

## Partial Test of the Universality Hypothesis: The Case of Different Coupling Strengths in Different Lattice Directions\*

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(Received 19 July 1971; revised manuscript received 2 November 1971)

High-temperature series expansions are used to examine the dependence of critical-point exponents upon *lattice anisotropy* (different interaction strengths in different directions in the lattice). The two-spin correlation function  $C_2(\vec{r})$  is calculated to tenth order in  $(1/k_B T)$  for the Ising Hamiltonian

$$\mathcal{H}_{\text{anis}} = -J_{xy} \sum_{\langle ij \rangle}^{xy} S_i^z S_j^z - J_R \sum_{\langle ij \rangle} S_i^z S_j^z$$

for a wide range of anisotropy parameters  $R \equiv J_R/J_{xy}$  and for both the sc and fcc lattices; here the first summation is over all pairs of nearest-neighbor sites whose relative displacement vector  $\vec{r}_{ij}$  has no  $z$  component, while the second summation is over all other pairs of nearest-neighbor sites. Hence for  $R=0$ , both the sc and fcc lattices reduce to the two-dimensional square lattice, while in the limit  $R \rightarrow \infty$ , the sc becomes a one-dimensional linear chain and the fcc becomes two noninteracting three-dimensional bcc lattices. The series for  $C_2(\vec{r})$  are then used to obtain series of corresponding lengths for the specific heat, susceptibility, and second moment. Analysis of these series yields results consistent with the universality hypothesis of critical-point exponents. Specifically, it is found that when lattice anisotropy is introduced, the critical-point exponents studied (the susceptibility exponent  $\gamma$  and the correlation length exponent  $\nu$ ) do not appear to change from their values for an isotropic lattice. The problem of *next-nearest-neighbor interactions* is treated using similar methods in Paper II of this series (and briefly discussed in this paper).

### I. INTRODUCTION

Much recent activity in the field of critical phenomena has focused on characterizing, in terms of critical-point exponents, the properties of thermodynamic and correlation functions near a critical point.<sup>1-3</sup>

Concerning these exponents, one question that has been asked is: "Are there relations between exponents associated with different physical quantities?" Many rigorous inequalities and various non-rigorous scaling hypotheses have been proposed to answer this question.<sup>4-8</sup> These hypotheses lead to the well-known scaling laws which allow one to express any exponent in terms of no more than two other exponents.

An even more fundamental question, however, is: "Upon precisely what features of an interaction Hamiltonian do the individual critical-point exponents depend?" The universality hypothesis has been designed to deal with this second question.<sup>9-11</sup> The universality hypothesis makes predictions concerning when exponents should or should not change as a parameter in the system Hamiltonian is varied.

Aside from its own inherent interest, we are motivated to study the question of universality because many of the heuristic arguments proposed for the validity of the scaling hypotheses are *also* the bases for the universality hypothesis.<sup>10</sup> Thus a failure in some predictions of the universality hypothesis might indicate possible weaknesses in the

justifications usually presented<sup>6,10</sup> for scaling. One must calculate at least *two* exponents in order to test the scaling hypothesis, whereas the universality hypothesis may be tested (partially) if one can calculate a *single* exponent for different values of some parameter in the Hamiltonian.

In this work we apply high-temperature series-expansion techniques in order to test those predictions of the universality hypothesis that deal with the presence of (a) "lattice anisotropy" (i.e., different coupling strengths in different lattice directions), and (b) "further-neighbor interactions." We have treated these two specific problems because of the following reasons (each of which is discussed more fully in later sections).

(i) Exact results consistent with universality exist for two-dimensional models with lattice anisotropy but not for the corresponding three-dimensional models. Since certain of the so-called two-exponent "scaling relations" (which are actually *not* consequences of the homogeneity hypothesis) are believed to hold in two dimensions but not in three,<sup>12</sup> it is important to see if a similar breakdown occurs for the universality predictions.

(ii) Analysis of rather short high-temperature series expansions for a quantum-mechanical Heisenberg model with next-nearest-neighbor interactions indicates an apparent serious violation of the universality hypothesis (next-nearest-neighbor interactions are treated in Paper II of this series).<sup>13</sup> We would like to know whether this violation is real or

due to knowledge of an insufficient number of terms in the series.

(iii) Analyses of high-temperature series for next-nearest-neighbor Ising and classical-Heisenberg models have led various authors to conclude that the universality hypothesis is obeyed (Paper II).<sup>13</sup> We feel that some of this analysis is biased in favor of universality and that more extensive analysis is needed.

(iv) For certain magnetic materials which have further-neighbor interactions or lattice anisotropy, experimental results are at variance with the predictions of high-temperature series expansions for the corresponding models without further neighbors or lattice anisotropy. It is important to determine if this disagreement is due to a breakdown in the universality hypothesis or is due to other reasons (such as the inability of the experimentalist to reach temperatures near enough to the critical temperature to measure the true exponent) (see Sec. IC and Paper II).<sup>13</sup>

In the remainder of Sec. I we define precisely the models that we have considered, state the predictions of universality for these models, and review the relevant research literature. In Sec. II we describe the techniques we have employed to analyze the new high-temperature series expansions we have obtained. Results of this analysis are presented in Sec. III. Our results and conclusions are summarized in Sec. IV. In Paper II we will consider the problem of next-nearest-neighbor interactions.<sup>13</sup>

#### A. Models Treated and Predictions of Universality

A large portion of the models that are of experimental interest can be described by the classical Hamiltonian<sup>14</sup>

$$\mathcal{H} = - \sum_{\vec{r}, \vec{r}'} \sum_{\alpha=1}^D J_{\vec{r}-\vec{r}'}^{\alpha} S_{\vec{r}}^{\alpha} S_{\vec{r}'}^{\alpha}, \quad (1.1)$$

where the vectors  $\vec{r}$ ,  $\vec{r}'$  label sites on a  $d$ -dimensional lattice of  $N$  sites,  $S_{\vec{r}}^{\alpha}$  is the  $\alpha$ th component of a spin vector in a  $D$ -dimensional spin space, and  $J_{\vec{r}-\vec{r}'}^{\alpha}$  denotes an exchange constant. For  $D=1, 2, 3$ , and  $\infty$  the Hamiltonian (1.1) reduces to the Ising, plane rotator, classical-Heisenberg, and spherical models, respectively.<sup>14</sup>

Since current evidence<sup>15</sup> strongly favors the conjecture that the critical-point exponents are independent of spin quantum number  $S$ , we have considered only the *classical* ( $S=\infty$ ) Hamiltonian (1.1). Thus essentially the only parameters upon which critical-point exponents might depend are (i) the lattice dimensionality  $d$ , (ii) the spin-space dimensionality  $D$ , (iii) the "lattice anisotropy" or dependence of  $J_{\vec{r}-\vec{r}'}^{\alpha}$  upon the *direction* of  $\vec{r}-\vec{r}'$ , (iv) the "spin-space anisotropy" or dependence of  $J_{\vec{r}-\vec{r}'}^{\alpha}$  upon  $\alpha$ , and (v) the range of interaction or dependence of  $J_{\vec{r}-\vec{r}'}^{\alpha}$  upon  $|\vec{r}-\vec{r}'|$ .

The universality hypothesis would predict that critical-point exponents depend upon (ii) and (iv) only through the symmetry of the ordered phase, so that one can assign an "effective  $D$ " to an arbitrary anisotropic interaction (as Jasnow and Wortis<sup>16</sup> concluded from high-temperature series expansions). As stated above, it is the purpose of this work to study the possible dependence of critical-point exponents upon (iii), lattice anisotropy, and (v), the range of interaction.

