PHYSICAL REVIEW B VOLUME 7, NUMBER 1 1 JANUARY 1973

General-R High-Temperature Series for the Susceptibility, Second Moment, and Specific Heat of sc and fcc Ising Models with Lattice Anisotropy*

Fredric Harbus† and H. Eugene Stanley
Physics Department, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
(Received 30 August 1972)

Of particular current interest is the critical behavior of functions on crossing over from one lattice dimensionality to another. To this end, we report high-temperature series for an Ising model with lattice anisotropy—i.e., with different exchange constants for different lattice directions. The Hamiltonian is $\mathcal{K}_{\mathrm{I\,anis}} = -J_{xy}\sum_{\langle ij\rangle}^{xy} s_i s_j - J_z \sum_{\langle ij\rangle}^{z} s_i s_j \equiv -J_{xy}(\sum_{\langle ij\rangle}^{xy} s_i s_j + R\sum_{\langle ij\rangle}^{z} s_i s_j)$ where $s_i = \pm 1$, the first summation is over all nearest-neighbor pairs in the xy plane, and the second sum is over pairs coupled in the z direction. The susceptibility, second moment, and specific-heat series are explicitly presented for *arbitrary* J_{xy} and J_z for the simple cubic (sc) and face-centered cubic (fcc) lattices to tenth order in inverse temperature. The general-R series are essential if one wishes to study the Riedel–Wegner crossover exponent appropriate to changing lattice dimensionality, since for $R \equiv J_z/J_{xy} = 0$, both the sc and fcc lattices reduce to two-dimensional square lattices, while in the limit $R \to \infty$, the sc reduces to noninteracting linear chains.

I. INTRODUCTION

Ising-model Hamiltonians with "lattice anisotropy," i.e., different exchange constants in different lattice directions, have recently been considered in two different but related contexts in the field of critical phenomena. The first context concerns testing the "universality hypothesis,"[1–3] which was put forth to describe just which features of the interaction Hamiltonian determine the critical indices. For example, according to universality, the exponents should retain their values for the nearest-neighbor (nn) isotropic model Hamiltonian when second-neighbor interactions or unequal exchange constants on the lattice are introduced. A change in the exponents is expected, however, when the effective dimensionality of the system is altered.[3]

In their investigations of these predictions, various authors[4–5] have utilized high-temperature series expansions to study the Ising Hamiltonian

$$\mathcal{K} = -J_{xy}\sum_{\langle ij\rangle}^{xy} s_i s_j - J_z \sum_{\langle ij\rangle}^{z} s_i s_j \equiv -J_{xy}\left(\sum_{\langle ij\rangle}^{xy} s_i s_j + R\sum_{\langle ij\rangle}^{z} s_i s_j\right), \tag{1.1}$$

where $s_i = \pm 1$, the first sum is over all nn pairs in an x-y plane, and the second sum is over all nn pairs whose relative displacement vector has a z component. High-temperature series were analyzed for a range of values of the parameter R by both groups.[4,5] In one case,[5] conclusions consistent with universality are reached, i.e., for all $R > 0$ the indices are three dimensional, and at $R = 0$ they change *discontinuously* to their two-dimensional values. The other work[4] claims to find exponents varying continuously with R for small R, in violation of the universality hypothesis. In view of this discrepancy in the literature (between Refs. 4 and 5), other workers should have available to

TABLE I. Coefficients a_{nj} in reduced susceptibility series for the sc lattice,

$$\bar{\chi} \equiv k_B T\chi/N\mu^2 = \sum_{n=0}^{\infty}\sum_{j=0}^{n} a_{nj}\tanh^{n-j}(\beta J_{xy})\tanh^{j}(\beta J_z).$$

$n \backslash j$	0	1	2	3	4	5	6	7	8	9	10
0	1										
1	4	2									
2	12	16	2								
3	36	80	32	2							
4	100	336	240	48	2						
5	276	1 264	1 392	512	64	2					
6	740	4 432	6 680	3 888	888	80	2				
7	1 972	14 768	29 136	23 600	8 544	1 376	96	2			
8	5 172	47 376	116 528	124 720	63 216	16 080	1 968	112	2		
9	13 492	147 504	442 368	593 856	400 032	142 416	27 216	2 672	128	2	
10	34 876	448 336	1595 896	2621 232	2224 312	1054 864	281 048	42 672	3480	144	2

them series for general R in order to conduct further tests of universality. While Ref. 4 obtained such series only for the simple cubic (sc) susceptibility $\bar{\chi}^{sc}$, we present here five additional general-R series: $\bar{\chi}^{fcc}$, μ_2^{sc}, μ_2^{fcc}, $\bar{C}_H^{sc}$, and $\bar{C}_H^{fcc}$, where $\bar{\chi}$, μ_2, and $\bar{C}_H$ (the reduced susceptibility, second moment of the correlation function, and the reduced specific heat) are defined below in Eqs. (2. 1)–(2. 3), respectively.

