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# 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\*

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Series for the reduced susceptibility  $\overline{\chi}$ , the reduced specific heat  $\overline{C}_H$ , and second moment  $\mu_2$  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  $\varphi$  describing the behavior of the critical temperature as a function of the anisotropy parameter R in the Hamiltonian  $\mathcal{K} = -J_{xy} \sum_{i \neq j}^{\infty} s_{is} - J_{z} \sum_{i \neq j}^{\infty} s_{is} - J_{xy} \left( \sum_{i \neq j}^{\infty} s_{is} s_{j} + R \sum_{i \neq j}^{\infty} s_{is} s_{j} \right)$ . 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  $\overline{\chi}$  and  $\overline{C}_H$  with respect to R confirms the exponent predictions of scaling in the parameter R for thermodynamic functions, while the results of the  $\mu_2$  series confirm the exponent predictions of scaling with respect to R for the two-spin correlation function. Our results agree with the predictions for  $\varphi$  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<sup>1-5</sup> on magnetic model systems with different coupling strengths in different lattice directions ("lattice anisotropy") described by the Hamiltonian

$$3C = -J_{xy} \sum_{\langle ij \rangle}^{xy} s_i s_j - J_z \sum_{\langle ij \rangle}^{z} s_i s_j$$

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

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 hypothe-

sis,"<sup>6</sup> and (b) to examine critical behavior upon crossing over from a three-dimensional to a two-dimensional lattice as  $R \to 0$ . Of particular interest is the "crossover exponent"  $\varphi$  giving the variation of critical temperature  $T_c(R)$  with R for small R,

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

and its relation to various scaling predictions.

In the preceding paper  $^1$  (hereafter referred to as Paper I), the reduced susceptibility  $\overline{\chi}$ , the reduced specific heat  $\overline{C}_H$ , and the second moment  $\mu_2$  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  $\tau \equiv T$ 

 $-T_c(R=0)$ , the magnetic field H, and the anisotropy parameter R were derived.

In Sec. II of the present paper we derive some of the predictions of scaling not covered in Paper I. Previous numerical work on the crossover problem, carried out on only the susceptibility series on only the sc lattice, 3,4 is reviewed in Sec. III. The previous results for the susceptibility exponents  $\gamma_n$ [defined below in Eq. (2.1)] are compared with some rigorous relations. In Sec. IV we describe the techniques we use to analyze all six series  $(\bar{\chi},$  $\mu_2$ ,  $\overline{C}_H$  for fcc and sc lattices), and present the results of this analysis. We believe this new numerical evidence made possible by the additional general-R series offers substantial support to the hypothesis of scaling in the parameter R for both thermodynamic functions and the pair correlation function. Finally, Sec. V contains a summary and concluding remarks.

#### II. PREDICTIONS OF SCALING

As was shown in Paper I, scaling of thermodynamic functions predicts that the exponents  $\gamma_n$  defined by

$$\overline{\chi}^{(n)} \equiv \left(\frac{\partial^n \overline{\chi}}{\partial R^n}\right)_{R=0} \sim \tau^{-\gamma_n} \tag{2.1}$$

should obey the relation [Eq. (1.9) of Paper I]

$$\gamma_n = \gamma_0 + n\varphi \,, \tag{2.2}$$

where  $\varphi$  is the same as the exponent in Eq. (1.2), and  $\gamma_0$  is the exponent for the two-dimensional zero-field susceptibility; claimed<sup>7</sup> to be exactly 1.75 for the Ising model.

In addition, there is an elementary rigorous result  $^{8}$  which states that

$$\gamma_1 = 2\gamma_0 . \tag{2.3}$$

Coupling this result with the scaling prediction, Eq. (2.2) yields

$$\varphi = \gamma_0 , \qquad (2.4)$$

$$\gamma_n = (n+1)\gamma_0. \tag{2.5}$$

For purposes of later comparison, it is worthwhile to point out that the above relations Eq. (2.5) have also been shown<sup>8</sup> to be rigorously true for n = 2, 3,

$$\gamma_2 = 3\gamma_0, \qquad \gamma_3 = 4\gamma_0. \tag{2.6}$$

In a manner similar to Eq. (2.1), one may define the exponents  $\alpha_n$  which characterize the divergence near the critical point of the quantities

$$\overline{C}_{H}^{(n)} \equiv \left(\frac{\partial^{n} \overline{C}_{H}}{\partial R^{n}}\right)_{R=0} \sim \tau^{-\alpha_{n}}. \tag{2.7}$$

Again, scaling of thermodynamic functions with respect to the parameter R predicts that

$$\alpha_n = \alpha_0 + n\varphi , \qquad (2.8a)$$

which, combined with Eq. (2.4), yields

$$\alpha_n = \alpha_0 + n\gamma_0 \,, \tag{2.8b}$$

where  $\alpha_0 = 0$  corresponds to the well-known logarithmic divergence of the two-dimensional specific heat. <sup>9</sup> The proof of Eq. (2.8a) proceeds exactly as the proof of Eq. (2.2).