Specifically, we have calculated high-temperature series expansions for the two-spin correlation function  $C_2(\vec{r})$  for two interaction Hamiltonians chosen to test (iii) and (v), respectively,

$$\begin{aligned} \mathcal{H}_{\text{anis}} &= - \sum_{\langle ij \rangle}^{xy} J_{xy} S_i^x S_j^x - \sum_{\langle ij \rangle}^z J_z S_i^z S_j^z \\ &\equiv -J_{xy} \left( \sum_{\langle ij \rangle}^{xy} S_i^x S_j^x + R \sum_{\langle ij \rangle}^z S_i^z S_j^z \right) \end{aligned} \quad (1.2)$$

and

$$\begin{aligned} \mathcal{H}_{\text{nnn}} &= -J_1 \sum_{\langle ij \rangle}^{nn} \vec{S}_i^{(D)} \cdot \vec{S}_j^{(D)} - J_2 \sum_{\langle ij \rangle}^{nnn} \vec{S}_i^{(D)} \vec{S}_j^{(D)} \\ &\equiv -J_1 \left( \sum_{\langle ij \rangle}^{nn} \vec{S}_i^{(D)} \cdot \vec{S}_j^{(D)} + R' \sum_{\langle ij \rangle}^{nnn} \vec{S}_i^{(D)} \cdot \vec{S}_j^{(D)} \right), \end{aligned} \quad (1.3)$$

where  $R \equiv J_z/J_{xy}$  and  $R' \equiv J_2/J_1$ .

In Eq. (1.2), the Ising model, the first summation is over pairs of nearest-neighbor sites whose relative displacement vector  $\vec{r}_{ij}$  has no  $z$  component, while the second summation is over all other pairs of nearest-neighbor sites. We treat the simple cubic (sc) and the face-centered cubic (fcc) lattices. Note that in the limit  $R \rightarrow 0$ , the sc and fcc lattices reduce to noninteracting planes ( $d=2$ ); in the limit  $R \rightarrow \infty$ , the sc lattice reduces to an array of noninteracting chains ( $d=1$ ), and the fcc lattice reduces to two noninteracting bcc lattices ( $d=3$ ).

In Eq. (1.3) we have isotropically interacting  $D$ -dimensional classical spins. The first and second summations are over nearest-neighbor and next-nearest-neighbor pairs of lattice sites. We treat the sc, bcc, and fcc lattices which reduce, respectively, in the limit  $R' \rightarrow \infty$  to two noninteracting fcc, sc, and sc lattices.<sup>13</sup>

For  $\mathcal{H}_{\text{anis}}$  the universality hypothesis predicts that the critical exponents depend on  $J_{xy}$  and  $J_z$  only insofar as these parameters determine the effective dimensionality of the system and the nature of the ordered state.

Consider first the case  $J_{xy} \geq 0$ ,  $J_z \geq 0$ , for which the ordered state is described by a nonzero value of the total magnetization. For finite nonzero values of  $R$  the exponents are predicted to be constant and equal to their  $R=1$  values. At  $R=0$  the exponents are predicted to change *discontinuously* to their values for a two-dimensional system. In the limit  $R \rightarrow \infty$  the exponents for the fcc lattice should main-

tain their three-dimensional values while the exponents for the sc lattice should jump discontinuously to one-dimensional values. Since in one dimension the singularity at  $T_c=0$  is not of the power law type the exponents are not defined in this case [cf. Eq. (3.4)]. The predictions of universality for  $\mathcal{H}_{I\text{anis}}$  are summarized in Fig. 1.

For other combinations of signs of  $J_{xy}$  and  $J_z$  similar predictions hold for the appropriately staggered counterpart of the function whose exponent is being considered. For example, if Fig. 1 refers to predictions for the exponent of the bulk susceptibility then for  $J_{xy} \geq 0$ ,  $J_z \leq 0$  this same figure (with  $R \rightarrow -R$ ) would apply to the exponent for the staggered susceptibility appropriate to a layered antiferromagnetic system described by a net magnetization per spin that alternates in sign along the  $z$  direction.

For  $\mathcal{H}_{\text{nnn}}$  the universality hypothesis predicts that the exponents are completely independent of  $R' \equiv J_2/J_1$  (with of course the same understanding as above that we consider staggered quantities when the signs of  $J_1$  and  $J_2$  are such that the ordered state has an antiferromagnetic structure).

The remainder of the present work is devoted to  $\mathcal{H}_{I\text{anis}}$ ; the Hamiltonian (1.3) will be treated in II.

## B. Previous Work

### 1. Exact Solutions

For the Ising model on a plane square lattice the exponents  $\alpha$  (specific heat),<sup>17</sup>  $\beta$  (spontaneous mag-

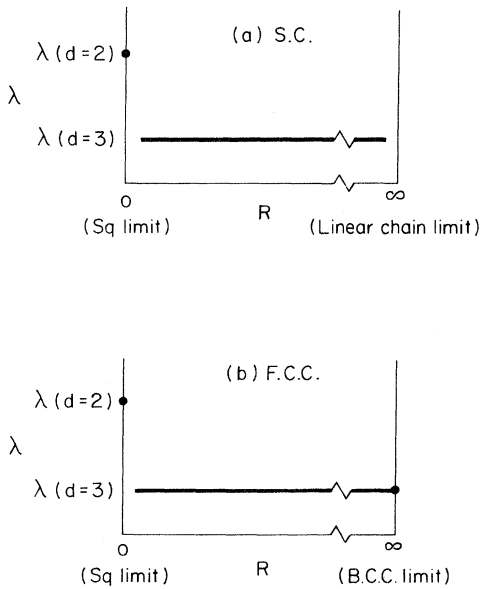


FIG. 1. Predictions of the universality hypothesis for  $\mathcal{H}_{I\text{anis}}$  for (a) sc and (b) fcc lattices. The exponent  $\lambda$  is predicted to change discontinuously at  $R=0$  (sc, fcc) and at  $R=\infty$  (sc).

netization),<sup>18</sup>  $\eta$  (correlation-function decay at  $T=T_c$ ),<sup>19-21</sup>  $\nu$  (correlation length),<sup>1,17,22</sup> and  $\gamma$  (susceptibility)<sup>1,23</sup> are claimed to be independent of the interaction strengths in the  $x$  and  $y$  directions (as long as they are nonzero and finite). This invariance has also been shown to hold for  $\alpha$  on a variety of other planar two-dimensional lattices (lattices with no crossing bonds).<sup>24-33</sup>

The only nontrivial three-dimensional model which is exactly soluble is the spherical model.<sup>34</sup> In Appendix A we show that for this model the exponents  $\gamma$  and  $\nu$  are independent of lattice anisotropy and next-nearest-neighbor interactions.

### 2. Extrapolations from Series Expansions

Of the various theoretical techniques for determining the properties of thermodynamic and correlation functions none has been as successful near the critical point as the method of extrapolation from exact series expansions.<sup>35-42</sup> So far as we know, however, this technique has not until now been applied to the problem of lattice anisotropy.

