.060 - 0.827(1-T_c/T)^{0.25}] \quad (33)$$

fits the same data equally well. Indeed (32) and (33) coincide numerically, to within 1%, over the range $0.20 \leq T_c/T \leq 0.95$ (and differ by only 2% even for $T_c/T = 0.98$). Nevertheless, we doubt if the impressive linearity of these plots is entirely accidental.

For the bcc lattice, if we take the mean of the [3, 4], [3, 5], [4, 3], [4, 4], and [5, 3] Padé values as providing the best estimates of $c(x)$, then, to within 1%, $C(0)/R$ is covered by the expression

$$C(0)/R = (T_c/T)^2[0.971 - 0.668(1-T_c/T)^{0.20}] \quad (34)$$

over the range $0.75 \leq T_c/T \leq 0.95$. On the other hand, inspection of the Padé tables suggests rather better convergence below the main diagonal. If we estimate $c(x)$ from the most frequently occurring Padé values

we are led to

$$C(0)/R=(T_c/T)^2[1.018-0.724(1-T_c/T)^{0.20}], \quad (35)$$

as reproducing $C(0)$ over the same temperature range. This, again, gives some indication of the measure of uncertainty in these coefficients.

We have not felt it worthwhile to analyze the sc lattice specific heat in this way, since the convergence of the Padé values is far from satisfactory. That the assumption (31), suggested by the hypothesis (30), is not to be ruled out by the specific-heat series themselves has, we believe, been adequately demonstrated, and this form of singularity in $C(0)$ would certainly account for the unsatisfactory features of the normal Padé analysis.

We show in Fig. 5 a plot of $C(0)$ for the bcc lattice, as estimated from the Padé tables, and indicate the temperature range over which the curve is covered by the expression (35). Although the peak is sharp, there is a long high-temperature tail, contributing to the entropy change between T_c and limitingly high temperatures. For all three lattices, we have determined this entropy change $\Delta S=S(\infty)-S(T_c)$ both graphically, from

$$\Delta S=\int_0^{x_c}\frac{C(0)}{x}\,dx, \quad (36)$$

and by evaluating, at x_c, PA's to the series expansion of the right-hand side of (36). The latter Padé tables are well converged, and, from both methods, we conclude:

for the fcc lattice, $\Delta S/R=0.238\pm0.004$,

for the bcc lattice, $\Delta S/R=0.242\pm0.004$,

for the sc lattice, $\Delta S/R=0.264\pm0.008$. (37)

10. DISCUSSION

Having presented our analysis in sufficient detail for it to tell its own story, we do not intend to add much by way of further discussion. Our conclusions rest on two main assumptions: that the basic coefficients have been calculated correctly, and that the series may be analysed along the lines of Eq. (19). On the former point, we have already noted the support we get from concurrent calculations by Domb and Wood, which certainly serve to confirm our ninth-order coefficients for open lattices. We believe our later coefficients are correct, but would observe that, while it is gratifying that all three lattices afford evidence of having the same critical indices, our conclusions are most firmly based on an analysis of the series (particularly the susceptibility series) for the close-packed lattice, and our checking procedures through ninth-order coefficients (when all basic graphs were drawn out) have been such that we believe an error here is unlikely. With regard to the assumptions underlying Eq. (19), we would claim only to follow precedent, in default of having anything more convincing to suggest. Only when the simplest assumptions fail to make sense of the data is a more elaborate assumption warranted, and we feel that this situation has not arisen. We have, in fact, looked briefly at the possibility that

$$\chi(0)\sim-\frac{A\ln[T/T_c-1]}{[T/T_c-1]^\gamma}$$

and then find smaller γ values, in the region of 1.25 rather than 1.43. But the convergence is not as good as without the logarithmic term. Indeed, if we try expressions of the form

$$\chi(0)\sim\frac{A[-\ln(T/T_c-1)]^p}{(T/T_c-1)^\gamma},$$

we find best convergence when p is very small, certainly less than 0.1. Thus our basic philosophy, expressed in Sec. 5, sends us back to our original postulate. Likewise, although one might wonder whether our values of x_c, 0.2492, 0.3963, and 0.5972, were approximations to the values 0.25, 0.4, and 0.6, the fact that use of these latter values leads to less well converged estimates of γ, and less agreement between the three lattices, dissuades us from pursuing this possible hypothesis.

Our conclusions, then, are $\gamma=1.43\pm0.01$ and $2\Delta=3.63\pm0.03$, for all three lattices.

