

Some Critical Properties of the Nearest-Neighbor, Classical Heisenberg Model for the fcc Lattice in Finite Field for Temperatures Greater than T_C [†]

M. Ferer,* M. A. Moore,† and Michael Wortis

Department of Physics, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801

(Received 2 April 1971)

Using renormalization techniques on the Englert linked-cluster expansion, we have derived high-temperature series for the spin-spin correlation function of the spin-infinity Heisenberg model in finite field. Analysis of our tenth-order zero-field series, which are two terms longer than previous spin-infinity series, favors values of the critical indices γ , ν , and $-\alpha$ higher than previous spin-infinity work but in closer agreement with spin- $\frac{1}{2}$ results. We find $\gamma=1.405 \pm 0.020$, $\nu=0.717 \pm 0.007$, and $\alpha=-0.14 \pm 0.06$. Our finite-field series to eighth order in the interaction and second order in the field allow us to determine the gap index Δ for the spin-infinity Heisenberg system; we assert $2\Delta=3.54 \pm 0.03$. Our results are compared with experiment and with the predictions of scaling theory.

I. INTRODUCTION

Much of our theoretical knowledge of the nature of the critical point derives from the investigation of certain idealized models such as the Ising model and the Heisenberg model.^{1,2} These models are normally characterized by spins at all sites of a lattice, interacting through a Hamiltonian

$$\mathcal{H} = -\frac{1}{2} \sum_{i,j} [J_x(\vec{r}_{ij})S_x(\vec{r}_i)S_x(\vec{r}_j) + J_y(\vec{r}_{ij})S_y(\vec{r}_i)S_y(\vec{r}_j) + J_z(\vec{r}_{ij})S_z(\vec{r}_i)S_z(\vec{r}_j)] - mH \sum_i S_z(\vec{r}_i), \quad (1.1)$$

$\vec{S}(\vec{r}_i)$ being the spin operator at the i th lattice site, $J_x(\vec{r}_{ij})$ the interaction between $S_x(\vec{r}_i)$ and $S_x(\vec{r}_j)$, and H an external field applied in the z direction. The familiar models are special cases of this Hamiltonian; that is, in the Ising model only one of the three $J_x(\vec{r})$, $J_y(\vec{r})$, or $J_z(\vec{r})$ is nonzero, while in the Heisenberg model the coupling is isotropic, $J_x(\vec{r}) = J_y(\vec{r}) = J_z(\vec{r})$.

On three-dimensional lattices, these models are believed to have a second-order phase transition. Unfortunately, there exists no exact solution for any of these three-dimensional models. Thus, after Domb and others, we use the only nonexact approach whose results agree well with the exact solution of the spin- $\frac{1}{2}$ Ising model in two dimensions: exact enumeration series.²

The method used in obtaining our high-temperature series is an extension of the procedure previously used on the three-dimensional Ising model.³ That is, we used the Englert⁴ linked-cluster expansion completely renormalized in the sense of DeDominicis.⁵ The computer program used was a straightforward adaptation of an earlier program which correctly produces Ising-model series. The

only modification of the earlier program was the minor one of decorating, within the program, each line of a diagram with all three Cartesian indices.⁶ This prescription turned out to be very inefficient, as it required the lattice count for each decoration of a diagram, thus making series longer than tenth order in βJ prohibitive. Even so, this prescription was used because the routine nature of the modification lessened the possibility of error. We are confident of the correctness of our series because our series are produced by slightly modifying a working program, because our zero-field susceptibility series agrees with existing nine-term series,⁷ and because all consistency checks reveal no difficulties. Using this method for the classical (spin-infinity) Heisenberg model on the fcc lattice, with nearest-neighbor interaction J , we derived series for the spin-spin correlation function,

$$\Gamma(\vec{r}, T, H) = \langle S_x(\vec{0})S_x(\vec{r}) \rangle - \langle S_x(\vec{0}) \rangle \langle S_x(\vec{r}) \rangle, \quad (1.2)$$

as a double power series in $v = \beta J$ and $h = \beta mH$, that is,

$$\Gamma(\vec{r}, v, h) = \sum_{n,m=0}^{\infty} Q_{n,m}(\vec{r}) v^n h^m, \quad (1.3)$$

where all the coefficients $Q_{n,0}(\vec{r})$ have been derived for $n \leq 10$ and the coefficients $Q_{n,2}(\vec{r})$ have been derived for $n \leq 8$.⁸

In this paper we will attempt to determine the Curie temperature T_C and the conventionally defined^{1,2} critical indices ν , γ , η , α , and 2Δ for this system. That is, we will investigate the leading singularity of the following physical quantities: the zero-field susceptibility

$$\chi = \sum_{\vec{r}} \Gamma(\vec{r}, v, h=0) \propto \epsilon^{-\gamma}, \quad \epsilon \equiv 1 - \frac{T_C}{T} = 1 - \frac{v}{v_C}; \quad (1.4)$$

the zero-field specific heat

$$C = \frac{\partial}{\partial T} \left(-\frac{1}{2} \sum_j \sum_\beta J_\beta(\vec{r}_j) \Gamma(\vec{r}_j, \nu, h=0) \right) \propto \epsilon^{-\alpha}; \quad (1.5)$$

the zero-field spherical moments

$$\mu_n = \sum_{\vec{r}} |\vec{r}|^n \Gamma(\vec{r}, \nu, h=0) \propto \epsilon^{-\gamma-n\nu}; \quad (1.6)$$

and the second-field derivative of the spherical moments which determines the gap index,

$$\mu_{n,2} = \sum_{\vec{r}} |\vec{r}|^n \left. \frac{\partial^2 \Gamma(\vec{r}, \nu, h)}{\partial h^2} \right|_{h=0} \propto \epsilon^{-\gamma-n\nu-2\Delta}. \quad (1.7)$$

The series $\mu_0 \equiv \chi$, μ_2 , C , $\mu_{0,2}$ and $\mu_{2,2}$ ⁷ are presented in Table I so that the reader might easily check our more important assertions; however, we caution him that we feel that the results of certain methods of analysis can be misleading for this system, especially for the large positive moments like μ_2 . In the following paper,⁹ hereafter referred to as II, we present our series for $\Gamma(\vec{r}, \nu, h)$ from which all series presented and analyzed in this paper may be derived; and we attempt to determine the critical form of the zero-field spin-spin correlation function.