## C. Relevant Experimental Results

$\text{CrBr}_3$  is an insulating ferromagnet which is well represented by the spin- $\frac{3}{2}$  Heisenberg model with interactions in the  $xy$  plane approximately 17 times stronger than the interactions in the  $z$  direction.<sup>43,44</sup> Recent experiments on  $\text{CrBr}_3$ <sup>45</sup> have indicated that  $\gamma = 1.215 \pm 0.02$  in contrast to the appreciably larger estimates for  $\gamma$  from high-temperature series expansions for the corresponding isotropic model<sup>46</sup> ( $R=1$ ).

In Paper II, after reviewing the results of our analysis, we will discuss a possible reason for this apparent disagreement between theory and experiment.<sup>47</sup>

Recent experiments on the layered antiferromagnet,  $\text{K}_2\text{NiF}_4$  have indicated that it can be described by a nearest-neighbor Heisenberg system with coupling between planes at least 270 times smaller than the intraplanar interactions.<sup>48</sup> Unfortunately we will not have much to say about this interesting system because due to the smallness of  $J_z/J_{xy}$ , much longer high-temperature series than those we have obtained would be necessary to obtain useful information (cf. the discussion in Sec. II F).

## D. Present Work

Using the technique of bond and vertex renormalization,<sup>12</sup> we have calculated the coefficients in the high-temperature series expansion for the two-spin correlation function,

$$C_2(\vec{r}) = \sum_{n=0}^{\infty} g_n(\vec{r}) x^n, \quad (1.4)$$

through order  $g_{10}$  for  $\mathcal{H}_{I\text{anis}}$ . Here  $x \equiv 1/k_B T$ . The coefficients  $g_n(\vec{r})$  were then utilized to calculate

series of corresponding lengths for the reduced zero-field isothermal susceptibility,

$$\bar{\chi}_T \equiv \sum_{\vec{r}} C_2(\vec{r}) \equiv \sum_{n=0}^{\infty} a_n x^n \sim \epsilon^{-\gamma}, \quad (1.5)$$

for the "second moment,"

$$\mu_2 \equiv \sum_{\vec{r}} |\vec{r}|^2 C_2(\vec{r}) \equiv \sum_{n=0}^{\infty} b_n x^n \sim \epsilon^{-(2\nu+\gamma)}, \quad (1.6)$$

and for the reduced zero-field specific heat,

$$\bar{C}_H \equiv -\frac{1}{2} T \frac{\partial}{\partial T} \sum_{\vec{r}} J_{\vec{r}} C_2(\vec{r}) = \sum_{n=0}^{\infty} c_n x^n \sim \epsilon^{-\alpha}, \quad (1.7)$$

where  $\epsilon \equiv (x_c - x)/x_c = (T - T_c)/T_c$  in this work.

The coefficients  $g_n(\vec{r})$  were obtained not in the general form of polynomials in  $R$  but were calculated separately for each value of  $R$  considered. For this purpose we modified a computer program used by Ferer, Moore, and Wortis to treat nearest-neighbor isotropic lattices.<sup>12,49</sup> Rather strong checks on the calculation were made by verifying that in the limits  $R \rightarrow 0$  and  $R \rightarrow \infty$  the computer program generated the series for the corresponding isotropic problem (see Sec. IA).

For purposes of comparison we have also calculated 20 coefficients in the high-temperature series expansions of  $\bar{\chi}_T$  and  $\mu_2$  for the exactly soluble spherical model. These coefficients were generated directly from the exact solution (see Appendices A and B).

To the best of our knowledge the present work is the first treatment of  $\mathcal{H}_{I, \text{anis}}$  using high-temperature series expansions.

The series for  $\bar{\chi}_T$ ,  $\mu_2$ , and  $\bar{C}_H$  may be obtained from NAPS.

## II. TECHNIQUES OF ANALYSIS

It is by now conventional to obtain estimates for critical-point exponents by making extrapolations based upon a finite number of exactly calculated terms, and many ingenious methods have been proposed to render this step possible.<sup>1,3,50</sup> In this Sec. we discuss the methods we have used to provide predictions for  $\gamma$  and  $\nu$ ; where appropriate we note the advantages and disadvantages of these methods. We also briefly consider the problems associated with making estimates for exponents which change discontinuously when a parameter in the Hamiltonian is varied.

In what follows we will consider generally that we know  $N$  terms in the expansion

$$f(x) = \sum_{n=0}^{\infty} a_n x^n, \quad (2.1)$$

where  $f$  is a physical quantity such as the susceptibility or specific heat and  $x \equiv 1/k_B T$ . In addition it is assumed that<sup>51</sup>

$$f(x) \sim (1 - x/x_c)^{-\lambda} \quad (2.2)$$

near  $x = x_c$ , where  $x_c \equiv 1/k_B T_c$  and  $\lambda$  is the critical-point exponent for  $f$ .

### A. Ratio Method

The simplest method and the one first used to obtain exponents from series expansions<sup>52</sup> is the ratio method, which has its theoretical foundation in a theorem of classical analysis by Darboux.<sup>53-55</sup> This theorem states that if

$$f(x) = (1 - x/x_c)^{-\lambda} \phi(x) + \psi(x), \quad (2.3)$$

and  $\phi(x)$  and  $\psi(x)$  are analytic in the disc  $|x| \leq x_c$ , then the asymptotic form of the coefficients in the expansion of  $f(x)$ ,

$$a_n^{\text{asympt}} = a_n (1 + O(1/n)), \quad (2.4)$$

is given by

$$\begin{aligned} a_n^{\text{asympt}} &= \frac{1}{n!} \left. \frac{d^n}{dx^n} \left(1 - \frac{x}{x_c}\right)^{-\lambda} \right|_{x=0} \phi(x_c) \\ &= \frac{\lambda(\lambda+1) \cdots (\lambda+n-1)}{n! x_c^n}. \end{aligned} \quad (2.5)$$

Forming the ratios  $\rho_n$  of successive terms one finds

$$\rho_n \equiv \frac{a_n}{a_{n-1}} = \frac{1}{x_c} + \frac{\lambda-1}{n} \frac{1}{x_c} + O\left(\frac{1}{n^2}\right). \quad (2.6)$$

Thus a plot of  $\rho_n$  versus  $1/n$  should asymptotically approach a straight line with intercept  $x_c^{-1}$  at  $1/n = 0$  and with a slope equal to  $(\lambda-1)/x_c$ . We can thus form a series of estimates for  $1/x_c$ ,

$$\left(\frac{1}{x_c}\right)_n \equiv n\rho_n - (n-1)\rho_{n-1} = \frac{1}{x_c} + O\left(\frac{1}{n^2}\right). \quad (2.7)$$

Once we believe we have an accurate estimate of  $x_c$  we can then obtain a series of estimates for  $\lambda$ :

$$\lambda_n \equiv 1 - n(1 - \rho_n x_c^{\text{est}}). \quad (2.8)$$

It is important to estimate the effect of an error in  $x_c^{\text{est}}$  on the accuracy of the  $\{\lambda_n\}$  obtained from Eq. (2.8). Let

$$x_c^{\text{est}} = x_c + \Delta x_c. \quad (2.9)$$

Using  $\rho_n \sim 1/x_c$ , the error in  $\lambda_n$  due to an error in  $x_c^{\text{est}}$  is found to be<sup>56</sup>

$$(\Delta\lambda)_n \sim n\rho_n \Delta x_c \sim n(\Delta x_c/x_c). \quad (2.10)$$

The result (2.10) is at first sight rather alarming because it says that the error in  $\lambda_n$  increases with the length of the series. However, from (2.7),  $\Delta x_c \sim 1/n^2$  so that as expected we should obtain better estimates for  $\lambda$  with longer series.