The anisotropic Hamiltonian (1. 1) has also received considerable attention in connection with a "crossover" exponent[2,6,7] φ and, in our view, an even more compelling motivation to focus upon the general-R series is their applicability to calculations of φ. The exponent φ describes the singular behavior of the quantity $T_c(R) - T_c(R=0)$ as the system "crosses over" from one universality class[2] to another, i. e., as the system approaches its two-dimensional limit ($R \to 0$).

To derive the equation defining φ, we start from the assumption that the Gibbs potential is a generalized homogeneous function (GHF) in the variable R as well as in the variables $\tau = [T - T_c(0)]/T_c(0)$ and H,

$$G(\lambda^{a_\tau}\tau,\ \lambda^{a_H}H,\ \lambda^{a_R}R) = \lambda G(\tau, H, R) \ . \qquad (1.\,2)$$

Equation (1. 2) is assumed to hold for all $\lambda > 0$ and small values of the arguments (i. e., in the vicinity of the two-dimensional critical point $\tau = H = R = 0$). Now, for a given value of $R_0 > 0$, the right-hand side of (1. 2) certainly has a singularity at the value of temperature critical for a system with this R, that is, for a value $\tau_0(R_0) = [T_c(R_0) - T_c(0)]/T_c(0) = cR_0$, where c is some constant. But then by the functional form of (1. 2), there exists an entire *line* of singularities given by $\tau_0(R) \sim R^{a_\tau/a_R}$, or

$$T_c(R) - T_c(0) \sim R^{1/\varphi} \ , \qquad (1.\,3)$$

where φ is defined to be a_R/a_τ.

A second prediction of the GHF hypothesis for the parameter R is that there exists a constant "gap" exponent for successive derivatives with respect to R of the thermodynamic functions derived from the Gibbs potential. Consider, e. g., the reduced susceptibility $\bar{\chi}$, for which we define

$$\bar{\chi}^{(n)} = \left(\frac{\partial^n \bar{\chi}}{\partial R^n}\right)_{\tau, H} \ . \qquad (1.\,4)$$

First we find the two-dimensional susceptibility exponent $\gamma_0 = \frac{7}{4}$ in terms of the scaling powers. To do this, differentiate (1. 2) twice with respect to H and set $H = 0$,

$$\bar{\chi}^{(0)}(\lambda^{a_\tau}\tau,\ 0,\ \lambda^{a_R}R) = \lambda^{1-2a_H}\,\bar{\chi}^{(0)}(\tau, 0, R). \qquad (1.\,5)$$

Now setting $\lambda^{a_\tau}\tau$ equal to a small positive constant, and letting $R = 0$, we get for the asymptotic form of $\bar{\chi}^{(0)}$

TABLE II. Coefficients a_{nj} in reduced susceptibility series for the fcc lattice, $\bar{\chi} \equiv k_B T\chi/N\mu^2 = \sum_{n=0}^{\infty}\sum_{j=0}^{n} a_{nj} \tanh^{n-j}(\beta J_{xy}) \tanh^{j}(\beta J_z)$.

n \ j	0	1	2	3	4	5	6	7	8	9	10
0	1										
1	4	8									
2	12	64	56								
3	36	320	656	392							
4	100	1 344	4 544	6 016	2 648						
5	276	5 056	24 720	52 896	50 304	17 864					
6	740	17 728	116 288	353 024	535 568	404 224	118 760				
7	1 972	59 072	495 504	1 987 168	4 235 872	5 045 856	3 119 984	789 032			
8	5 172	189 504	1 964 352	9 942 656	27 760 032	46 095 360	44 673 920	23 593 536	5 201 048		
9	13 492	590 016	7 369 168	45 593 696	159 435 424	344 472 640	462 863 408	380 935 552	174 446 208	34 268 104	
10	34 876	1 793 344	26 462 688	195 429 888	829 616 496[a]	2 231 941 152[a]	3 884 437 504[a]	4 411 833 200[a]	3 135 441 872[a]	1 273 786 304[a]	224 679 864

[a]Uncertainty in last quoted digit.