The use of high-temperature series in investigating these models has proven quite convincing and successful for the Ising model^{1,2,3,10}; unfortunately, it has proven less so for the Heisenberg model. In part, this is because the derivation of series for the Heisenberg model is more tedious, which restricts the length and number of available series. More importantly, the Heisenberg series are less well behaved; hence the extrapolation procedures are less effective and less convincing.

Early work on the classical Heisenberg model, which was based on a six-term susceptibility series, indicated¹¹ $\gamma \sim 1.33$; later, eight-term series indicated the higher value 1.375 ± 0.002 .^{6,12-14} The analysis of Baker *et al.*¹⁵ indicates $\gamma = 1.43 \pm 0.01$ for the spin- $\frac{1}{2}$ Heisenberg model in strong disagreement with the universality hypothesis, which opts for spin independence of the critical indices. The considerable differences between these values and the desire for information about more of the critical properties prompted the derivation and analysis of our longer series; these series indicate $\gamma = 1.405 \pm 0.020$, again higher than previous results.

In later sections of this paper we consider the following matters. First, we discuss our methods of analysis^{10,16} which are based primarily on the familiar ratio methods with certain modifications. In many cases, these modifications allow us to form sequences, for one physical quantity, which do not depend on assumed values of any other physical quantity, for example a sequence for ν which does

TABLE I. Selected series.

X	μ_2	$\frac{C}{18k} = \frac{1}{18k} \frac{\partial E}{\partial T}$	$2\mu_{0,2}$	$2\mu_{2,2}$
0.333 333 333 333	0.0	0.0	-0.066 666 666 667	0.0
1.333 333 333 333 ^v	1.333 333 333 333 ^v	0.0	-1.066 666 666 67 ^v	-0.533 333 333 333 ^v
4.888 888 888 89 ^{v2}	10.666 666 666 7 ^{v2}	0.111 111 111 111 ^{v2}	-10.115 555 555 6 ^{v2}	-10.536 296 296 3 ^{v2}
17.244 444 444 4 ^{v3}	60.503 703 703 7 ^{v3}	0.296 296 296 296 ^{v3}	-74.287 407 407 4 ^{v3}	-120.541 234 568 ^{v3}
59.486 419 753 1 ^{v4}	295.111 111 111 ^{v4}	0.792 592 592 592 ^{v4}	-466.952 973 545 ^{v4}	-1 045.971 677 84 ^{v4}
202.248 465 608 ^{v5}	1 319.799 082 89 ^{v5}	2.106 995 884 77 ^{v5}	-2 640.958 457 38 ^{v5}	-7 634.883 323 54 ^{v5}
680.700 137 174 ^{v6}	5 576.175 645 70 ^{v6}	5.606 270 821 08 ^{v6}	-13 833.537 668 0 ^{v6}	-49 429.791 059 8 ^{v6}
2 273.984 280 10 ^{v7}	22 628.632 054 9 ^{v7}	15.181 783 264 7 ^{v7}	-68 352.052 271 7 ^{v7}	-292 868.887 329 ^{v7}
7 553.120 309 76 ^{v8}	89 102.650 034 8 ^{v8}	41.921 498 552 0 ^{v8}	-322 553.299 676 ^{v8}	-1 620 457.660 27 ^{v8}
24 973.767 737 8 ^{v9}	342 728.749 695 ^{v9}	117.563 133 644 ^{v9}		
82 267.515 404 8 ^{v10}	1 293 805.851 95 ^{v10}	333.628 207 628 ^{v10}		
		955.855 616 474 ^{v11}		

not depend on a value of T_C . We feel that it was just this sort of interdependence of physical quantities which allowed previous analysis to indicate $\gamma = 1\frac{3}{8}$ with such apparent precision.¹² Secondly, we present T_C analysis of our zero-field spherical-moment series using methods of analysis which do not depend upon assumed values of γ and ν . This analysis favors $T_C = 3.1753 \pm 0.0020$ as opposed to 3.18016 ± 0.00007 .¹² We also observe trends in the sequences for the different moments and attempt to ascertain the effect of these trends on the later sequences for the indices. Thirdly, we present analysis for the critical indices ν and $2\nu - \gamma$ using the method of " T_C renormalization"^{3,17,18} for which the analysis does not depend on our value for T_C . Lastly, we present analysis for the indices ν , γ , α , and 2Δ using our value for T_C . The results of this analysis for the indices, as well as the results of earlier series work^{6,7,12,14,15,19} and experiment,²⁰ are shown in Table II.

II. METHODS OF ANALYSIS

If a series

$$\chi = \sum_{n=0}^{\infty} a_n v^n$$

has as its leading singularity

$$\left(1 - \frac{v}{v_C}\right)^{-\gamma} = \sum_{n=0}^{\infty} \binom{n+\gamma-1}{n} \left(\frac{v}{v_C}\right)^n,$$

then

$$\rho_n \equiv \frac{a_n}{a_{n-1}} \approx \frac{1}{v_C} \left(1 - \frac{\gamma-1}{n}\right),$$

so that

$$\rho_n = \frac{1}{v_C} \left(1 + \frac{\gamma-1+f(n)}{n}\right),$$

where $f(n) \rightarrow 0$, $n \rightarrow \infty$.¹⁶ From this, we can derive two sequences which have $T_C \equiv 1/v_C$ as their limit:

$$n\rho_n - (n-1)\rho_{n-1} = \frac{v}{v_C} [1+f(n)-f(n-1)] - \frac{1}{v_C}, \quad n \rightarrow \infty \quad (2.1)$$

$$\frac{n\rho_n}{n+\gamma-1} = \frac{1}{v_C} \left(1 + \frac{f(n)}{n+\gamma-1}\right) - \frac{1}{v_C}, \quad n \rightarrow \infty. \quad (2.2)$$

Note that in both cases the remainder goes to zero more rapidly than $1/n$. We can also form a sequence the limit of which is γ :

$$nv_C \rho_n - n + 1 = \gamma + f(n) - \gamma, \quad n \rightarrow \infty. \quad (2.3)$$

We can form other sequences for T_C and γ using the log-derivative series

$$\frac{d \ln \chi}{dv} = \sum_{n=0}^{\infty} (da)_n v^n,$$

TABLE II. Critical indices for various Heisenberg systems.