The important point is that if we estimate an  $x_c$  we must be careful about extrapolating the series  $\{\lambda_n\}$ . Specifically (2.6) and (2.10) yield

$$\lambda_n \sim \lambda + n(\Delta x_c/x_c) + O(1/n), \quad (2.11)$$

and if the amplitude of the first correction term in (2.11) (due to an error in  $x_c^{\text{est}}$ ) is greater than the amplitude of the second correction term [due to higher-order terms in (2.4)], a spurious trend will be introduced. Forming linear extrapolants we would then find

$$\begin{aligned} \lambda_n^{\text{extrap}} &\equiv n\lambda_n - (n-1)\lambda_{n-1} \\ &= \lambda + (2n-1)\frac{\Delta x_c}{x_c} + O\left(\frac{1}{n}\right), \end{aligned} \quad (2.12)$$

and the estimates for  $\lambda$  would be worse, not better.

Another consideration concerning the convergence of the series is the effect of singularities on the negative real axis. These singularities, which are usually related to the existence of an antiferromagnetic phase transition in the system for which all exchange constants are of sign opposite to those of the system under consideration,<sup>57-59</sup> cause the series (2.7) and (2.8) to oscillate (with decreasing amplitudes as  $n \rightarrow \infty$ ) around their limiting values.

As has been pointed out, these oscillations can be reduced by considering the estimates<sup>59</sup>

$$\left(\frac{1}{x_c}\right)_n^{\text{alt}} \equiv \frac{n\rho_n - (n-2)\rho_{n-2}}{2} \quad \text{for } x_c \quad (2.13)$$

and the extrapolants

$$\lambda_n^{\text{alt}} \equiv \frac{n\lambda_n - (n-2)\lambda_{n-2}}{2} \quad \text{for } \lambda. \quad (2.14)$$

The theoretical basis for (2.13) has been given by Guttman.<sup>60</sup>

There is another method, used by various authors,<sup>61</sup> in which one forms the "ratios"

$$\tilde{\rho}_n \equiv \left(\frac{a_n}{a_{n-2}}\right)^{1/2} \quad (2.15)$$

and then uses (2.7) with  $\rho_n$  replaced by  $\tilde{\rho}_n$ .

In Sec. II E we will discuss a method more effective than those described above for reducing the effect of unphysical singularities.

#### B. Park's Method

Park's<sup>62,63</sup> method is essentially the ratio method applied to a "logarithmic derivative" of the original series to be analyzed. If

$$f(x) \sim (1 - x/x_c)^{-\lambda}, \quad (2.16)$$

then

$$\frac{d \ln f(x)}{d \ln x} \sim \lambda \frac{x}{x_c} \frac{1}{1 - x/x_c} = \lambda \sum_{n=1}^{\infty} \left(\frac{1}{x_c}\right)^n x^n \equiv \sum_{n=1}^{\infty} b_n x^n. \quad (2.17)$$

Therefore we expect

$$x_c = \lim_{n \rightarrow \infty} (x_c)_n \equiv \lim_{n \rightarrow \infty} \frac{b_n}{b_{n+1}} \quad (2.18)$$

and

$$\lambda = \lim_{n \rightarrow \infty} \lambda_n \equiv \lim_{n \rightarrow \infty} \frac{(b_n)^{n+1}}{(b_{n+1})^n}. \quad (2.19)$$

One virtue of (2.18) and (2.19) is that estimates of  $\lambda_n$  are found that are independent of those for  $x_c$  and vice versa. However, the estimates for  $\lambda_n$  seem to converge more slowly than the corresponding estimates from (2.8) with an accurate value of  $x_c$ . On the other hand if  $x_c$  is known accurately we can form

$$\lambda = \lim_{n \rightarrow \infty} \bar{\lambda}_n \equiv \lim_{n \rightarrow \infty} b_n x_c^n \quad (2.20)$$

which may converge more rapidly.

Again we note the error in  $\lambda_n$  due to an error in  $x_c$

$$(\Delta \lambda)_n \cong n \frac{\Delta x_c}{x_c} \lambda, \quad (2.21)$$

is essentially the same as in (2.10) since the exponents we will consider are usually of order unity.

#### C. Padé Approximants

The Padé approximant (PA)  $P_D^N(x)$  to a function  $g(x)$  is defined as

$$P_D^N(x) = \frac{\sum_{n=0}^N p_n x^n}{\sum_{d=0}^D q_d x^d}, \quad (2.22)$$

where the coefficients  $p_n$  and  $q_d$  are determined by requiring that the first  $N+D$  terms in the expansion of  $P_D^N$  in a Taylor series in  $x$  match the corresponding number of coefficients in the expansion of  $g(x)$ .

If  $f(x) \sim (x_c - x)^{-\lambda}$  as in (2.16) and we define

$$g(x) = \frac{d}{dx} \ln f(x) \sim \frac{\lambda}{x_c - x}, \quad (2.23)$$

then the PA's to  $g(x)$  might be expected to have poles at  $x = x_c$  with residues of  $-\lambda$ .

The power of the PA method is that if the function to be analyzed has exactly the form

$$f(x) = \prod_{i=1}^I (x_i - x)^{-\lambda_i}, \quad (2.24)$$

then the PA can represent  $(d/dx) \ln f(x)$  exactly (so long as  $D \geq I$  and  $N \geq I - 1$ ) independent of how well separated the singularities are. Furthermore, because it can represent the function exactly we can determine the physical singularity (i.e., the nearest singularity on the positive real axis) even when there are nonphysical singularities that lie closer to the origin.

In general, however, the function under consideration does not have the form (2.24), in which case very little is known *a priori* about the ability of the PA to represent the function. In fact it is possible that further PA's (obtained by increasing the number of terms in the series) may not give more accurate values for  $x_c$  and  $\lambda$ , but may better approximate the function in regions of the  $x$  plane near singularities other than the one of interest.<sup>1</sup>

Given these problems the method does seem to work. It seems to work best when the singularity of interest factors, although it need not be the closest singularity to the origin, i. e., for functions of the form

$$f(x) = (x_c - x)^{-\lambda} \phi(x), \quad (2.25)$$

where  $\phi(x)$  is not necessarily analytic for  $|x| \leq |x_c|$  [cf. Eq. (2.3)].

In cases where PA's are unreliable for estimating exponents the PA's are still extremely valuable in determining the general positions of singularities so that the series may be intelligently analyzed using other methods.