TABLE III. Coefficients b_{nj} in second-moment series for the sc lattice,

$$\mu_2 \equiv \sum |\vec{r}|^2 \overline{C}_2(\vec{r}) = \sum_{n=0}^{\infty} \sum_{j=0}^{n} b_{nj} \tanh^{n-j}(\beta J_{xy}) \tanh^{j}(\beta J_z).$$

$n \backslash j$	0	1	2	3	4	5	6	7	8	9	10
0	0										
1	4	2									
2	32	32	8								
3	164	272	128	18							
4	704	1 696	1 248	352	32						
5	2 708	8 816	9 168	4 032	768	50					
6	9 696	40 608	56 160	34 656	10 368	1 440	72				
7	32 948	171 504	301 488	245 936	103 328	22 688	2 432	98			
8	107 648	678 432	1 468 704	1 517 408	840 576	259 744	44 128	3 808	128		
9	340 916	2549 552	6 630 368	8 412 544	5 889 248	2 398 416	574 320	78 512	5 632	162	
10	1052 960	9193 120	28 179 552	42 859 360	36 779 200	18 910 752	5966 816	1149 792	130 368	7968	200

$$\overline{\chi}^{(0)} \sim \tau^{(1-2a_H)/a_\tau} = \tau^{-\gamma_0}. \quad (1.6)$$

Differentiating Eq. (1.5) n times with respect to R changes the scaling power on the right-hand side by na_R, so that

$$\overline{\chi}^{(n)}(\lambda^{a_\tau}\tau,\ 0,\ \lambda^{a_R}R) = \lambda^{1-2a_H-na_R}\overline{\chi}^{(n)}(\tau,\ 0,\ R). \quad (1.7)$$

Then setting $R=0$,

$$\overline{\chi}^{(n)}(\tau,\ 0,\ 0) \sim \tau^{-(1-2a_H-na_R)/a_\tau} = \tau^{-\gamma_n}, \quad (1.8)$$

where

$$\gamma_n = \gamma_0 + n\varphi. \quad (1.9)$$

Similar equations hold for the specific-heat derivatives; for all n

$$\overline{C}_H^{(n)}(\tau,\ 0,\ 0) \equiv \left(\frac{\partial^n \overline{C}_H}{\partial R^n}\right)_{\tau, H=R=0} \sim [T - T_c(0)]^{-\alpha_n}, \quad (1.10)$$

where

$$\alpha_n = \alpha_0 + n\varphi \quad (1.11)$$

and α_0 is the two-dimensional specific-heat index $\alpha_0 = 0$.

The same homogeneity arguments for the variable R applied to the pair correlation function make predictions for the second-moment function μ_2:

$$\mu_2^{(n)}(\tau, 0, 0) \equiv \left(\frac{\partial^n \mu_2}{\partial R^n}\right)_{\tau, H=R=0} \sim [T - T_c(0)]^{-(\gamma_0 + 2\nu_0 + n\varphi)}, \quad (1.12)$$

where $\nu_0 = 1$, $\gamma_0 = \frac{7}{4}$ as before, and φ must be the same crossover exponent as for thermodynamic functions by virtue of the fluctuation-dissipation theorem connecting the correlation function to the bulk susceptibility.

Abe[6] and Suzuki[7] first presented arguments implying $\varphi = \gamma_0$ based upon an additional assumption concerning "scaling" properties of multispin correlation functions. However, more recently φ has been proven[8] rigorously equal to γ_0 without making the Abe–Suzuki assumptions. The latter work[8] starts directly from the high-temperature expansion of the susceptibility and considers graphical contributions with one out-of-plane bond to show $\overline{\chi}^{(1)} \sim \tau^{-2\gamma_0}$. By Eq. (1.9) it follows that if a constant gap exponent exists it must equal γ_0.