	γ	ν	η	α	2Δ	β	δ
Spin infinity							
Bowers and Woolf	1.375 ± 0.002	$0.6875 \leq \nu \leq 0.7125$	$0 \leq \eta \leq 0.07^a$	$-\frac{1}{8} \leq \alpha \leq -\frac{1}{16}$			
Jasnow and Wortis	1.38 ± 0.01	0.700 ± 0.007	0.03 ± 0.03^a			0.38 ± 0.03	
Stephenson and Wood	1.38				3.45	0.373 ± 0.014^a	4.9 ± 0.4^a
Ferer, Moore, and Wortis	1.405 ± 0.020	0.717 ± 0.007	0.040 ± 0.008^a	-0.14 ± 0.06	3.54 ± 0.03		
Spin $\frac{1}{2}$							
Baker <i>et al.</i>	1.43 ± 0.01				3.63 ± 0.03	0.35 ± 0.05	5.0 ± 0.2
RbMnF ₃							
Corliss <i>et al.</i>	1.397 ± 0.034	0.724 ± 0.008	0.067 ± 0.010			0.316 ± 0.008	

^aThese indices were derived using scaling relations.

which has

$$\frac{1}{1 - v/v_c} = \sum_{n=0}^{\infty} \gamma \left(\frac{v}{v_c}\right)^n$$

as its leading singularity.¹⁰ Therefore, the terms of the exact series $(da)_n$ have as their limit γ/v_c^n and thus $(da)_n = [\gamma + g(n)]/v_c^n$, where $g(n) \rightarrow 0$ as $n \rightarrow \infty$. The ratio of consecutive terms forms a sequence for T_c ,

$$\begin{aligned} \frac{(da)_n}{(da)_{n-1}} &= \frac{v}{v_c} \frac{\gamma + g(n)}{\gamma + g(n-1)} \\ &\approx \frac{1}{v_c} \left(1 + \frac{1}{\gamma} [g(n) - g(n-1)]\right) - \frac{1}{v_c}, \end{aligned} \quad n \rightarrow \infty; \quad (2.4)$$

and $v_c^n (da)_n$ is a sequence which has γ as its limit,

$$v_c^n (da)_n = \gamma + g(n) - \gamma, \quad n \rightarrow \infty. \quad (2.5)$$

Of course we have only a finite number of terms in these sequences, and we must use some extrapolation technique to find their limit. We use the most common such method, the Neville table,²¹ which assumes that the remainders are analytic functions of $1/n$. As an example, consider the sequence (2.3). The Neville table assumes that the sequence is of the form

$$l_n^0 \equiv n \rho_n v_c^{-n+1} = \gamma + \frac{c_1^0}{n} + \frac{c_2^0}{n^2} + \frac{c_3^0}{n^3} + \dots \quad (2.6)$$

The Neville table is the two-dimensional array

$$l_n^i \equiv [n l_n^{i-1} - (n-1) l_{n-1}^{i-1}] / i, \quad i \neq 0 \quad (2.7)$$

where, if the remainder is of the form (2.6), then

$$l_n^i = \gamma + \frac{c_{i+1}^i}{n^{i+1}} + \frac{c_{i+2}^i}{n^{i+2}} + \dots, \quad (2.8)$$

where the c_m^i depend on c_m^0 and all c_n^j for $j < i$ and $n < m$. Thus l_n^1 is the linear extrapolant, l_n^2 the quadratic, and so forth. Note that in the sequences (2.1), (2.2), and (2.4) for T_c the remainder goes to zero more rapidly than $1/n$, so that if the remainder is analytic, it has the form

$$\frac{c_2^0}{n^2} + \frac{c_3^0}{n^3} + \frac{c_4^0}{n^4} + \dots$$

Of course the Neville table is an approximation which assumes that the remainder is analytic in $1/n$. If one has a nonanalytic remainder, the Neville table will not extrapolate the sequence correctly. To give an idea of the sort of error that is made, Table III shows a Neville table of the sequence $l_n^0 = 1 + 1/\sqrt{n}$. Note that the l_n^i decrease monotonically as a function of n and i towards 1 but that the true limit is not apparent from the table. It will be seen in later sections that some of our Neville-table extrapolations behave in this fashion.

Another characteristic behavior we will observe in our extrapolations is a lack of smoothness which may be due to singularities at complex values of v .

Note that of the sequences for T_c only one, (2.2), is not self-contained; that is, the sequence (2.2) depends on a value of γ . If one chooses γ a bit small, the terms of the sequence will be too large, and the leading term in the remainder will go as $1/n$ and will be poorly approximated by a Neville table, which assumes the leading term goes as $1/n^2$. Thus, for an irregular sequence like (2.2) for the susceptibility series, the choice of an incorrect γ may cause the Neville table to indicate an incorrect value of T_c . We believe that the difference between our results and those of Bowers and Woolf¹² may be due to this sort of effect. Their methods for T_c were affected because they chose γ a bit low ($1/8$); and the value of T_c thus arrived at indicated, not surprisingly, $\gamma = 1/8$ when it was used in determining a value of γ . To support this assertion we present in Table IV the Neville table of sequence (2.2) for our ten-term susceptibility series, with γ taken to be $1/8$. The first eight rows of this table are replicas of Table XII of Bowers and Woolf, which they felt indicated $T_c = 3.180 \pm 0.001$.¹² However, we note that the ninth and tenth terms in the second column begin to decrease, and that even the maximum is below the allowed values quoted by Bowers and Woolf. Thus, this table indicates a lower value of T_c which would, in turn, indicate a higher value of γ , and so forth.

Aware of these difficulties, we determine our value of T_c relying solely on sequences (2.1) and (2.4). We also have a method, T_c renormalization,^{3,17,18} of deriving fairly regular sequences for the indices ν and $2\nu - \gamma$ that are independent of T_c . As an example of this method, let us consider the two moment series

$$\mu_x = \sum_{n=0}^{\infty} \mu_x(n) v^n \propto \epsilon^{-\gamma - x\nu}$$

and

$$\mu_y = \sum_{n=0}^{\infty} \mu_y(n) v^n \propto \epsilon^{-\gamma - y\nu}.$$

TABLE III. This Neville table of the sequence $l_n^0 = 1 + 1/\sqrt{n}$ exhibits the slow monotonic convergence characteristic of some later extrapolations.

		l_n^i				
n^i	0	1	2	3	4	
6	1.4082					
7	1.3780	1.1963				
8	1.3536	1.1827	1.1419			
9	1.3333	1.1716	1.1327	1.1143		
10	1.3162	1.1623	1.1251	1.1073	1.0969	

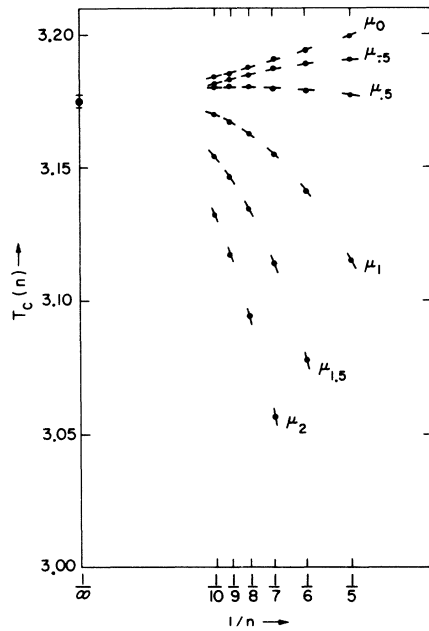


FIG. 1. $1/n$ plot of sequence (2.1) for the moment series.