#### D. Forming Series with $x_c=1$ (" $T_c$ Renormalization")

As seen earlier a small error in the estimate of  $x_c$  can lead to significant errors in the estimates for the critical exponents. We now describe a method which circumvents this problem by forming a new series which has critical point  $x_c = 1$ .<sup>12,16,22,49</sup>

Consider two series

$$f(x) = \sum_{n=0}^{\infty} a_n x^n, \quad (2.26)$$

$$g(x) = \sum_{n=0}^{\infty} b_n x^n \quad (2.27)$$

for two quantities  $f(x)$  and  $g(x)$  which both have a singularity at  $x = x_c$ ,

$$f(x) \sim (1 - x/x_c)^{-\lambda_1}, \quad (2.28)$$

$$g(x) \sim (1 - x/x_c)^{-\lambda_2}. \quad (2.29)$$

Then

$$a_n \sim \lambda_1(\lambda_1 + 1) \cdots (\lambda_1 + n - 1) / x_c^n n! \sim n^{\lambda_1 - 1} / x_c^n \Gamma(\lambda_1) \quad (2.30)$$

and

$$b_n \sim \lambda_2(\lambda_2 + 1) \cdots (\lambda_2 + n - 1) / x_c^n n! \sim n^{\lambda_2 - 1} / x_c^n \Gamma(\lambda_2). \quad (2.31)$$

Now form the generating function

$$h(x) \equiv \sum_{n=0}^{\infty} c_n x^n, \quad (2.32)$$

with

$$c_n \equiv a_n / b_n \sim n^{\lambda_1 - \lambda_2}. \quad (2.33)$$

By Appell's comparison theorem<sup>64</sup> we then have

$$h(x) \sim (1 - x)^{1 + \lambda_1 - \lambda_2}. \quad (2.34)$$

Thus we have obtained a series [Eq. (2.32)] with known critical point  $x_c = 1$ . We can now apply any of the methods described above to the new series for  $h(x)$ . Of course this technique is of value only if one of the exponents  $\lambda_1$ ,  $\lambda_2$  are known, or if the quantity  $\lambda_1 - \lambda_2$  is of interest. Later we will see cases when both of these statements apply.

#### E. Transformation Techniques

In many cases convergence of a series is slowed by the presence of singularities close to the physical singularity.<sup>46,50,65-70</sup> In other cases, the physical singularity is not closest to the origin so that we cannot find  $x_c$  or  $\lambda$  from the ratio method or Park's method—two methods which we would like to use because convergence theorems exist for them. It would thus be helpful if we could obtain a new series with the same exponent for which the singularities are more favorably located.

In order to achieve this we consider a new series

$$g(y) = f(x(y)) = \sum_{n=0}^N b_n y^n, \quad (2.35)$$

where

$$x(y) = \frac{y}{1 - by}, \quad y(x) = \frac{x}{1 + bx}. \quad (2.36)$$

Note that any singularity near  $x = -1/b$  will be transformed away from the origin and will have a reduced effect on the asymptotic behavior of the new series.

If  $f(x) \sim (x_c - x)^{-\lambda}$  then

$$g(y) \sim \left( \frac{y_c}{1 - by_c} - \frac{y}{1 - by} \right)^{-\lambda} \\ = \text{const} (y - y_c)^{-\lambda} \left( \frac{1}{b} - y \right)^{\lambda}, \quad (2.37)$$

with  $y_c = x_c / (1 + bx_c)$ . We note that in addition to the physical singularity at  $y = y_c$  we have introduced a spurious singularity at  $y = 1/b$  (cf. Fig. 2). However, the position of this singularity is known exactly and we can reduce its effect by considering

$$h(y) \equiv \left( \frac{1}{b} - y \right)^{-\lambda^{\text{est}}} f(x(y)), \quad (2.38)$$

where  $\lambda^{\text{est}}$  is an estimated value for  $\lambda$ . Estimating a value  $\lambda$  in no way prejudices the results of the calculation but merely determines how quickly the series will converge.

The transformation (2.36) is only one of many possible transformations that can be used. The only important restrictions on the transformation are that (i) the transformed function have a singularity with either the same exponent or one that is simply related to that of the original series and (ii) that  $c_0 = 0$ , where

$$y = \sum_n c_n x^n. \quad (2.39)$$

The second condition assures that we can find  $g(y)$  to order  $N$  in  $y$ , given  $f(x)$  to order  $N$  in  $x$ .

Once the transformed series is obtained it can then be treated with any of the methods described above. The various combinations of techniques that can be used are shown in Fig. 3.

We will make extensive use of the transformation (2.36) to reduce the effect of the antiferro-

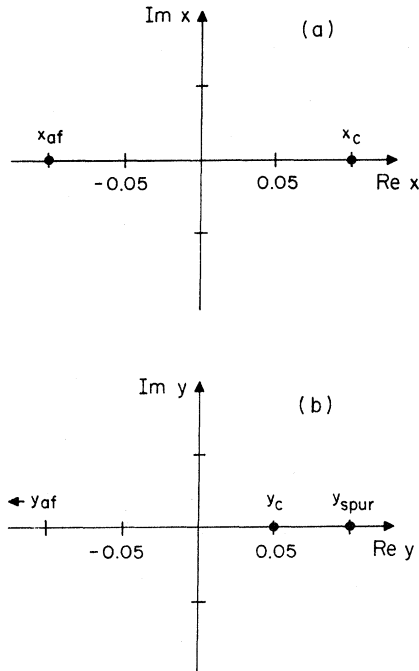


FIG. 2. Example of transformation method ( $x_c = -x_{af} = 1$ ). If the transformation (2.36) with  $b=1$  is applied to a function with physical singularity at  $x=x_c=1$  and an antiferromagnetic singularity at  $x=x_{af}=-1$  as shown in (a), the transformed function has the analytic structure indicated in (b). In (b) the antiferromagnetic singularity in the transformed plane ( $y$  plane) is now at  $y=y_{af}=\infty$  while a spurious singularity has been introduced at  $y=y_{spur}=1$ . The effect of the spurious singularity can be reduced by using Eq. (2.38).

magnetic singularity discussed in Sec. IIA.

F. Analysis of Series Expansions which Depend on a Parameter

An important question we must ask is: "Over what range of the parameter  $R$  can we expect to get reliable information about  $x_c$  and  $\lambda$ ?" Although we will not be able to answer this question exactly—we would need an expression for the form of the function  $f(x)$ —some elementary considerations give an idea of what might be expected in general.

Because the coefficients of the series we obtain are polynomials in  $R$  (or  $1/R$ ), the finite series for  $f(x)$  will be little changed from the  $R=0$  ( $R=\infty$ ) series when  $R$  is very small (very large). For these values of  $R$  it will thus be unreasonable to expect to get accurate predictions for  $\lambda$  if the exponent changes discontinuously at  $R=0$  (sc and fcc) and  $R=\infty$  (sc).<sup>71</sup>

More specifically consider the *model* function

$$f(x) = \epsilon^{-a}(RA + \epsilon^b), \tag{2.40}$$

where  $a, b > 0$ , and  $\epsilon \equiv [x_c(R) - x]/x_c(R)$ , with  $x_c(R)$  a continuous function of  $R$ . For (2.40)

$$\lambda \equiv -\lim_{\epsilon \rightarrow 0} \frac{\ln f(x)}{\ln \epsilon} = \begin{cases} a, & R \neq 0 \\ a - b \equiv c, & R = 0 \end{cases} \tag{2.41}$$

so that  $\lambda$  changes discontinuously at  $R=0$ , a property that the true  $f(x)$  should have if universality holds. Asymptotically the coefficients of the expansion for (2.40) are

$$a_n \sim \frac{AR a(a+1) \cdots (a+n-1)}{x_c^n(R) n!} + \frac{c(c+1) \cdots (c+n-1)}{x_c^n(R) n!} \\ \sim \frac{AR n^{a-1}}{x_c^n(R) \Gamma(a)} + \frac{n^{c-1}}{x_c^n(R) \Gamma(c)}. \tag{2.42}$$

In order to see the true asymptotic behavior of the series we must have the first term of (2.42) much greater than the second, which implies

$$n \gg \left[ \frac{\Gamma(a)}{\Gamma(c)A} \frac{1}{R} \right]^{1/b}. \tag{2.43}$$

Thus as  $R$  decreases we need an increasing number of coefficients to determine  $\lambda$  correctly. For example if  $b=1$  we need *ten* times as many coefficients for  $R=0.1$  as for  $R=1.0$ .