Hence the general-R high-temperature series for $\overline{\chi}$, $\overline{C}_H$, and μ_2 serve several worthwhile purposes with regard to the crossover problem. They are useful in determining whether a constant gap index φ exists at all, and, if it does, whether it checks with the expected value of γ_0. This provides a sensitive test of scaling in the parameter R for both thermodynamic functions and the two-spin correlation function. Previous work has been restricted to the existing general-R $\overline{\chi}^{\mathrm{sc}}$ series,[4] which have been analyzed[9,10] by various techniques with the conclusions in dispute. In Paper II following,[11] all *six* functions $\overline{\chi}^{\mathrm{sc}}$, $\overline{\chi}^{\mathrm{fcc}}$, $\overline{C}_H^{\mathrm{sc}}$, $\overline{C}_H^{\mathrm{fcc}}$, μ_2^{sc}, and μ_2^{fcc} are considered, and it is concluded there is stronger evidence in favor of a constant gap exponent of $\varphi = \gamma_0 = \frac{7}{4}$.

II. METHOD OF CALCULATION

We use a computer program based upon the renormalized linked-cluster expansion theory of Wortis, Jasnow, and Moore.[12] The two-spin correlation function $\overline{C}_2(\vec{r}) \equiv \langle s_0 s_{\vec{r}} \rangle - \langle s_0 \rangle \langle s_{\vec{r}} \rangle$ was expanded to tenth order in inverse temperature for a range of specific values for J_{xy} and J_z in the Hamiltonian (1.1).

From $\overline{C}_2(\vec{r})$, series for the reduced zero-field isothermal susceptibility

$$\overline{\chi} = \overline{\chi}(J_{xy},\ J_z) = \sum_{\vec{r}} \overline{C}_2(\vec{r}), \quad (2.1)$$

the "second moment" of the correlation function

$$\mu_2 = \mu_2(J_{xy},\ J_z) = \sum_{\vec{r}} |\vec{r}|^2 \overline{C}_2(\vec{r}), \quad (2.2)$$

and reduced specific heat

TABLE IV. Coefficients b_{nj} in second-moment series for the fcc lattice,

$$\mu_2 \equiv \sum |\vec{r}|^2 \bar{C}_2(\vec{r}) = \sum_{n=0}^{\infty} \sum_{j=0}^{n} b_{nj} \tanh^{n-j}(\beta J_{xy}) \tanh^j(\beta J_z).$$

n \ j	0	1	2	3	4	5	6	7	8	9	10
0	0										
1	4	8									
2	32	128	128								
3	164	1 088	2 240	1 416							
4	704	6 784	21 920	29 120	13 568						
5	2 708	35 264	159 584	332 192	324 128	119 240					
6	9 696	162 432	964 736	2 791 232	4 249 984	3 261 248	992 768				
7	32 948	686 016	5 125 216	19 289 440	40 609 344	48 473 696	30 639 872	794 840			
8	107 648	2 713 728	24 741 856	116 102 080	316 188 800	520 119 872	509 670 048	273 549 440	61 865 216		
9	340 916	10 198 208	110 909 248	629 896 416[a]	2 126 995 712[a]	4 510 445 636[a]	6 072 599 068[a]	5 038 560 000	2 349 806 144[a]	470 875 848	
10	1 052 960	36 772 480	468 578 816[a]	3 150 446 672[a]	12 806 963 904[b]	33 555 757 568[c]	58 073 240 288[c]	66 042 641 872[c]	47 492 359 200[b]	19 572 937 312[b]	3 521 954 816

[a]Uncertainty in last quoted digit.
[b]Uncertainty in last two quoted digits.
[c]Uncertainty in last three quoted digits.

$$\bar{C}_H = \bar{C}_H(J_{xy}, J_z) = -\tfrac{1}{2} T \frac{\partial}{\partial T} \sum_{\vec{r}} J_{\vec{r}} \bar{C}_2(\vec{r}) \qquad (2.3)$$

were calculated. Here the coefficients of the respective high-temperature series depend upon the particular values of J_{xy} and J_z set at the beginning of the computer program. Given the coefficients for eleven different combinations of J_{xy} and J_z, we were able to solve simultaneous linear equations to determine the general series coefficients for arbitrary values of these parameters to tenth order.