For the derivatives with respect to R of the second moment  $\mu_2$ , we define the exponents  $\nu_n$  by

$$\mu_2^{(n)} \equiv \left(\frac{\partial^n \mu_2}{\partial R^n}\right)_{R=0} \sim \tau^{-(\gamma_0 + 2\nu_n)} , \qquad (2.9)$$

where  $\nu_0 = 1$  exactly. Assuming the pair correlation function to scale in the variable R [as well as in H,  $\tau$ , and the lattice distance  $\vec{r}$ ] yields

which, combined with Eq. (2.4), yields

$$2\nu_n = 2\nu_0 + n\gamma_0 \,. \tag{2.10b}$$

The proof of Eq. (2.10a) begins with the assumption that the pair correlation function  $\overline{C}_2(\tau, H, \dot{r}, R)$  is a GHF of its four variables, for small values of  $\tau$ , H, R, and  $1/|\dot{r}|^{10,11}$ :

$$\overline{C}_{2}(\lambda^{b\tau}\tau, \lambda^{bH}H, \lambda^{b\tau}\dot{\overline{\tau}}, \lambda^{bR}R) = \lambda^{1+3b\tau}\overline{C}_{2}(\tau, H, \dot{\overline{\tau}}, R),$$
(2.11)

where the scaling power of the function is chosen to conform with the notation of Ref. 11, in which the correlation function  $C_2(\tau, H, \tilde{r}, R)$  defined by

$$\overline{\chi} = \sum_{\text{all } \vec{r}} \overline{C}_2(\tau, H, \vec{r}, R) \equiv \int C_2(\tau, H, \vec{r}, R) d\vec{r}$$
(2.12)

has a scaling power of unity.

It is then easy to show that the *j*th moment  $\mu_j$  is also a GHF:

$$\mu_{j}(\lambda^{b\tau}\tau, \lambda^{bH}H, \lambda^{bR}R)$$

$$= \sum_{\vec{r}} |\vec{r}|^{j} \overline{C}_{2}(\lambda^{b\tau}\tau, \lambda^{bH}H, \vec{r}, \lambda^{bR}R)$$

$$= \sum_{\vec{r}} |\lambda^{b\vec{r}}\vec{r}|^{j} \overline{C}_{2}(\lambda^{b\tau}\tau, \lambda^{bH}H, \lambda^{b\vec{r}}\vec{r}, \lambda^{bR}R)$$

$$= \lambda^{1+(3+j)b\tau} \sum_{\vec{r}} |\vec{r}|^{j} \overline{C}_{2}(\tau, H, \vec{r}, R)$$

$$= \lambda^{1+(3+j)b\tau}\mu_{j}(\tau, H, R). \qquad (2.13)$$

Given that  $\mu_j$  is a GHF, it follows that the derivatives  $\mu_j^{(n)} \equiv (\partial^n \mu_j / \partial R^n)_{R=0}$  are also GHF's:

$$\mu_{f}^{(n)}(\lambda^{b\tau}\tau, \lambda^{bH}H) = \left(\frac{\partial^{n}\mu_{f}}{\partial R^{n}} (\lambda^{b\tau}\tau, \lambda^{bH}H, R)\right)_{R=0}$$

$$= \left(\frac{\partial^{n}\mu_{f}}{\partial R^{n}} (\lambda^{b\tau}\tau, \lambda^{bH}H, \lambda^{b}RR)\right)_{R=0} \lambda^{-nbR}$$

$$= \lambda^{1+(3+f)b_{r}-nb_{R}}\mu_{f}^{(n)}(\tau, H). \qquad (2.14)$$

In order to consider the divergence of  $\mu_j^{(n)}$  with  $\tau$ , we set  $\lambda \equiv |\tau|^{-1/b\tau}$  in the above equation, and let H=0:

$$\mu_{i}^{(n)}(1, 0) = |\tau|^{-[1+(3+j)b_{r}-nb_{R}]/b_{\tau}}\mu_{i}^{(n)}(\tau, 0). \quad (2.15)$$