Although (2.40) is only a model function and it is possible that conditions more favorable than (2.43) will hold in reality, the above considerations do show the problems involved in analyzing series for functions that have exponents that change discontinuously when a parameter is varied.

In practice it will be necessary to have a criterion for determining for what values of  $R$  the techniques of series analysis we use will be valid and thus yield reliable results. The idea which first comes to mind is that if a number of different methods each yields consistent results which are in agreement with one another, then there is a good chance that the result

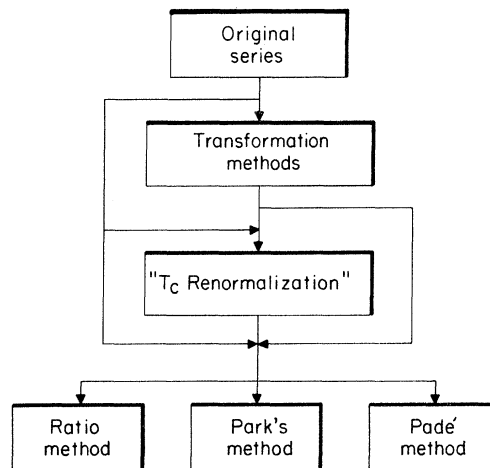


FIG. 3. Various combinations of methods that we have used to analyze series expansions.

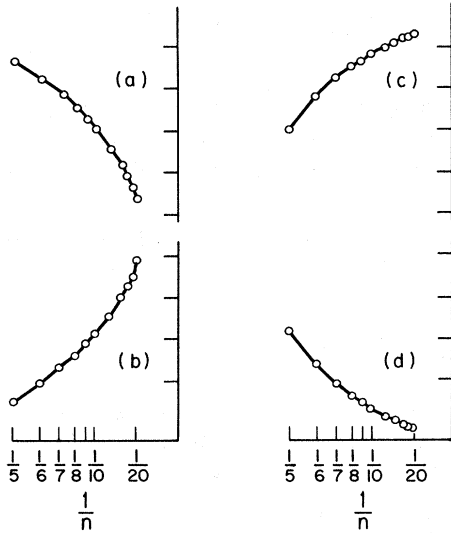


FIG. 4.  $(x_c)_n$  vs  $1/n$ . In (a) and (b) the series  $(x_c)_n$  and the extrapolants either both increase or both decrease, indicating nonasymptotic behavior. In (c) and (d) the series  $(x_c)_n$  indicate possible asymptotic behavior. This test, described in Sec. II of the text, is thus a "necessary but not sufficient" condition for asymptotic behavior.

will be reliable. We will see, however, that there are a number of cases when there is consistency but the results should *not* be believed.

If the results obtained from series analysis are to be valid we must have enough terms so that the series has settled down to its asymptotic behavior. That is, we must have some coefficients  $a_n$  for  $n > m$ , where a lower bound on  $m$  is given [cf. Eq. (2.7)] by

$$(x_c)_n = x_c [1 + O(1/n^2)], \quad n > m. \quad (2.44)$$

In other words, if the series has settled down to its true asymptotic behavior, corrections to  $(x_c)_n$  are of order  $1/n^2$  or smaller. (Note that the converse is not necessarily true.) We can easily test to see if (2.43) holds by forming the linear extrapolants

$$(x_c^{\text{extrap}})_n = n(x_c)_n - (n-1)(x_c)_{n-1}. \quad (2.45)$$

Assume first that

$$(x_c)_n = x_c \pm C/n^q, \quad (2.46)$$

where  $C$  and  $q$  are constants. Then

$$\begin{aligned} (x_c^{\text{extrap}})_n &= x_c \pm C \left[ \frac{1}{n^{q-1}} - \frac{1}{(n-1)^{q-1}} \right] \\ &\equiv x_c + (\Delta x_c^{\text{extrap}})_n. \end{aligned} \quad (2.47)$$

Thus we have

$$(\Delta x_c^{\text{extrap}})_n = \begin{cases} 0, & q = 1 \\ \geq 0, & q < 1 \\ \leq 0, & q > 1 \end{cases} \quad (2.48)$$

where the upper and lower direction in the inequalities correspond to the  $\pm$  in (2.46).

From (2.48) we then have the following "rule": If the estimates (2.44) and (2.45) for  $(x_c)_n$  and  $(x_c^{\text{extrap}})_n$ , respectively, are either both increasing or decreasing or if the estimates (2.48) are constant, then the series has not yet settled down to its asymptotic behavior. This is illustrated graphically in Fig. 4.

### III. ANALYSIS OF SERIES

#### A. Padé Approximants

In order first to obtain an idea of the analytic structure of the functions being considered we calculated PA's to  $(d/dx) \ln \bar{\chi}(x)$ ,  $(d/dx) \ln [x^{-1} \mu_2(x) / \bar{\chi}(x)]$ , and  $(d/dx) \ln [\mu_2(x) / x]$ . The constant term in the expansion of  $\mu_2(x)$  vanishes, implying a zero in  $\mu_2(x)$  and thus a pole in  $(d/dx) \ln \mu_2(x)$  [and  $(d/dx) \ln \mu_2(x) / \bar{\chi}(x)$ ] at  $x=0$ . Because we are not interested in the behavior at  $x=0$ , we have considered the logarithmic derivatives of the *reduced* functions  $x^{-1} \mu_2(x)$  and  $x^{-1} \mu_2(x) / \bar{\chi}(x)$  indicated above. These logarithmic derivatives will be analytic at  $x=0$ .

For the range of  $R$  we have considered ( $0.01 \lesssim R \lesssim 100$ ) (sc),  $0.01 \lesssim R$  (fcc), the PA's consistently indicated that the singularity nearest to the origin is on the positive real axis (the ferromagnetic singularity at  $x = x_c$ ). The only other singularity, the presence of which was consistently indicated by the PA's, is on the negative real axis (the antiferromagnetic singularity at  $x = x_{\text{af}}$ ). For the sc lattice, the zero-field free energy  $G(T, H=0, J_{xy}, J_z)$  has the symmetry property

$$G(T, H=0, J_{xy}, J_z) = G(T, H=0, -J_{xy}, -J_z), \quad (3.1)$$

indicating that  $x_{\text{af}} = -x_c$ . However, for all  $R$  (sc) the PA's consistently indicated  $x_{\text{af}}$  slightly greater than  $x_c$ . This slight disagreement may be due to the fact that the singularity at  $x = x_{\text{af}}$  is believed not to factor,<sup>57,58</sup> and is thus less amenable to PA analysis than the singularity at  $x_c$ .<sup>1,50</sup> For the fcc lattice, Eq. (3.1) holds only in the limits  $R=0$  (square) and  $R=\infty$  (bcc) while at  $R=1$  it is believed that  $x_{\text{af}}(R) = \infty$  (i. e., the nonexistence of an antiferromagnetic transition).<sup>72-74</sup> We thus expect that  $x_c(R)/x_{\text{af}}(R)$  increases monotonically from 0 at  $R=1$  to 1 at  $R=0$  ( $R=\infty$ ). This behavior was confirmed by the PA's although it became increasingly difficult to estimate  $x_{\text{af}}$  as  $R$  approached 1.