Recently Widom, Kadanoff, and others have advanced a number of so-called "homogeneity" or "scaling" arguments, whereby all critical indices can be expressed in terms of just two of them, for example γ and Δ; and Fisher's "microdomain" model of ferromagnetism leads to similar conclusions. We shall not give detailed references to the rather extensive literature, but refer only to the recent review article by Kadanoff *et al.*[32] The existence, and constancy, of a gap parameter Δ, is intrinsic to these theories, which entail the equation

$$\alpha_s=2-2\Delta+\gamma, \quad (38)$$

where α_s is the index of the singular part of the specific heat [equal to -0.20 in Eq. (32)]. Further, if β denotes the degree of the magnetic phase boundary, δ the degree of the critical isotherm, and ν and η are indices related to the long-range form of the correlation function, which is written as $e^{-\lambda r}/r^{1+\eta}$, where $\lambda\sim|T-T_c|^\nu$ (we confine this discussion to three-dimensional lattices), then, on these theories,

$$\beta=\Delta-\gamma, \qquad \delta=\Delta/(\Delta-\gamma), \quad (39)$$

$$\nu=(2\Delta-\gamma)/3, \qquad \eta=(4\Delta-5\gamma)/(2\Delta-\gamma). \quad (40)$$

With $\gamma=1.43\pm0.01$ and $2\Delta=3.63\pm0.03$, Eqs. (38),

[32] L. P. Kadenoff, W. Götze, D. Hamblen, R. Hecht, E. A. S. Lewis, V. V. Palciauskas, M. Rayl, J. Swift, D. Aspnes, and J. Kane, Rev. Mod. Phys. **39**, 395 (1967).

(39), and (40) lead to

$$-0.24 \leq \alpha_s \leq -0.16,$$
$$0.36 \leq \beta \leq 0.41,$$
$$4.46 \leq \delta \leq 5.00,$$
$$0.72 \leq \nu \leq 0.75,$$
$$0 \leq \eta \leq 0.10.$$

We could leave the matter here. But experience with the Ising problem, and particularly the exact results pertaining to the two-dimensional Ising problems, prompts the search for simple fractions which do justice to the conclusions which we have, so far, expressed in decimal form. There are two possible sets of fractions which are not unattractive (even though they lie marginally outside the confidence limits we have chosen). These are (a) $\gamma=\frac{17}{12}=1.417$, $2\Delta=\frac{11}{3}=3.67$; and (b) $\gamma=\frac{10}{7}=1.429$, $2\Delta=\frac{25}{7}=3.57$. On hypothesis (a), we find

$$\alpha_s=-\tfrac{1}{4}=-0.25, \quad \beta=\tfrac{5}{12}=0.417, \quad \delta=\tfrac{22}{5}=4.4,$$
$$\nu=\tfrac{3}{4}=0.75, \quad \text{and} \quad \eta=\tfrac{1}{9}=0.11;$$

while on hypothesis (b) we find

$$\alpha_s=-\tfrac{1}{7}=-0.14, \quad \beta=\tfrac{5}{14}=0.357, \quad \delta=5,$$
$$\nu=\tfrac{5}{7}=0.71, \quad \text{and} \quad \eta=0.$$

We must, however, emphasize that the predictions of the "homogeneity" and "scaling" arguments may well be wrong. These theories involve a symmetry, in the critical indices, above and below T_c, which is not supported by the most recent work on the three-dimensional Ising problem.[33] Fisher[31] has very tentatively suggested that the second of the Eqs. (39), for δ, may remain valid under less restrictive hypotheses, and that the first, for β, should perhaps be multiplied on the right-hand side by γ'/γ (where γ' is the analog of γ for $T \leq T_c$). If this is so, then, since for the three-dimensional Ising problem γ' seems to be slightly larger than γ, we should conclude that our lower estimates for β are certainly not excessive and rule out the possibility, sometimes suggested,[34] that $\beta=\frac{1}{3}$.

We have compiled[35] most of the graph data used in this work. The collection falls into five parts: (1) figures; (2) a dictionary giving numerical descriptions, serial numbers, etc.; (3) the T matrix; (4) the irreducible parts of the partition functions; (5) the lattice constants.

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[33] G. A. Baker, Jr., and D. S. Gaunt, Phys. Rev. **155**, 545 (1967).

[34] C. Domb, Ann. Acad. Sci. Fennicae AVI, No. 210 (1966). (A useful introduction to the more detailed discussions of Ref. 31.)

[35] G. A. Baker, Jr., H. E. Gilbert, J. Eve, and G. S. Rushbrooke, Brookhaven National Laboratory Report No. BNL 50053, 1967 (unpublished).