It is not hard to show that the series

$$\sum_{n=0}^{\infty} \frac{\mu_x(n)}{\mu_y(n)} Z^n$$

has $(1 - Z)^{-1-x\nu+y\nu}$ as its leading singularity. Therefore this series has $Z_C = 1$, and sequences (2.3) and (2.5) can be used to determine ν .

III. DETERMINATION OF T_C

We base our determination of T_C on sequences (2.1) and (2.4) for the zero-field spherical moments

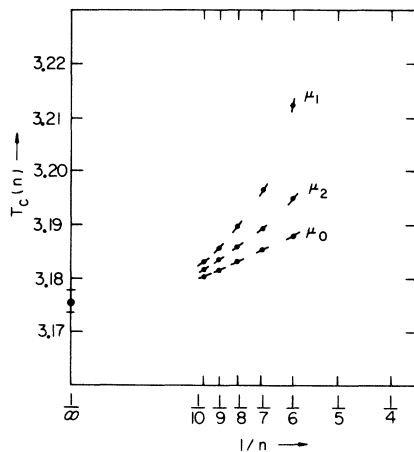


FIG. 2. $1/n$ plot of sequence (2.4) for some moment series; the moments not included here behave similarly.

TABLE IV. This is an extension, using our ninth and tenth terms of χ , of Table XII of Bowers and Woolf, which shows a Neville table of the sequence $n\rho_n/(n + \gamma - 1)$ for T_C with γ taken to be $1\frac{3}{8}$. Note that the second column begins to decrease in tenth order and has not reached the value quoted by Bowers and Woolf, 3.180 ± 0.001 , while the third column decreases monotonically from the seventh-order term.

$n \setminus i$	0	1	2
1	2.909 09		
2	3.087 72		
3	3.135 35		
4	3.153 92	3.172 48	
5	3.162 71	3.175 89	3.178 16
6	3.167 68	3.177 63	3.179 38
7	3.170 79	3.178 56	3.179 80
8	3.172 81	3.178 87	3.179 38
9	3.174 16	3.178 89	3.178 92
10	3.175 09	3.178 81	3.178 64

μ_n for n from -1 to $+2$ in increments of $\frac{1}{2}$. Neville tables of these sequences are shown in Table V. As can be seen, these extrapolations are not smooth; however, we feel we can say with some confidence that $T_C = 3.1753 \pm 0.0020$ especially from sequence (2.4) for the susceptibility and the positive moments. Moreover, none of the other extrapolations appears inconsistent with this value.

This is an appropriate place to discuss some trends in the behavior of the remainders which will affect later extrapolations. Shown in Fig. 1 (2) are plots of the sequence (2.1) [(2.4)] for the moments in question vs $1/n$. Figure 1 and the corresponding extrapolations show significantly different behavior of the sequence (2.1) for the different moment series. The remainders of this sequence are large and depend strongly on $1/n$, especially for the large positive moments. Also, the extrapolations for these positive moments appear to have both a certain lack of smoothness and the sort of behavior encountered in Table III, associated with a non-analytic remainder. At the same time, from Fig. 2 and the corresponding extrapolations, the remainders $g(n) - g(n - 1)$ for the different moments behave very much alike and are neither so large nor so strongly $1/n$ dependent as the $f(n) - f(n - 1)$; however, these sequences are less smooth than sequences (2.1). These trends will be of interest in further sections because the behavior of the Neville-table extrapolation of $g(n) - g(n - 1)$ [$f(n) - f(n - 1)$] will be very similar to that of $g(n)$ [$f(n)$]. Thus we will observe the same lack of smoothness in $g(n)$ as well as the same "nonanalytic" behavior in $f(n)$.

IV. DETERMINATION OF ν USING T_C RENORMALIZATION

Shown in Table VI are Neville tables of sequences

TABLE V. Analysis of the zero-field moment series μ_n for T_C using Neville tables of the last six terms of sequences (2.4) and (2.1). Because of the irregularity of these series, we will normally present only the first three columns of the Neville table except when later columns are indicative of important trends.

$n \downarrow$	Sequence (2.4)			Sequence (2.1)			
	0	1	2	0	1	2	3
μ_{-1}							
5	3.1081			3.1519			
6	3.1315	3.1784		3.1657	3.1933		
7	3.1445	3.1768	3.1747	3.1714	3.1855	3.1752	
8	3.1512	3.1713	3.1620	3.1724	3.1753	3.1582	
9	3.1553	3.1700	3.1677	3.1724	3.1725	3.1669	
10	3.1584	3.1708	3.1730	3.1726	3.1733	3.1751	
$\mu_{-1/2}$							
5	3.1894			3.1906			
6	3.1885	3.1870		3.1892	3.1863		
7	3.1872	3.1837	3.1793	3.1873	3.1827	3.1780	
8	3.1851	3.1787	3.1707	3.1849	3.1775	3.1688	
9	3.1832	3.1767	3.1723	3.1828	3.1756	3.1718	
10	3.1818	3.1760	3.1753	3.1814	3.1756	3.1755	
μ_0							
5	3.1925			3.2011			
6	3.1877	3.1779		3.1944	3.1810		
7	3.1853	3.1792	3.1809	3.1906	3.1811	3.1812	
8	3.1831	3.1768	3.1726	3.1877	3.1790	3.1755	
9	3.1814	3.1755	3.1730	3.1855	3.1776	3.1750	
10	3.1803	3.1755	3.1756	3.1838	3.1772	3.1761	
$\mu_{1/2}$							
5	3.2654			3.1775			
6	3.2278	3.1523		3.1791	3.1822		
7	3.2090	3.1620	3.1749	3.1801	3.1828	3.1835	
8	3.1984	3.1667	3.1743	3.1805	3.1815	3.1793	3.1752
9	3.1919	3.1690	3.1733	3.1804	3.1800	3.1771	3.1744
10	3.1877	3.1707	3.1747	3.1801	3.1791	3.1770	3.1767
μ_1							
5	3.2509			3.1148			
6	3.2124	3.1355		3.1412	3.2134		
7	3.1967	3.1576	3.1876	3.1551	3.1896	3.1579	
8	3.1895	3.1677	3.1843	3.1629	3.1863	3.1808	3.2040
9	3.1854	3.1713	3.1787	3.1675	3.1837	3.1783	3.1755
10	3.1829	3.1730	3.1770	3.1704	3.1819	3.1777	3.1767
$\mu_{1.5}$							
5	3.2196			3.0079			
6	3.1957	3.1479		3.0788	3.2207		
7	3.1883	3.1699	3.1991	3.1143	3.2032	3.1798	
8	3.1852	3.1759	3.1860	3.1344	3.1945	3.1801	3.1804
9	3.1832	3.1760	3.1763	3.1466	3.1893	3.1789	3.1773
10	3.1817	3.1755	3.1743	3.1545	3.1860	3.1782	3.1773
μ_2							
5	3.2112			2.8508			
6	3.1949	3.1624		2.9891	3.2656		
7	3.1889	3.1738	3.1853	3.0565	3.2252	3.1713	
8	3.1857	3.1762	3.1800	3.0942	3.2073	3.1773	3.1833
9	3.1834	3.1754	3.1738	3.1172	3.1976	3.1783	3.1794
10	3.1817	3.1750	3.1742	3.1321	3.1918	3.1783	3.1783