Selected results of the PA analysis for the exponents  $\gamma$  and  $2\nu$  are presented in Tables I-IV. From these results we might conclude

$$\gamma \simeq 1.25, \quad 2\nu \simeq 1.30 \quad (3.2)$$

for  $0.2 \lesssim R \lesssim 5$  (sc) and

$$\gamma \simeq 1.25, \quad 2\nu \simeq 1.28 \quad (3.3)$$

for  $0.08 \lesssim R$  (fcc). The currently accepted values



TABLE I. Estimates (in units of  $10^{-2}$ ) for the critical-point exponent  $\gamma$  from PA's to  $(d/dx)\ln\bar{\chi}(x)$  for the sc Ising model for various values of the parameter  $R$ . Here and in all PA tables which follow, the notation "0" indicates that either the closest singularity to the origin was not on the positive real axis or that there were two singularities on the positive real axis very close to each other making determination of an estimate of the exponent difficult. For  $0.2 \lesssim R \lesssim 5$  the PA tables show good consistency and indicate  $\gamma(R) \cong \gamma(R=1) \cong 1.25$ . For other values of  $R$  the tables are in general less consistent, especially for  $R \gg 1$ .

$\gamma$ : Ising, sc, $R=0.01$								$\gamma$ : Ising, sc, $R=0.05$							
$N$	1	2	3	4	5	6	7	$N$	1	2	3	4	5	6	7
(a)	$D$							(b)	$D$						
	2	158	187	156	150	160	171		2	152	167	138	131	135	137
	3	196	172	147	154	149	164		3	170	157	127	134	138	135
	4	144	157	160	165	158			4	133	138	137	136	134	
	5	177	161	0	161				5	141	137	133	139		
	6	186	166	163					6	125	136	137			
	7	165	152						7	135	131				
	8	160							8	133					
$\gamma$ : Ising, sc, $R=0.10$								$\gamma$ : Ising, sc, $R=0.20$							
$N$	1	2	3	4	5	6	7	$N$	1	2	3	4	5	6	7
(c)	$D$							(d)	$D$						
	2	145	152	129	123	236	127		2	137	138	123	120	124	124
	3	153	147	120	125	127	126		3	138	137	119	122	124	131
	4	127	128	128	126	126			4	123	122	125	124	125	
	5	128	128	128	90				5	122	123	124	124		
	6	128	128	127					6	125	124	124			
	7	127	112						7	124	124				
	8	123							8	124					
$\gamma$ : Ising, sc, $R=0.40$								$\gamma$ : Ising, sc, $R=0.60$							
$N$	1	2	3	4	5	6	7	$N$	1	2	3	4	5	6	7
(e)	$D$							(f)	$D$						
	2	129	127	123	123	125	125		2	126	125	124	126	126	125
	3	127	129	123	123	125	125		3	125	124	124	126	126	125
	4	124	123	125	124	126			4	124	125	125	125	125	
	5	123	124	125	125				5	126	126	125	125		
	6	125	125	126					6	126	126	125			
	7	125	125						7	125	125				
	8	125							8	125					
$\gamma$ : Ising, sc, $R=0.80$								$\gamma$ : Ising, sc, $R=1.00$							
$N$	1	2	3	4	5	6	7	$N$	1	2	3	4	5	6	7
(g)	$D$							(h)	$D$						
	2	125	124	125	127	126	125		2	125	124	125	127	126	124
	3	124	124	123	126	100	125		3	124	124	124	126	118	125
	4	125	123	125	125	125			4	125	123	125	126	125	
	5	127	126	125	125				5	127	126	126	125		
	6	126	102	125					6	126	118	125			
	7	125	125						7	124	125				
	8	125							8	125					
$\gamma$ : Ising, sc, $R=1.25$								$\gamma$ : Ising, sc, $R=5/3$							
$N$	1	2	3	4	5	6	7	$N$	1	2	3	4	5	6	7
(i)	$D$							(j)	$D$						
	2	125	124	125	127	126	125		2	126	124	124	126	126	125
	3	124	124	123	126	101	125		3	124	124	123	126	126	125
	4	125	123	125	125	125			4	124	123	125	125	125	
	5	127	126	125	125				5	126	126	125	125		
	6	126	102	125					6	126	126	125			
	7	125	125						7	125	125				
	8	125							8	125					

TABLE I. (Continued)

$\gamma$ : Ising, sc, $R=2.50$								$\gamma$ : Ising, sc, $R=5.00$							
$N$	1	2	3	4	5	6	7	$N$	1	2	3	4	5	6	7
(k)	$D$							(l)	$D$						
	2	126	123	124	124	126	126		2	123	118	127	125	123	126
	3	123	124	124	124	127	126		3	119	121	125	121	124	128
	4	124	124	124	0	125			4	122	128	124	124	125	
	5	124	124	0	125				5	125	125	125	124		
	6	126	127	125					6	124	125	125			
	7	126	126						7	125	123				
	8	126							8	127					
$\gamma$ : Ising, sc, $R=10.00$								$\gamma$ : Ising, sc, $R=50.00$							
$N$	1	2	3	4	5	6	7	$N$	1	2	3	4	5	6	7
(m)	$D$							(n)	$D$						
	2	108	112	131	134	119	122		2	48	0	0	157	147	132
	3	111	107	134	131	121	118		3	80	0	0	149	166	143
	4	111	118	125	124	124			4	104	111	137	133	17	
	5	129	127	124	124				5	103	101	133	138		
	6	127	130	124					6	101	104	123			
	7	123	122						7	141	143				
	8	122							8	142					
$\gamma$ : Ising, sc, $R=100.00$															
$N$	1	2	3	4	5	6	7								
(o)	$D$														
	2	28	0	0	152	161	117								
	3	61	0	0	188	164	179								
	4	95	105	165	139	26									
	5	100	91	145	200										
	6	102	109	126											
	7	168	0												
	8	0													

are  $\gamma(R=1) \cong 1.25$ ,  $2\nu(R=1) \cong 1.28$  for all cubic lattices. Although one can always question whether the PA's are converging, we feel that the apparent invariance of  $\gamma$  and  $\nu$  over the range of  $R$  indicated above is significant. It would be hard to understand why the PA estimates should "lock in" on the  $\gamma(R=1)$  values if the series were *not* asymptotic, especially since the PA method is believed to work for  $R=1$ .

For  $R$  outside the range where  $\gamma$  and  $\nu$  appear constant, the residues of the PA's become less consistent in general, although there are values of  $R$  for which one might attempt to estimate  $\gamma$  and  $\nu$ . For example from Tables I(a) and III(a), we *might* conclude  $\gamma_{sc}(R=0.01) \sim 1.6$ ,  $\gamma_{fcc}(R=0.01) \sim 1.4$ . However, below we will show that for  $R \leq 0.2$ ,  $\geq 5$  (sc),  $\leq 0.08$  (fcc) we probably do not have enough coefficients in the series to see true asymptotic behavior.

The increasing number of coefficients it takes to see asymptotic behavior is illustrated by the PA's for the spherical model for which  $\gamma_{\text{exact}} = 2$  for all finite  $R$ . While the residues of the PA's to  $(d/dx) \ln \bar{\chi}(x)$  converge rather rapidly for  $R=1$ , it takes considerably more terms to see asymptotic be-

havior for  $R=0.2$  (cf. Table V). Exactly the same behavior will be true of the estimates for  $2\nu$  (cf. Appendix A).

#### B. Park's Method and " $T_c$ Renormalization"

In order to determine trends in our series we used Park's method for which convergence theorems exist<sup>50</sup> (as opposed to PA's), and for which we do not have to choose a value of  $x_c$  (as opposed to the ratio method).