Thus the exponents  $\nu_n$  defined in Eq. (2.9) are given by

$$-(\gamma_0 + 2\nu_n) = (1 + 5b_r - nb_R)/b_\tau. \tag{2.16}$$

To express the right-hand side of (2.16) in terms of known quantities  $\gamma_0$ ,  $\nu_0$ , and  $\varphi$ , we first set j=n=0 in Eq. (2.15). Then, since the susceptibility is the zeroth moment of  $\overline{C}_2$  [cf. Eq. (2.1) of I], we have for  $\gamma_0$ 

$$-\gamma_0 = (1+3b_r)/b_\tau. (2.17)$$

Next we use the definition 12

$$\xi^2 = \mu_2 / \overline{\chi} \tag{2.18}$$

for the correlation length  $\xi$ . Setting j=2, n=0 in Eq. (2.15) we find from Eqs. (2.17) and (2.18) that

$$-2\nu_0 = (1+5b_r)/b_\tau + \gamma_0 = 2b_r/b_\tau. \tag{2.19}$$

Finally, to obtain an expression involving  $\varphi$ , it is easiest to set j=0 in Eq. (2.13), let H=0, and set  $\lambda \equiv |R|^{-1/b}R$ . Then,

$$|R|^{(1+3b_T)/b_R} \overline{\chi}(\tau/|R|^{b_T/b_R}, 0, 1) = \overline{\chi}(\tau, 0, R).$$
(2.20

Now, if the right-hand side of Eq. (2.20) has a singularity at a temperature  $T_c(R)$ , corresponding to a value of  $\tau = \tau_c(R) = [T_c(R) - T_c(0)]/T_c(0)$  for some R > 0, the functional form of Eq. (2.20) requires there to be singularities over the entire line where the first argument of the left-hand side has a constant value. Thus

$$T_c(R)/|R|^{b_T/b_R} = \text{const}$$

or

$$T_c(R) - T_c(0) \sim |R|^{b_T/b_R},$$
 (2.21)

so that from Eq. (1.2),

$$\varphi = b_R / b_{\tau}. \tag{2.22}$$

Using the results Eqs. (2.16), (2.19), and (2.22) in (2.15) we obtain the desired result Eq. (2.10a).

Equation (2.10b) is actually rigorous for the case n=1, by virtue of the relation<sup>8</sup>

$$\mu_2^{(1)} \propto \chi_{\rm sq}^2 + 2\mu_{2,\rm sq} \chi_{\rm sq} \,, \tag{2.23}$$

where  $\mu_{2,sq}$  denotes the second moment on the twodimensional square lattice. This equation holds for either the sc or fcc lattices, with the constant of proportionality differing between them.

We note that the scaling powers for the Gibbs potential of Paper I  $(a_{\tau}, a_{H}, a_{R})$  are not independent of the b scaling powers for  $\overline{C}_{2}$ . From Eq. (1.5) of I with  $H \neq 0$  and Eq. (2.13) of the present paper with j=0, it follows that

$$(1 - 2a_H)/a_\tau = (1 + 3b_\tau)/b_\tau$$
, (2.24a)

$$(1 - 2a_H)/a_R = (1 + 3b_r)/b_R$$
, (2.24b)

$$(1 - 2a_H)/a_H = (1 + 3b_r)/b_H$$
. (2.24c)

Thus the a's are expressible in terms of the b's, but the converse is not true.

## III. PREVIOUS WORK

There is currently a controversy in the literature<sup>3,4</sup> concerning whether the predictions of scaling in the parameter  $R \equiv J_z/J_{xy}$  for the exponents  $\varphi$  and  $\gamma_n$  stated in Eqs. (2.4) and (2.5) are borne out by series analyses of the susceptibility on the sc lattice.

One group of workers,  $^3$  using an 11-order high-temperature series in R and  $\tanh(J_{xy}/kT)$ , reports the following values for the exponents  $\gamma_n$ :

$$\gamma_1 = 3.50$$
,  $\gamma_2 = 5.0 \pm 0.1$ ,  $\gamma_3 = 6.5 \pm 0.2$ ,  $\gamma_4 = 8.0 \pm 0.3$ . (3.1)

The last three are in disagreement with both the scaling predictions, Eq. (2.5), and the rigorous equalities, Eq. (2.6), for n=2 and 3.

The same group<sup>3</sup> reports a value for  $\varphi$  of 1.2  $\pm$ 0.1, obtained from a log-log plot of  $T_c(R) - T_c(0)$  vs R. This result is again in disagreement with the scaling result Eq. (2.4). We believe this low estimate for  $\varphi$  to be a consequence of improperly low estimates of the  $T_c(R)$  for small R. These low estimates are consistent with the same group's estimates of the exponent  $\gamma(R)$  describing the critical behavior of the susceptibility

$$\overline{\chi}(R) \sim [T - T_c(R)]^{-\gamma(R)}. \tag{3.2}$$

Their<sup>3</sup> estimates for  $\gamma(R)$  show continuous variation with R for small R, contradicting the universality prediction<sup>6,13</sup> of 1.25 for all R > 0. Low estimates of  $T_c(R)$  would lead to high estimates of  $\gamma(R)$  (values > 1.25) on a ratio plot. [In Sec. IV, we will present an estimate for  $\varphi$  using a different set of  $T_c(R)$ .] Another author, <sup>4</sup> using Padé approximant (PA) techniques on the same general-R sc susceptibility series, claims results for the  $\gamma_n$  that are at least consistent with the scaling predictions, Eq. (2.5).