Tables I and II present coefficients a_{nj} through $n = 10$ for the reduced susceptibility series

$$\bar{\chi} = \sum_{n=0}^{\infty} \sum_{j=0}^{n} a_{nj} \tanh^{n-j}(\beta J_{xy}) \tanh^j(\beta J_z), \qquad (2.4)$$

with $\beta \equiv 1/k_B T$ and the a_{nj} integers related to a class of graphs on the lattice with $(n-j)$ bonds in the $x-y$ plane and j bonds in the z direction.[13]

Tables III and IV present the corresponding integer coefficients b_{nj} in the second-moment series:

$$\mu_2 = \sum_{\vec{r}} |\vec{r}|^2 \bar{C}_2(\vec{r}) = \sum_{n=0}^{\infty} \sum_{j=0}^{n} b_{nj} \tanh^{n-j}(\beta J_{xy}) \tanh^j(\beta J_z). \qquad (2.5)$$

From the double tanh expansions one may reexpand to obtain for the coefficient of β^n a polynomial in R through R^n.

While $\bar{\chi}$ and μ_2 have contributions to tenth order from correlation functions to lattice points up to ten lattice spacings away from the origin, the specific heat has contributions from the correlation function to only the nearest neighbors of the origin. On the sc lattice, the form for $\bar{C}_H$ is

$$\bar{C}_H^{sc} = T C_H^{sc}/N = \sum_{n=2}^{\infty} \sum_{j=0}^{n} c_{nj} J_{xy}^{n-j} J_z^j \beta^{n-1}$$

$$= \sum_{n \text{ even}} J_{xy}^n (c_{n0} + c_{n2} R^2 + \cdots + c_{nn} R^n) \beta^{n-1}, \qquad (2.6)$$

since all odd n coefficients vanish and only even

TABLE V. Coefficients c_{nj} in reduced specific heat series for the sc lattice,

$$\bar{C}_H \equiv T C_H/N = \sum_{n=2}^{\infty} \sum_{j=0}^{n} c_{nj} J_{xy}^{n-j} J_z^j \beta^{n-1} \equiv \sum_{n=2}^{\infty} J_{xy}^n \left(\sum_{j=0}^{n} c_{nj} R^j \right) \beta^{n-1};$$

coefficients with n or j odd are zero.

n \ j	0	2	4	6	8	10
2	2	1				
4	10	24	−1			
6	$21\frac{1}{3}$	500	20	$\frac{2}{3}$		
8	$94\frac{4}{9}$	$5306\frac{14}{45}$	$2831\frac{1}{9}$	$4\frac{44}{45}$	$-\frac{17}{45}$	
10	$363\frac{199}{315}$	$50688\frac{4}{7}$	$81322\frac{2}{3}$	$5466\frac{2}{3}$	$\frac{4}{7}$	$\frac{62}{315}$

TABLE VI. Coefficients c_{nj} in reduced specific heat series for the fcc lattice,

$$C_H \equiv TC_H/N = \sum_{n=2}^{\infty} \sum_{j=0}^{n} c_{nj} J_{xy}^{n-j} J_z^j \beta^{n-1} \equiv \sum_{n=2}^{\infty} J_{xy}^n \sum_{j=0}^{n} c_{nj} R^j \beta^{n-1};$$

coefficients with j odd are zero.

$n \backslash j$	0	2	4	6	8	10
2	2	4				
3	0	48				
4	10	240	140			
5	0	$1066\frac{2}{3}$	$2133\frac{1}{3}$			
6	$21\frac{1}{3}$	3920	18680	$3962\frac{2}{3}$		
7	0	$13484\frac{4}{5}$	$123946\frac{2}{3}$	$88942\frac{14}{15}$		
8	$94\frac{4}{9}$	$43655\frac{1}{9}$	$693441\frac{7}{9}$	$1109895\frac{1}{9}$	$124004\frac{8}{9}$	
9	0	$135789\frac{5}{7}$	3437056	$10147242\frac{2}{3}$	$3708635\frac{3}{7}$	
10	$363\frac{199}{315}$	$406877\frac{5}{7}$	$15538010\frac{2}{3}$	$75708842\frac{2}{3}$	$60036413\frac{5}{7}$	$4127967\frac{29}{45}$
11[a]	0	1186519.99	65349340.11	487998490.56	696672551.98	153890822.39

[a]Computer round-off error was too great to allow determination of the exact fractions for the $n = 11$ coefficients.

powers of R enter for the even n. For the fcc, odd-order n are now nonzero as well:

$$\overline{C}_H^{\text{fcc}} = TC_H^{\text{fcc}}/N = \sum_{n=2}^{\infty} \sum_{j=0}^{n} c_{nj} J_{xy}{}^{n-j} J_z^j \beta^{n-1}$$

$$= \sum_{n=2}^{\infty} J_{xy}{}^n (c_{n2} R^2 + c_{n4} R^4 + \cdots + c_{nn'} R^{n'}) \beta^{n-1} , \tag{2.7}$$

where $n' = n$ if n is even, $n' = n - 1$ if n is odd. Here $c_{n0} \equiv 0$, and again only even powers of R contribute. The specific heat coefficients c_{nj} appear in Tables V and VI.