(2.3) and (2.5) for the ratio series

$$\sum_{i=0}^{\infty} \frac{\mu_n(i)}{\mu_m(i)} Z^i,$$

$(n, m) = (0, -1), (0, -\frac{1}{2}), (\frac{1}{2}, 0), (1, 0), (1\frac{1}{2}, 0), (2, 0)$.²² Note that the sequences are normalized so

that the limit of all sequences is ν and not $1 + (n - m)\nu$.

As was expected from the behavior of the tables of Sec. III, the extrapolation of sequence (2.3) depends strongly on the moment in question. These tables for the large positive moments show the overshoot and slow monotonic convergence characteristic of the corresponding tables of Sec. III. Thus, the entries in the last column of the tables will be below the limit of the sequence, which tendency will increase as the label of the moment increases. At the same time, the tables of sequence (2.5) are somewhat less smooth, but they do not exhibit such pronounced trends and appear to be

TABLE VI. Analysis for ν from the ratio series $\sum_{i=0}^{\infty} [\mu_n(i)/\mu_m(i)]Z^i$. Presented are Neville tables of sequences (2.3) and (2.5) for the ratio series (n, m) shown in the table.

$n \downarrow$	Sequence (2.5)			Sequence (2.3)			
	0	1	2	0	1	2	3
$(0, -1)$							
5	0.6164			0.6823			
6	0.6435	0.7792		0.6852	0.7000		
7	0.6589	0.7514	0.6818	0.6867	0.6955	0.6844	
8	0.6693	0.7422	0.7146	0.6881	0.6976	0.7039	0.7364
9	0.6771	0.7395	0.7301	0.6895	0.7009	0.7123	0.7290
10	0.6831	0.7371	0.7274	0.6909	0.7033	0.7130	0.7146
$(0, -\frac{1}{2})$							
5	0.5739			0.6744			
6	0.6010	0.7363		0.6775	0.6933		
7	0.6190	0.7275	0.7055	0.6795	0.6916	0.6874	
8	0.6323	0.7254	0.7191	0.6813	0.6940	0.7011	0.7241
9	0.6427	0.7253	0.7250	0.6831	0.6970	0.7075	0.7204
10	0.6509	0.7250	0.7238	0.6847	0.6993	0.7087	0.7114
$(\frac{1}{2}, 0)$							
5	0.5854			0.6931			
6	0.6080	0.7209		0.6911	0.6807		
7	0.6235	0.7166	0.7058	0.6900	0.6834	0.6899	
8	0.6350	0.7157	0.7130	0.6896	0.6869	0.6974	0.7098
9	0.6440	0.7159	0.7168	0.6896	0.6902	0.7018	0.7105
10	0.6512	0.7161	0.7170	0.6900	0.6928	0.7035	0.7075
$(1, 0)$							
5	0.6299			0.7240			
6	0.6466	0.7301		0.7156	0.6734		
7	0.6573	0.7218	0.7012	0.7103	0.6786	0.6915	
8	0.6651	0.7194	0.7119	0.7069	0.6832	0.6969	0.7060
9	0.6711	0.7190	0.7175	0.7047	0.6870	0.7006	0.7078
10	0.6758	0.7187	0.7175	0.7032	0.6901	0.7023	0.7063
$(\frac{3}{2}, 0)$							
5	0.6566			0.7556			
6	0.6673	0.7207		0.7404	0.6644		
7	0.6741	0.7146	0.6993	0.7308	0.6727	0.6935	
8	0.6792	0.7148	0.7154	0.7243	0.6788	0.6971	0.7031
9	0.6833	0.7163	0.7217	0.7197	0.6835	0.7000	0.7058
10	0.6866	0.7169	0.7193	0.7165	0.6871	0.7016	0.7052
$(2, 0)$							
5	0.6669			0.7885			
6	0.6752	0.7167		0.7660	0.6536		
7	0.6805	0.7123	0.7015	0.7517	0.6657	0.6959	
8	0.6848	0.7151	0.7235	0.7419	0.6737	0.6978	0.7008
9	0.6884	0.7176	0.7261	0.7350	0.6795	0.6999	0.7042
10	0.6914	0.7177	0.7185	0.7299	0.6838	0.7012	0.7042

TABLE VII. Analysis for $2\nu - \gamma$ using Neville tables of sequences (2.3) and (2.5) for the two ratio series shown.