These discrepancies between Refs. 3 and 4 seem to us sufficient motivation to undertake a further study of the crossover exponent. Furthermore, the series from Paper I give us the opportunity to study the additional scaling predictions of Eqs. (2.8) and especially (2.10). Our study of (2.10) provides a test of correlation-function scaling in the parameter R, and constitutes to our knowledge the first such test of its kind.

## IV. TECHNIQUES OF SERIES ANALYSIS AND PRESENT

In order to estimate the exponents  $\gamma_n$ ,  $\alpha_n$ , and  $\nu_n$  we proceed to test the series of Paper I by the ratio

method, 14 by Padé approximants (PA's) to their logarithmic derivatives, 15 and by Park's method, 16 In addition, each series is raised to a number of trial powers near the inverses of the exponents predicted by scaling. We look for powers which produce in their respective Padé tables consistent simple poles which are closest to the exactly known  $T_c(0)$ . <sup>17</sup> Each series to a power was also studied by the ratio test and Park's method. Finally, bilinear transformations are used to improve convergence.

We found that the series for  $\overline{\chi}_{sc}$  had better convergence to the correct  $T_c(0)$  when expressed in the variable  $\mathfrak{J} \equiv J_{xy}/kT$  rather than  $v \equiv \tanh(\mathfrak{J})$ . Hence, we expand all the series of Paper I in J.

#### A. Ratio Tests

Consider a finite series, e.g., the susceptibility

$$\overline{\chi} \simeq \sum_{l=0}^{L} A_l \mathcal{J}^l$$
,  $\mathcal{J} \equiv J_{xy}/kT$ , (4.1) with

$$A_1 \equiv \sum_{i=0}^{l} a_{l,j} R^j, \quad a_{00} = 1.$$
 (4.2)

Then the *n*th derivative with respect to R, at R=0, is given by

$$\overline{\chi}^{(n)} \simeq n! \sum_{l=n}^{l} \alpha_{l,n} \vartheta^{l}$$

$$= n! \vartheta^{n} \sum_{l=0}^{l-n} \alpha_{l+n,n} \vartheta^{l}. \tag{4.3}$$

The ratios  $\rho_{n,l}$  are formed,

$$\rho_{n,l} \equiv a_{l+n,n}/a_{l+n-1,n}, \quad l=1,\ldots, L-n$$
(4.4)

and plotted versus 1/l. A useful sequence of exponent estimates  $\gamma_{n,l}$  is obtained by using the formula<sup>14</sup>

$$\rho_{n,l} = g_c^{-1} [1 + (\gamma_{n,l} - 1)/l]. \tag{4.5}$$

This sequence  $\gamma_{n,l}$  corresponds to the slopes of a sequence of straight lines passing through successive ratios  $\rho_n$ , and the exactly known<sup>17</sup>  $\mathcal{J}_c^{-1}$ , where

$$\mathcal{J}_c \equiv J_{rv}/kT_c(0) = \operatorname{arctanh}(\sqrt{2} - 1). \tag{4.6}$$

Upon arriving at a set of estimates  $\gamma_{n,l}$  ( $l=1,\ldots$ , L-n), we form a Neville table <sup>18,19</sup> of extrapolated estimates of the  $\gamma_{n,l}$ . The linear extrapolants  $\lambda_{n,l}$ are given by

$$\lambda_{n,l} = l \gamma_{n,l} - (l-1) \gamma_{n,l-1}, \qquad (4.7)$$

the quadratic extrapolants  $\zeta_{n,l}$  by

$$\zeta_{n,l} = \frac{1}{2} \left[ l \lambda_{n,l} - (l-2) \lambda_{n,l-1} \right], \qquad (4.8)$$

and so on.

### B. Park's Method

In the Park's-method studies the exact  $T_c(0)$  of Eq. (4.6) is again used to estimate the exponents, according to Eq. (2.20) of Ref. 5. The lth estimate of  $\gamma_n$  by Park's method,  $\gamma_{n,l}^P$ , is given by

$$\gamma_{n,l}^{P} = b_{l}^{(n)} \mathcal{J}_{c}^{l},$$
 (4.9)

where

$$b_{l}^{(n)} = \left(la_{l+n,n} - \sum_{i=1}^{l-1} a_{l+n-j,n} b_{j}^{(n)}\right) / a_{n,n}$$
 (4.10)

is the coefficient of  $\mathfrak{I}^{l}$  in the expansion for the logarithmic derivative of the series under study,

$$\frac{d \ln \overline{\chi}^{(n)}}{d \ln \vartheta} \simeq \sum_{l=1}^{L-n} b_l^{(n)} \vartheta^l + n, \qquad (4.11)$$

and  $b_1^{(n)} \equiv a_{n+1,n}/a_{n,n}$ .