III. CHECKS ON SOLUTIONS

The series in the limits $R = 0$ and $R = \infty$ are known, as is the isotropic $R = 1$ case. For $R = 0$, both the anisotropic sc and fcc lattices reduce to two-dimensional square lattices. The $R = \infty$ limit ($J_{xy} = 0$, J_z finite) on the anisotropic sc gives a set of noninteracting one-dimensional linear chains, and on the fcc it gives a body-centered cubic (bcc) lattice.

We verified that the general series for $\overline{\chi}$, μ_2, and $\overline{C}_H$ reproduced the expected known series in all cases. For example, reading down the "zeroth" column in any table gives the Ising-square-lattice series, while summing the numbers in a given row across corresponds to $R = 1$ and yields the appropriate coefficient for the respective isotropic lattice (sc or fcc).[14] Reading the last entry in each row down a table checks the $R = \infty$ limits—for example, we immediately recognize the familiar linear chain results in the sc susceptibility table (cf. Table I).

Further checks on the tabulated numbers are provided by the very recent rigorous results of Liu and Stanley,[8] who show

$$\overline{\chi}^{(1)} = g\beta J_{xy} (\overline{\chi}^{(0)})^2, \tag{3.1}$$

$$\mu_2{}^{(1)} = g\,\beta J_{xy} [(\overline{\chi}^{(0)})^2 + 2\overline{\chi}^{(0)} \mu_2{}^{(0)}] , \tag{3.2}$$

where g is the number of out-of-plane nn bonds ($g = 2$, 8 for the sc, fcc, respectively). Here, of course, $\overline{\chi}^{(0)}$ and $\mu_2{}^{(0)}$ are the reduced susceptibility and second moment for the square lattice (obtained by reading down the zeroth column), and $\overline{\chi}^{(1)}$ and $\mu_2{}^{(1)}$ are as defined in Eqs. (1.4) and (1.12). We have verified that the numbers in Tables I–IV satisfy Eqs. (3.1) and (3.2).

Note added in proof. The reader will note that all the entries except the main diagonal and the first column of Tables I and III (sc lattice) are divisible by 8, while for Tables II and IV (fcc lattice) they are divisible by 16.

ACKNOWLEDGMENTS

We gratefully acknowledge helpful conversations with Dr. G. Paul and particularly L. Liu, who kindly assisted in some of the numerical checking procedures. We also wish to thank D. Karo, D. Lambeth, and M. H. Lee for discussions.

---

*Work forms a portion of a Ph.D. thesis to be submitted by Fredric Harbus to the Physics Department of MIT. Work supported by NSF, ONR, and AFOSR.

†NSF Predoctoral Fellow.

[1]D. Jasnow and M. Wortis, Phys. Rev. 176, 739 (1968).

[2]E. Riedel and F. Wegner, Z. Phys. 225, 195 (1969).
[3]R. B. Griffiths, Phys. Rev. Letters 24, 1479 (1970); L. P. Kadanoff (unpublished).
[4]J. Oitmaa and I. G. Enting, Phys. Letters 36A, 91 (1971); J. Phys. C 5, 231 (1972).
[5]G. Paul and H. E. Stanley, Phys. Letters 37A, 347 (1971); Phys. Rev. B 5, 2578 (1972).
[6]R. Abe, Progr. Theoret. Phys. (Kyoto) 44, 339 (1970).
[7]M. Suzuki, Progr. Theoret. Phys. (Kyoto) 46, 1054 (1971).
[8]L. L. Liu and H. E. Stanley, Phys. Letters 40A, 272 (1972); Phys. Rev. Letters 29, 927 (1972). A relation similar to Eq. (3.1) is mentioned in Ref. 10 without proof.
[9]D. C. Rapaport, Phys. Letters 37A, 407 (1971).
[10]I. G. Enting and J. Oitmaa, Phys. Letters 38A, 107 (1972).
[11]R. Krasnow, F. Harbus, L. Liu, and H. E. Stanley, following paper, Phys. Rev. B 7, 370 (1973).
[12]M. Wortis, D. Jasnow, and M. A. Moore, Phys. Rev. 185, 805 (1969).
[13]See, for example, C. Domb, Advan. Phys. 9, 149 (1960); H. E. Stanley, *Introduction to Phase Transitions and Critical Phenomena* (Oxford U. P., Oxford, England, 1971), Chap. 9.
[14]M. A. Moore, D. Jasnow, and M. Wortis, Phys. Rev. Letters 22, 940 (1969).