		Sequence (2.5)				Sequence (2.3)			
		$\sum_{n=0}^{\infty} \left[\left(\frac{\mu_{1.5}}{\mu_{-0.5}}(n) \right) / \mu_0(n) \right] Z^n$							
n	i	0	1	2	3	0	1	2	3
5		-0.0088				-0.0040			
6		-0.0010	0.0377			0.0015	0.0232		
7		0.0040	0.0339	0.0244		0.0054	0.0250	0.0295	
8		0.0075	0.0324	0.0279	0.0235	0.0084	0.0261	0.0294	0.0293
9		0.0102	0.0316	0.0287	0.0302	0.0107	0.0267	0.0290	0.0280
10		0.0123	0.0311	0.0291	0.0299	0.0125	0.0272	0.0290	0.0292
		$\sum_{n=0}^{\infty} \left[\left(\frac{\mu_2}{\mu_0}(n) \right) / \mu_0(n) \right] Z^n$							
5		0.0754				0.0763			
6		0.0703	0.0444			0.0716	0.0527		
7		0.0656	0.0378	0.0211		0.0673	0.0456	0.0277	
8		0.0616	0.0338	0.0220	0.0235	0.0635	0.0407	0.0260	0.0243
9		0.0583	0.0318	0.0248	0.0303	0.0602	0.0376	0.0267	0.0275
10		0.0556	0.0307	0.0262	0.0297	0.0575	0.0355	0.0271	0.0278

more rapidly convergent. Thus, as before, we tend to have more confidence in the log-derivative sequences.

We feel that value $\nu = 0.717 \pm 0.007$ is consistent with these tables, which, we reiterate, are self-contained, being independent of an assumed value of T_C .

V. DETERMINATION OF $2\nu - \gamma$ USING T_C RENORMALIZATION

It has been observed in experiment²³ and Ising-model calculations^{3,18} that γ is only slightly smaller than 2ν for three-dimensional systems.²⁴ We investigate the difference $2\nu - \gamma$ by forming, from the series μ_n/μ_{n-2} and μ_0 , the ratio series

$$\sum_{i=0}^{\infty} \left[\left(\frac{\mu_n}{\mu_{n-2}}(i) \right) / \mu_0(i) \right] Z^i,$$

which has $(1 - Z)^{-1-2\nu\gamma}$ as its leading singularity.

Shown in Table VII are Neville tables of sequences (2.3) and (2.5) for two of these ratio series. The sequences are normalized so their limit is $2\nu - \gamma$. Other such ratio series were investigated; and, although they were not inconsistent with those presented, their sequences were less well behaved. We feel the analysis presented indicates $2\nu - \gamma = 0.029 \pm 0.006$ which, with the result of Sec. IV, implies $\gamma = 1.405 \pm 0.020$. Also, using the scaling law $\gamma = (2 - \eta)\nu$,¹ we find $\eta = 0.040 \pm 0.008$.

VI. ANOTHER DETERMINATION OF ν AND γ

In this section, we attempt to determine the indices γ and ν from the same moment series con-

sidered in Secs. III and IV, using $T_C = 3.1753 \pm 0.0020$ as determined in Sec. III. Neville tables of the sequences (2.3) and (2.5), with $T_C = 3.1753$, for these moments as well as our readings of these extrapolations are shown in Table VIII. These extrapolations behave as discussed previously, causing the sequence (2.3) for the large positive moments to appear to indicate lower values than sequence (2.5).

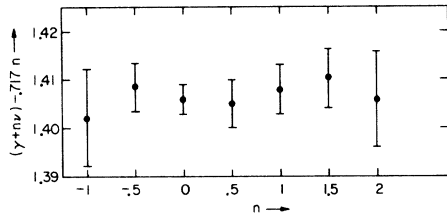
The values thus obtained are consistent with each other and with the results of Secs. IV and V. A plot of $\gamma + n\nu - 0.717n$ vs n , which is shown in Fig. 3, indicates $\nu = 0.717 \pm 0.002$ and $\gamma = 1.406 \pm 0.004$. These uncertainties are due only to the uncertainty in reading the above extrapolations, which assume $T_C = 3.1753$. When proper account is taken of the uncertainty in T_C , it is found that $\gamma = 1.406 \pm 0.020$ and $\nu = 0.717 \pm 0.007$, which agree with the results of the T_C renormalization method.

VII. DETERMINATION OF α USING $T_C = 3.1751 \pm 0.0020$

Specific-heat series are notoriously hard to analyze^{15,25}; the series for this model is no exception. Sequences (2.3) and (2.5) for the specific-heat series using $T_C = 3.1753$ are listed in Table IX and are shown in Fig. 4 plotted vs $1/n$. We do not present Neville tables for these sequences because they are so badly behaved; from Fig. 4, we feel safe in estimating $\alpha = -0.14 \pm 0.06$, the rather large uncertainties being dictated by the irregularity of the sequences. If we use the Josephson inequality $d\nu \geq 2 - \alpha$,²⁶ we can limit the uncertainty, $-\alpha \leq d\nu - 2 \leq 0.166$. Therefore, given the inequality, we have $\alpha = -0.14_{-0.03}^{+0.06}$.

TABLE VIII. Analysis of the zero-field moments μ_n for $\gamma + n\nu$. Shown are Neville tables of sequences (2.3) and (2.5) for the moments with $T_C = 3.1753$. Also shown are our readings of the extrapolations of μ_n for $\gamma + n\nu$.