The Park's-method estimates for the exponents exhibit large oscillations about a mean value. One may then perform sequential averages of the estimates; i.e., one can calculate the quantities

$$p_{n,l} = \frac{1}{2} \left( \gamma_{n+l}^{P} + \gamma_{n,l+1}^{P} \right). \tag{4.12}$$

This procedure can be repeated successively. Very good convergence is obtained even after the first such averaging. Such oscillations in the  $\gamma_{n,l}^{P}$  can also be eliminated by doing a bilinear transformation on the original series; this procedure is described in Sec. IVD.

## C. Pade Approximants

The Padé tables for the logarithmic derivatives of each series exhibit less pronounced convergence than either of the above two methods. We thus use the log-Padé method only as a check of our results. One measure of the reliability of the log-PA results for the exponents is provided by how well the estimate of the critical temperature compares with the exact value  $T_c(0)$ .

In the case of raising the series to various trial powers. 20 we find that if the power is not the one predicted by scaling, then convergence to a particular singularity is generally observed, but the corresponding critical temperature is different from  $T_c(0)$ . Each series was raised to powers equal to, and on both sides of, the inverse of the exponent predicted by scaling. Convergence was not always the best for the scaling value, but the pole produced was always closest to  $T_c(0)$ . This is an example of how good convergence alone is not sufficient to draw definitive conclusions.

## D. Bilinear Transformations

When a series is examined by the ratio test or by Park's method, there often exist large oscillations in the successive ratios and estimates for the exponents. This can be due to a "nonphysical" singularity in the complex-9 plane situated closer to the origin than the ferromagnetic singularity  $\mathbf{J}_c$  of Eq. (4.6). Such a spurious singularity may often

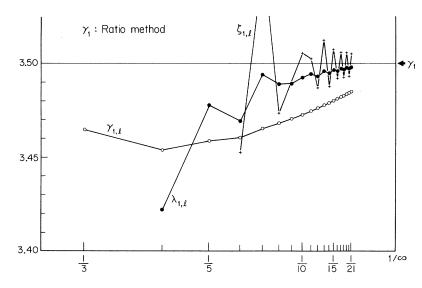


FIG. 1. Estimates of the exponent  $\gamma_1$  by ratio method. First two Neville table entries are also shown [cf. Eqs. (4.7) and (4.8)]. Arrow at right indicates limiting value from Eq. (2.3).

be "transformed away" by a bilinear transformation. Here the original series in  $\bf 3$  is reexpressed in the variable  $\bf 18$ 

$$\tilde{\mathfrak{J}} \equiv \mathfrak{J}/(1+b\mathfrak{J}), \qquad (4.13)$$

with b suitably chosen to move the interfering singularity further from the origin and hence diminish its effect. The location of the singularity, and thus the proper value of b, can be estimated from the Padé table for the original series in  $\beta$ .

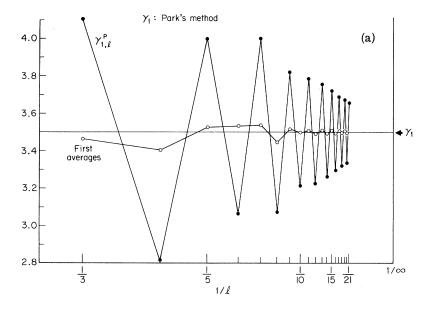
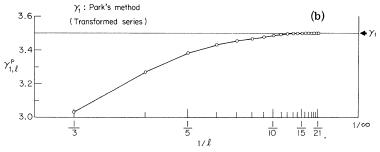


FIG. 2. (a) Estimates  $\gamma_{1,I}^{p}$  (0) for the exponent  $\gamma_{1}$ , by Park's method. Only the first averages ( $\bullet$ ) are shown for clarity. (b) Estimates by Park's method after the transformation of Eq. (4.13), where the choice b=2.17 was based on the log-Padé estimates. These points are without averaging.



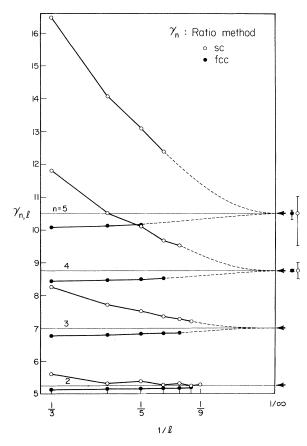


FIG. 3. Ratio-method estimates  $\gamma_{n,l}$  for n=2-5 (O)sc, ( $\blacksquare$ )fcc. Arrows at right indicate the values predicted by scaling. For  $n \le 3$ , these are also rigorous equalities. Dashed lines are guides to the eye, and vertical bars indicate confidence limits based on all methods of analysis.