PHYSICAL REVIEW B VOLUME 7, NUMBER 1 1 JANUARY 1973

Scaling with Respect to a Parameter for the Gibbs Potential and Pair Correlation Function of the $S=\frac{1}{2}$ Ising Model with Lattice Anisotropy*

Richard Krasnow, Fredric Harbus,† Luke L. Liu, and H. Eugene Stanley
Physics Department, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
(Received 24 May 1972; revised mansucript received 30 August 1972)

Series for the reduced susceptibility $\bar{\chi}$, the reduced specific heat $\bar{C}_H$, and second moment μ_2 of the static correlation function for the three-dimensional $S=\frac{1}{2}$ Ising model on both the simple cubic (sc) and face-centered cubic (fcc) lattices with different coupling strengths in different lattice directions have been analyzed to determine the crossover exponent φ describing the behavior of the critical temperature as a function of the anisotropy parameter R in the Hamiltonian $\mathcal{H}=-J_{xy}\sum_{\langle ij\rangle}^{xy} s_i s_j - J_z\sum_{\langle ij\rangle}^{z} s_i s_j \equiv -J_{xy}(\sum_{\langle ij\rangle}^{xy} s_i s_j + R\sum_{\langle ij\rangle}^{z} s_i s_j)$. Here $s_i=\pm 1$, the first sum is over all nearest-neighbor pairs in the xy plane, and the second sum is over all pairs coupled in the z direction. The constant gap exponent we obtain for successive derivatives of $\bar{\chi}$ and $\bar{C}_H$ with respect to R confirms the exponent predictions of scaling in the parameter R for thermodynamic functions, while the results of the μ_2 series confirm the exponent predictions of scaling with respect to R for the two-spin correlation function. Our results agree with the predictions for φ of Abe and Suzuki, and also with rigorous relations satisfied by the exponents describing the derivatives of the various functions. Our results do not agree with previously published results, which are based on an analysis of only the susceptibility on only the sc lattice.

I. INTRODUCTION

Interest has recently focused[1-5] on magnetic model systems with different coupling strengths in different lattice directions ("lattice anisotropy") described by the Hamiltonian

$$\mathcal{H}=-J_{xy}\sum_{\langle ij\rangle}^{xy} s_i s_j - J_z\sum_{\langle ij\rangle}^{z} s_i s_j$$

$$\equiv -J_{xy}\left(\sum_{\langle ij\rangle}^{xy} s_i s_j + R\sum_{\langle ij\rangle}^{z} s_i s_j\right), \qquad (1.1)$$

thereby defining $R\equiv J_z/J_{xy}$ as the ratio of interplanar to intraplanar coupling strengths. Here $s_i=\pm 1$, the first sum is over nearest-neighbor (nn) spins in the xy plane, while the second sum is over spins whose relative displacement vector has a z component. The Hamiltonian (1.1) has previously been studied[1-5] with two purposes in mind: (a) to test the predictions of the "universality hypothesis,"[6] and (b) to examine critical behavior upon crossing over from a three-dimensional to a two-dimensional lattice as $R\rightarrow 0$. Of particular interest is the "crossover exponent" φ giving the variation of critical temperature $T_c(R)$ with R for small R,

$$T_c(R)-T_c(0)\sim R^{1/\varphi}, \qquad (1.2)$$

and its relation to various scaling predictions.

In the preceding paper[1] (hereafter referred to as Paper I), the reduced susceptibility $\bar{\chi}$, the reduced specific heat $\bar{C}_H$, and the second moment μ_2 were defined, and high-temperature series for arbitrary R were presented for these quantities on both the sc and fcc lattices. The implications of scaling of thermodynamic functions and of the pair correlation function with respect to the parameter R were discussed. In particular, the consequences of assuming the Gibbs potential to be a generalized homogeneous function (GHF) of the variables $\tau\equiv T$