n	Sequence (2.5)			Sequence (2.3)			
	0	1	2	0	1	2	3
$\mu_{-1}, \gamma - \nu = 0.695 \pm 0.010$							
5	0.7825			0.7108			
6	0.7717	0.7177		0.7078	0.6927		
7	0.7642	0.7192	0.7229	0.7066	0.6991	0.7151	
8	0.7584	0.7177	0.7131	0.7056	0.6990	0.6990	
9	0.7536	0.7154	0.7074	0.7047	0.6973	0.6910	
10	0.7496	0.7135	0.7059	0.7038	0.6960	0.6908	
$\mu_{-1/2}, \gamma - \frac{1}{2}\nu = 1.050 \pm 0.005$							
5	1.0123			1.0154			
6	1.0166	1.0376		1.0198	1.0416		
7	1.0203	1.0430	1.0566	1.0235	1.0462	1.0578	
8	1.0235	1.0453	1.0523	1.0265	1.0476	1.0517	
9	1.0260	1.0463	1.0495	1.0289	1.0478	1.0484	
10	1.0281	1.0469	1.0495	1.0308	1.0479	1.0486	
$\mu_0, \gamma = 1.406 \pm 0.003$							
5	1.3702			1.3536			
6	1.3755	1.4021		1.3596	1.3897		
7	1.3798	1.4056	1.4144	1.3645	1.3933	1.4023	
8	1.3832	1.4070	1.4110	1.3683	1.3956	1.4025	
9	1.3859	1.4072	1.4079	1.3715	1.3971	1.4022	
10	1.3880	1.4074	1.4082	1.3742	1.3983	1.4030	
$\mu_{1/2}, \gamma + \frac{1}{2}\nu = 1.764 \pm 0.005$							
5	1.6523			1.7247			
6	1.6795	1.8159		1.7259	1.7318		
7	1.6973	1.8042	1.7749	1.7274	1.7364	1.7481	
8	1.7097	1.7961	1.7719	1.7670	1.7290	1.7403	1.7582
9	1.7186	1.7900	1.7683	1.7610	1.7306	1.7433	1.7570
10	1.7253	1.7853	1.7670	1.7639	1.7321	1.7456	1.7587
$\mu_1, \gamma + \nu = 2.125 \pm 0.005$							
5	2.0298			2.1288			
6	2.0536	2.1721		2.1181	2.0644		
7	2.0674	2.1505	2.0965	2.1117	2.0734	2.0958	
8	2.0766	2.1409	2.1123	2.1387	2.1078	2.1010	2.1096
9	2.0832	2.1359	2.1184	2.1306	2.1053	2.1039	2.1098
10	2.0882	2.1331	2.1217	2.1293	2.1037	2.1087	2.1115
$\mu_{3/2}, \gamma + \frac{3}{2}\nu = 2.485 \pm 0.005$							
5	2.3994			2.5672			
6	2.4148	2.4919		2.5369	2.3849		
7	2.4247	2.4840	2.4645	2.5176	2.4024	2.4462	
8	2.4323	2.4852	2.4889	2.5294	2.5048	2.4507	2.4583
9	2.4383	2.4865	2.4908	2.4945	2.4957	2.4232	2.4608
10	2.4432	2.4869	2.4886	2.4837	2.4891	2.4300	2.4632
$\mu_2, \gamma + 2\nu = 2.840 \pm 0.010$							
5	2.7459			3.0421			
6	2.7629	2.8475		2.9834	2.6901		
7	2.7746	2.8453	2.8399	2.9460	2.7215	2.8001	
8	2.7837	2.8472	2.8528	2.8742	2.9205	2.7417	2.8051
9	2.7908	2.8475	2.8487	2.8467	2.9022	2.7557	2.8103
10	2.7964	2.8471	2.8457	2.8385	2.8886	2.7660	2.8139

FIG. 3. Plot of $(\gamma + \nu) - 0.717n$ vs n .VIII. DETERMINATION OF 2Δ USING $T_C = 3.1753 \pm 0.0020$

In analyzing the series $\mu_{0,2}/\mu_0$, $\mu_{1,2}/\mu_1$, and $\mu_{2,2}/\mu_2$ for 2Δ , we found the sequence (2.5) was, apparently, rapidly convergent but very irregular, while sequence (2.3) seemed more slowly convergent but less irregular. Therefore, presented in Table X is sequence (2.5) and the Neville table of sequence (2.3). We feel these sequences indicate $2\Delta = 3.54 \pm 0.02$; when proper account is taken of the uncertainty in T_C , one finds $2\Delta = 3.54 \pm 0.03$.

IX. CONCLUSIONS

As a result of the analysis of Secs. III–VIII, we assert that the critical indices have the values $\nu = 0.717 \pm 0.007$, $\gamma = 1.405 \pm 0.020$, $\eta = 0.040 \pm 0.008$, $\alpha = -0.14 \pm 0.06$, $2\Delta = 3.54 \pm 0.03$ for the high-temperature nearest-neighbor classical Heisenberg model on the fcc lattice. We realize that, given some previous work, several of these assertions are rather controversial; but we feel that our results are reliable and that our work has the following advantages: (i) Our series are two terms longer than any of the previous series. (ii) We analyzed more series for T_C , ν , and γ , and we presented more analysis than would normally be necessary. We have presented analysis only for the fcc lattice because the series for the other lattices appear to be less well behaved and because there is little doubt that the indices are lattice independent.²⁷ (iii) We rely heavily on methods of analysis which

TABLE IX. Analysis for α using the specific-heat series. Shown are sequences (2.3) and (2.5) for the first derivative with respect to ν of the specific-heat series with $T_C = 3.1753$.

$n \setminus i$	Sequence (2.5)	Sequence (2.3)
	0	0
5	-0.0463	+0.0277
6	-0.0582	-0.0302
7	-0.0387	-0.0431
8	-0.0408	-0.0515
9	-0.0555	-0.0628
10	-0.0688	-0.0749

TABLE X. Analysis of the series $\mu_{n,2}/\mu_n$ for 2Δ . Shown is the sequence (2.5) and the Neville table of sequence (2.3).

$n \setminus i$	Sequence (2.5)		Sequence (2.3)	
	0	0	1	2
$\mu_{0,2}/\mu_0$				
3	3.515	3.625		
4	3.498	3.598	3.515	
5	3.504	3.580	3.510	3.504
6	3.522	3.569	3.511	3.512
7	3.530	3.560	3.514	3.520
8	3.530	3.555	3.516	3.524
$\mu_{1,2}/\mu_1$				
3	3.668	3.391		
4	3.623	3.445	3.552	
5	3.552	3.473	3.555	3.559
6	3.524	3.488	3.552	3.545
7	3.524	3.498	3.548	3.539
8	3.531	3.505	3.545	3.538
$\mu_{2,2}/\mu_2$				
3	3.470	3.640		
4	3.490	3.605	3.535	
5	3.511	3.584	3.522	3.510
6	3.508	3.571	3.517	3.509
7	3.523	3.562	3.517	3.516
8	3.530	3.555	3.518	3.522

are self-contained, making the assignment of uncertainties more transparent. (iv) We assign generous uncertainties to compensate for the natural tendency to have too much confidence in one's analysis. (v) We were careful that the different analysis methods were consistent; and, where apparent inconsistency was unavoidable, we feel we have offered a plausible explanation.