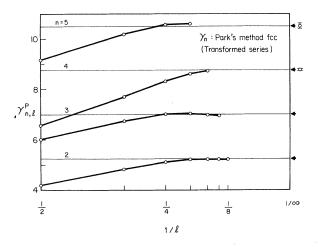


FIG. 4. Park's-method estimates  $\gamma_{n,l}^P$  for n=2-5 from fcc transformed series, Eq. (4.13). The choices b=1.58, 1.09, 2.00, 1.00 (for n=2, 3, 4, 5, respectively) were based on the log-Padé estimates. The case n=1 is shown in Fig. 2(b). Arrows and dashed lines as in Fig. 3.

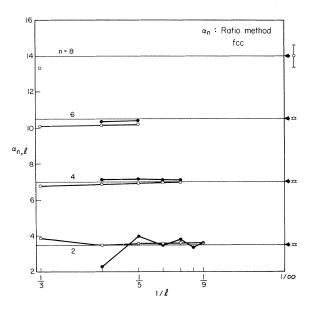


FIG. 5. Ratio-method estimates of  $\alpha_n$  for n=2, 4, 6, 8 for the untransformed fcc series (O).  $\bullet$ , first Neville extrapolants. Arrows at right indicate values predicted by scaling. Vertical bars indicate confidence limits on our estimates based on *all* methods of analysis.

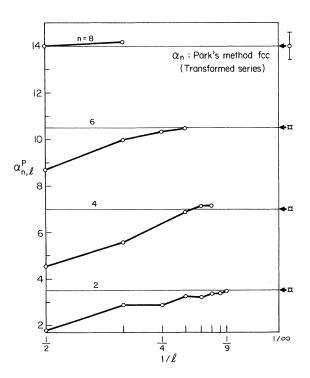


FIG. 6. Park's-method estimates of  $\alpha_n$  for n=2, 4, 6, 8 on the transformed fcc series. The parameter b of Eq. (4.13) equals 3.50, 3.00, 1.50, 0.25 for n=2, 4, 6, 8, respectively. Arrows at right indicate values predicted by scaling. Dashed lines are guides to the eye, and vertical bars at right are confidence limits.

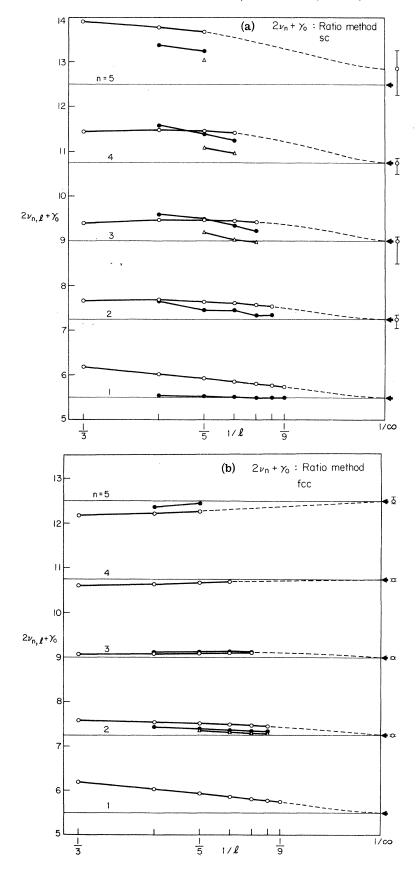


FIG. 7. Ratio-method estimates of  $2\nu_n+\gamma_0$ , for (a) sc lattice and (b) fcc lattice. Arrows at right indicate values predicted by scaling. For n=1 the limiting value is rigorous. Dashed lines are visual guides, not fits. Bars at right indicate confidence limits based on *all* methods of analysis. Higher Neville extrapolants are also shown, and their order can be inferred by the l at which they start: kth Neville extrapolant starts at l=3+k.

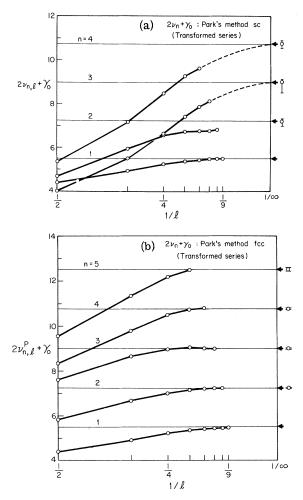


FIG. 8. Park's-method estimates for  $2\nu_n + \gamma_0$ , for (a) sc and (b) fcc lattices. Results for sc are obtained from transformed series, with the parameter b of Eq. (4.13) equal to 2.0, 4.0, 7.0, 6.0 for n=1, 2, 3, 4, respectively. Results for fcc use b values of 2.0, 1.5, 2.0, 2.0 for n=2, 3, 4, 5, respectively. Arrows at right indicate values predicted by scaling. Value for n=1 is rigorous. Dashed lines are visual guides, and vertical bars at right indicate our confidence limits based on all methods of analysis.

## E. Test Series

A particularly good test of the above methods is given by a lengthy series for  $\overline{\chi}^{(1)}$ , which we obtained from the rigorous relation<sup>8</sup>

$$\overline{\chi}^{(1)} \propto \Im \overline{\chi}_{sg}^2$$
, (4.14)

where  $\overline{\chi}_{sq}$ , the susceptibility for the two-dimensional square lattice, has very recently been calculated<sup>21</sup> through order 21. It is this relation that produces the rigorous result Eq. (2.3). It is valid for both sc and fcc lattices, with proportionality factors 2 and 8, respectively. Figure 1 shows the first few Neville table entries for this series

plotted versus 1/l. In Fig. 2(a) we display the estimates of the exponent  $\gamma_1$  obtained by Park's method and the first sequential averages of these estimates. Figure 2(b) shows the estimates of  $\gamma_1$  from the bilinearly transformed series.

## F. Evidence Supporting Scaling of Thermodynamic Functions: Exponents $\gamma_n$ and $\alpha_n$

Figure 3 shows ratio method estimates  $\gamma_{n,l}$  vs 1/l for n=2-5 for both the sc and fcc lattices. For n=1 the series estimates of the exact result 3.50 are shown in Fig. 1.

Figure 4 shows the Park's method estimates  $\gamma_{n,l}^P$  of Eq. (4.9) for the fcc series. These provide supportive evidence for the conclusions drawn from Fig. 3. The values shown are for the transformed  $\tilde{\mathbb{J}}$  series [cf. Eq. (4.13)], since the series in  $\mathbb{J}$  had oscillating estimates. The Park's estimates for the sc series are divergent, and upon transformation they become convergent, but too slowly to draw a firm conclusion.

When considering Figs. 3 and 4, it must be remembered that the correct exponents in each case must obey the rigorous equalities of Eq. (2.6) for n=2,3. Each equality is the value predicted by scaling, which is displayed by the arrow. If we had no such equalities, the combined methods of analysis would still lead us to the same values for the  $\gamma_n$ , albeit with confidence limits. Confidence limits are indicated in the right margin only for n=4,5.

The dashed lines in the figures are not fits, but merely guidelines. In considering the limiting value of the present estimates, it is important to distinguish these plots from "ratio plots." Since

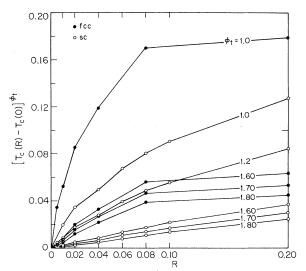


FIG. 9.  $T_c(R) - T_c(0)$  raised to various trial powers  $\varphi_t$ , for both the sc and fcc lattices.  $T_c(R)$  is expressed in units of the two-dimensional mean-field value,  $T_c^{\rm mf} = qJ_{xy}/k$ , where q=4 is the coordination number of the lattice.  $\varphi=1.2$  is the value from Ref. 3.

the present estimates are for the same quantity, the limiting slope of the dashed line must be zero. When plotting ratios, on the other hand, the limiting slope is in general nonzero.

In the case of the specific-heat exponents  $\alpha_n$ , we do not as yet have rigorous inequalities such as those for the  $\gamma_n$ , and therefore, we must place wider confidence limits on our estimates. Figures 5 and 6 exhibit the ratio and Park's estimates, respectively.

The  $\overline{C}_H$  series for the sc lattice proves to be too short for any meaningful results to be extracted, and that analysis is therefore not presented here.

## G. Evidence for Scaling of Correlation Function: Exponents $\nu_n$

Figures 7(a) and 7(b) show, for the sc and fcc lattices, respectively, ratio-method estimates for the  $\nu_n$ , for n=1-5. The exponents  $\nu_n$  are actually displayed in the form  $2\nu_n+\gamma_0$ , which are the exponents of  $\mu_2^{(n)}$ , as defined in Eq. (2.9). The case n=1 is identical for the two lattices because of the rigorous relation Eq. (2.23), and  $2\nu_1$  is thus known to be exactly  $2\nu_0+\gamma_0=3.75$ . Hence the n=1 case provides yet another test of our method. Figure 8 shows the Park's-method analysis.

TABLE I. (a) First three lines test the predictions of thermodynamic scaling with a parameter [Eqs. (2.5) and (2.8b)].

(b) Last line tests the predictions of correlation function scaling with a parameter [Eq. (2.10)].