How do our results agree with the predictions of scaling theory? Widom-Kadanoff scaling theory predicts relations between the indices which determine all but two of them.¹ These relations are exactly obeyed for the two-dimensional Ising model¹; but in three dimensions there exists convincing evidence that some of the relations are invalid for

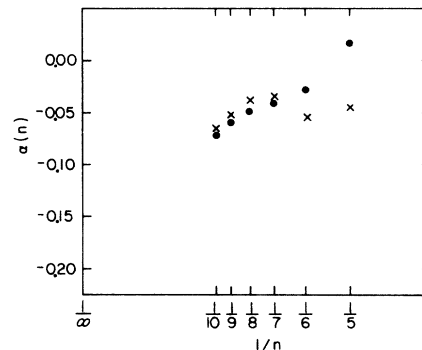


FIG. 4. $1/n$ plot of sequence (2.3) (●) and sequence (2.5) (×) for the specific-heat series, with $T_C = 3.1753$.

the Ising model.^{3,18,24,25} For example, $d\nu - 2 + \alpha$ and $d\nu + \gamma - 2\Delta$, $d=3$ being the dimensionality, are not zero as predicted by scaling but approximately 0.04. Testing these two relations for the Heisenberg model, we find

$$\begin{aligned} 3\nu - 2 + \alpha &= 0.01 \pm 0.08, \\ 3\nu + \gamma - 2\Delta &= 0.02 \pm 0.07. \end{aligned} \quad (9.1)$$

Thus, the relations are obeyed to within large uncertainties which would mask violations greater than those of the three-dimensional Ising model. Still, we can use scaling relations to predict the indices β and δ which determine the leading singularities of the equation of state, and we can have some confidence that the values will be correct to within the uncertainties quoted because any scaling violation will probably be smaller.

$$\begin{aligned} \beta &= \Delta - \gamma = 0.365 \pm 0.035, \\ \beta &= \frac{1}{2}(3\nu - \gamma) = 0.373 \pm 0.014, \end{aligned}$$

[†]Research supported in part by the National Science Foundation under Grant No. NSF GP-16886.

*Xerox Corporation Industrial Fellow.

[‡]Present address: Department of Theoretical Physics, University of Oxford, 12 Parks Road, Oxford OX1-3PQ, England.

¹L. P. Kadanoff *et al.*, Rev. Mod. Phys. **39**, 395 (1967).

²C. Domb, Advan. Phys. **9**, 149 (1960); M. E. Fisher, Rept. Progr. Phys. **30**, 615 (1967).

³M. A. Moore, D. Jasnow, and M. Wortis, Phys. Rev. Letters **22**, 940 (1969).

⁴F. Englert, Phys. Rev. **129**, 567 (1963).

⁵C. DeDominicis, J. Math. Phys. **3**, 983 (1962).

⁶D. Jasnow and M. Wortis, Phys. Rev. **176**, 739 (1968).

⁷Our zero-field susceptibility series agree with the ninth-order series of R. L. Stephenson [R. L. Stephenson and P. J. Wood, J. Phys. C **3**, 90 (1970)]. It should be noted here that our fifth- and seventh-order coefficients in $\mu_{0,2}$ do not agree with the results of Stephenson and Wood (Ref. 14). However, Stephenson and Wood have found an error, the correction of which brings their series into agreement with ours. This discrepancy is small, and they feel it should not materially affect their conclusions [P. J. Wood (private communication)].

⁸Only even powers in h enter the sum since $\Gamma(\vec{r}, \nu, h)$ is even in h for temperature above T_C .

⁹M. Ferer, following paper, Phys. Ref. B **4**, 3964 (1971).

¹⁰D. S. Gaunt, Proc. Phys. Soc. (London) **92**, 150 (1967).

¹¹C. Domb and M. F. Sykes, Phys. Rev. **128**, 168 (1962); J. Gammel, W. Marshall, and L. Morgan, Proc. Roy. Soc. (London) **A275**, 257 (1963).

¹²R. G. Bowers and M. E. Woolf, Phys. Rev. **177**, 917 (1969).

¹³H. E. Stanley, Phys. Rev. **158**, 546 (1967); **164**, 709 (1967). In the latter reference Stanley suggests that the variable $1/\nu - \coth\nu$ be used as the expansion param-

$$\delta = 2\Delta/(2\Delta - 2\gamma) = 4.9 \pm 0.4,$$

$$\delta = 6\nu/(3\nu - \gamma) - 1 = 4.8 \pm 0.4. \quad (9.2)$$

These results do not eliminate the attractive $\delta = 5$ and are in agreement with the results of previous work.^{7,15,19}

How do our series results agree with experiment? Unfortunately, the experimental situation for Heisenberg systems is not as good as that for Ising systems. Of the relatively few systems which are now believed to be well represented by the Heisenberg model, we know of only one, RbMnF₃, for which accurate determinations of γ , ν , and η have been made.²⁰ The results of analysis by Corliss *et al.* are shown in Table II. Their values of ν and γ agree well with ours; the difference in η may be due, as we will discuss in II, to their use of a poor approximation for the scattering function in analyzing their data; if their value of β is reliable, then it represents a dramatic violation of scaling and cannot be compared to ours, the derivation of which requires scaling.

eter for the spin-infinity model because it provides better-behaved sequences. We tried using this variable and found that in the present system its effect was not significant.

¹⁴R. L. Stephenson and P. J. Wood, Phys. Rev. **173**, 475 (1968).

¹⁵G. A. Baker, Jr., H. E. Gilbert, J. Eve, and G. S. Rushbrooke, Phys. Rev. **164**, 800 (1967).

¹⁶C. Domb and M. F. Sykes, Proc. Roy. Soc. (London) **A240**, 214 (1957).

¹⁷D. Jasnow, thesis (University of Illinois, 1969) (unpublished).

¹⁸M. E. Fisher and R. J. Burford, Phys. Rev. **156**, 583 (1967).

¹⁹G. A. Baker, Jr., J. Eve, and G. S. Rushbrooke, Phys. Rev. B **2**, 706 (1970).

²⁰L. M. Corliss, A. Delapalme, J. M. Hastings, H. Y. Lau, and R. Nathans, J. Appl. Phys. **40**, 1278 (1969).

²¹D. R. Hartree, *Numerical Analysis* (Oxford U. P., London, England, 1952).

²²Other combinations (n, m) were analyzed and found to give consistent results.

²³P. Heller, Rept. Progr. Phys. **30**, 731 (1967).

²⁴In attempting to explain the failure of the scaling of the three-dimensional Ising model, Migdal finds that, perhaps, very near T_C , $\gamma = 2\nu$: A. A. Migdal, Zh. Eksp. i Teor. Fiz. **59**, 1015 (1970) [Sov. Phys. JETP **32**, 552 (1971)].

²⁵M. F. Sykes, J. L. Martin, and D. L. Hunter, Proc. Phys. Soc. (London) **91**, 671 (1967).

²⁶B. D. Josephson, Proc. Phys. Soc. (London) **92**, 276 (1967).

²⁷From analysis of series for the sc and bcc lattices, we would be able to quote results for each lattice which are consistent with the results of analysis of our fcc series; but, because of the irregularity of the series for these lattices, we would only feel secure in quoting uncertainties several times larger than those quoted for the fcc lattice.