Definition of exponents	Scaling hypothesis plus $\gamma_1 = 2\gamma_0$ proof (Ref. 8)	Previous numerical results (sc lattice only)	Present work (sc and fcc lattices) sc fcc
(a) Test of thermodyna	mic scaling		
$T_c(R) - T_c(0) \sim R^{1/\varphi}$	$\varphi = \gamma_0$	$\varphi$ =1.2 <sup>(3)</sup>	$\varphi$ = 1.70 ± 0.1
	$[\gamma_0 = 1.75]$		
$\overline{\chi}^{(n)} \equiv (\partial^n \overline{\chi} / \partial R^n)_{R=0} \sim \tau^{-\gamma} n$	$\gamma_n = \gamma_0 + n\varphi$		
	$=(n+1)\gamma_0$		
	n = 1 3.50	3.50(3),(4)	3.500
	n = 2 5.25	$5.0 \pm 0.1^{(3)},  5.2 \pm 0.1^{(4)}$	5, 250
	n = 3 7.00	$6.5 \pm 0.2^{(3)}$ , $6.9 \pm 0.1^{(4)}$	7.000
	n = 4 8.75	$8.0 \pm 0.3^{(3)}$	$8.75 \pm 0.25$ $8.75 \pm 0.03$
	$n = 5 \ 10.50$		10.5 $\pm {0.50 \atop 1.00}$ 10.5 $\pm {0.1 \atop 0.2}$
$C_H^{(n)} \equiv (\partial^n C_H / \partial R^n)_{R=0} \sim \tau^{-\alpha_n}$	$\alpha_n = \alpha_0 + n\varphi$		
	$=\alpha_0+\gamma_0$		
	$[\alpha_0 = 0]$		
	n = 2 3.50		$3.5 \pm 0.05$
	n = 4  7.00		$\textbf{7.0} \pm \textbf{0.04}$
	$n = 6 \ 10.50$		10.5 $\pm$ 0.05
	n = 8 14.00		$14.0 \pm 0.6$
(b) Test of correlation-	function scaling		
$\mu_2^{(n)} \equiv (\partial^n \mu_2 / \partial R^n)_{R=0} \sim \tau^{-(\gamma_0 + 2\nu_n)}$	$\gamma_0 + 2\nu_n = \gamma_0 + 2\nu_0 + n\varphi$		
	$=2\nu_0+(\mu+1)\gamma_0$ , $[\nu_0]$	=1]	
	n = 1 5.50		5.500
	n=2 7.25		$7.25 \pm 0.10 \atop 0.20$ $7.25 \pm 0.02$
	n = 3 9.00		$9.0 \pm {0.10 \atop 0.50}$ $9.0 \pm 0.1$
	$n = 4 \ 10.75$		10.75 $\pm {0.10 \atop 0.25}$ 10.75 $\pm$ 0.03
	n = 5 12.50		12. $85 \pm {0.40 \atop 0.60}$ 12. $50 \pm {0.10 \atop 0.05}$

### H. Evidence Supporting $T_c(R) - T_c(0) \sim R^{1/\gamma_0}$

As a final step, we analyze values of  $T_c(R)$ , from Table VI of Ref. 5, in order to obtain a direct estimate of  $\varphi$  from Eq. (1.2) with  $T_c(0)$  being known exactly. <sup>17</sup> In Fig. 9 we plot  $T_c(R) - T_c(0)$  raised to various trial powers  $\varphi_t$  vs R, and seek the value of  $\varphi_t$  which produces the straightest line. This method was favored over a log-log plot, <sup>3</sup> since it allows the point (0, 0) to be included. We conclude that the best straight line occurs for

$$\varphi_t = 1.7 \pm 0.1, \qquad (4.15)$$

for both the sc and fcc lattices. This is consistent with results from our log-log plots. To arrive at this value of  $\varphi_t$  it is necessary to plot many more curves than those shown in Fig. 9, and observe the trend of the small-R region as the power is varied. While there is considerable scatter in any one curve, we believe the absence of curvature is most pronounced for the curve with  $\varphi_t$  given above. Although it is certainly not conclusive evidence for  $\varphi = \gamma_0$ , it casts doubt on the value  $\varphi = 1.2$  of Ref. 3.

#### V. SUMMARY AND CONCLUSIONS

We have analyzed the general-R series of Paper I for the susceptibility, specific heat, and second moment of the correlation function of the spin- $\frac{1}{2}$ Ising ferromagnet with directional anisotropy, on both the sc and fcc lattices. Our purpose was to determine the critical-point exponents  $\gamma_n$ ,  $\alpha_n$ , and  $\nu_n$  which characterize the divergence of the nth derivatives with respect to R of  $\overline{\chi}$ ,  $\overline{C}_H$ , and  $\mu_2$ . We find the  $\gamma_n$ ,  $\alpha_n$ , and  $\nu_n$  to be characterized by a constant crossover exponent  $\varphi$ . We have compared the results obtained above with those predicted by the scaling hypothesis for the parameter R, and find agreement. In particular, this work constitutes a test of scaling in R not only for thermodynamic functions but for the two-spin correlation function as well. Table I summarizes our results as well as the predictions of scaling.

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