Application of Park's method directly to the series for  $\bar{\chi}$ ,  $\mu_2$ , or  $\mu_2/\bar{\chi}$  is not useful because the antiferromagnetic singularity [for all  $R$  except  $R \approx 1$  (fcc)] causes the series to oscillate [cf. Fig. 5(a)]. While the amplitude of these oscillations should decrease as  $n \rightarrow \infty$ , as illustrated by the spherical model estimates, Fig. 5(b), our series for  $\mathcal{K}_t$  ant's (Ising) are not long enough to yield accurate estimates using Park's method on the original series.

We can obtain useful results with Park's method if we first eliminate the effects of the antiferromagnetic singularity by using the transformation, Eq. (2.36), with  $1/b = |x_{\text{af}}^{\text{est}}|$ , where  $x_{\text{af}}^{\text{est}}$  is an estimated value for  $x_{\text{af}}$ . For the sc lattice, accurate

TABLE II. Estimates (in units of  $10^{-2}$ ) for the critical-point exponent  $2\nu$  from PA's to  $(d/dx)\ln[x^{-1}\mu_2(x)/\bar{\chi}(x)]$  for the sc Ising lattice for various values of the parameter  $R$ . For  $0.2 \lesssim R \lesssim 5$  the PA tables show good consistency and indicate  $2\nu(R) \cong 2\nu(R=1) \cong 1.30$ .

2ν: Ising, sc, R=0.01							2ν: Ising, sc, R=0.05								
	N	1	2	3	4	5	6		N	1	2	3	4	5	6
(a)	D							(b)	D						
	2	161	197	183	184	185	188		2	155	174	159	170	156	153
	3	213	190	184	183	187			3	179	168	110	154	139	
	4	12	186	189	188				4	115	154	162	146		
	5	181	199	188					5	151	184	156			
	6	171	184						6	154	154				
	7	188							7	154					
2ν: Ising, sc, R=0.10							2ν: Ising, sc, R=0.20								
	N	1	2	3	4	5	6		N	1	2	3	4	5	6
(c)	D							(d)	D						
	2	149	159	148	148	141	138		2	141	151	139	135	133	131
	3	160	154	20	140	100			3	143	142	145	132	102	
	4	140	118	148	130				4	138	146	139	129		
	5	104	137	139					5	136	132	131			
	6	142	138						6	133	130				
	7	140							7	132					
2ν: Ising, sc, R=0.40							2ν: Ising, sc, R=0.60								
	N	1	2	3	4	5	6		N	1	2	3	4	5	6
(e)	D							(f)	D						
	2	132	132	132	130	130	130		2	129	128	130	130	130	130
	3	132	132	132	130	130			3	128	129	130	130	130	
	4	132	132	132	130				4	130	130	130	130		
	5	130	130	130					5	130	130	130			
	6	130	124						6	130	130				
	7	130							7	130					
2ν: Ising, sc, R=0.80							2ν: Ising, sc, R=1.00								
	N	1	2	3	4	5	6		N	1	2	3	4	5	6
(g)	D							(h)	D						
	2	127	127	129	130	130	130		2	127	127	129	130	130	130
	3	127	127	130	131	130			3	127	127	130	130	130	
	4	130	130	130	130				4	129	130	130	130		
	5	129	130	130					5	130	130	130			
	6	130	130						6	130	130				
	7	130							7	130					
2ν: Ising, sc, R=1.25							2ν: Ising, sc, R=5/3								
	N	1	2	3	4	5	6		N	1	2	3	4	5	6
(i)	D							(j)	D						
	2	127	127	129	130	130	130		2	129	128	130	130	130	130
	3	127	127	130	131	130			3	128	129	130	130	130	
	4	129	130	130	130				4	130	130	130	130		
	5	130	130	130					5	130	130	130			
	6	130	130						6	130	130				
	7	130							7	130					
2ν: Ising, sc, R=2.50							2ν: Ising, sc, R=5.00								
	N	1	2	3	4	5	6		N	1	2	3	4	5	6
(k)	D							(l)	D						
	2	133	131	131	129	130	130		2	140	147	132	130	130	131
	3	131	131	131	130	131			3	151	127	128	130	129	
	4	131	131	130	130				4	133	128	126	131		
	5	130	130	130					5	132	130	131			
	6	130	136						6	130	131				
	7	130							7	131					

TABLE II. (Continued)

2ν: Ising, sc, R=10.00							2ν: Ising, sc, R=50.00								
	N	1	2	3	4	5	6	N	1	2	3	4	5	6	
(m)	D							(n)	D						
	2	208	105	125	129	131	132		2	0	0	15	0	76	0
	3	124	141	128	0	132			3	114	197	140	124	129	
	4	136	132	131	131				4	165	161	116	128		
	5	137	131	132					5	162	165	132			
	6	133	130						6	186	149				
	7	132							7	136					
2ν: Ising, sc, R=100.00															
	N	1	2	3	4	5	6								
(o)	D														
	2	0	0	136	0	0	0								
	3	107	264	164	108	117									
	4	181	200	345	115										
	5	212	186	132											
	6	391	164												
	7	137													

estimates for  $x_{\text{af}}^{\text{est}}$  followed from  $|x_{\text{af}}^{\text{est}}| = x_c^{\text{est}}$ , where the  $x_c^{\text{est}}$  were obtained from the PA analysis. For the fcc lattice adequate, but slightly less accurate, estimates of  $x_{\text{af}}^{\text{est}}$  were obtained directly from the positions of the antiferromagnetic singularities as indicated by the PA's.

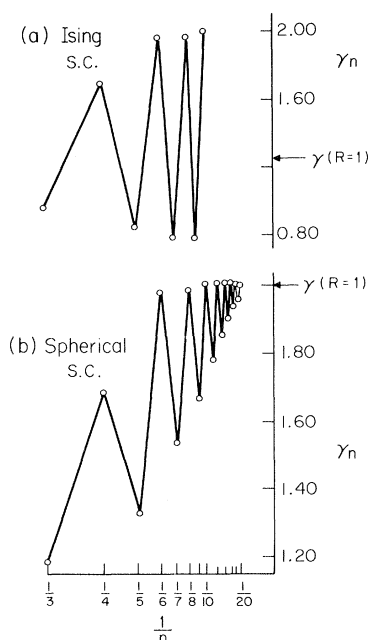


FIG. 5. Park's-method estimates for  $\gamma$  for the (a) Ising model and (b) spherical model on the sc lattice. The presence of the antiferromagnetic singularity at  $x = x_{\text{af}}$  causes the estimates  $\gamma_n$  to oscillate. Although the Ising model estimates do not appear to be converging, the estimates for the spherical model, for which we have longer series, are clearly converging to  $\gamma_{\text{exact}} = 2$ .

The estimates for  $\gamma$  and  $2\nu$  obtained by applying Park's method to the transformed series are shown in Figs. 6–9. For  $R < 1$  the behavior of the estimates  $\{\gamma_n\}$  are quite similar for the sc and fcc lattices. For  $R \ll 1$ , extrapolation of the first few estimates for  $\gamma$  would indicate a two-dimensional ( $\sim 1.75$ ) value for the exponent. Later terms, however, “bend over” and extrapolation of these estimates would indicate possible  $d=3$  behavior. Similar observations hold for the estimates  $\{2\nu_n\}$  except here it would appear that for a given  $R$  more terms are needed to see asymptotic behavior than for the  $\{\gamma_n\}$ . When  $R > 1$  the estimates  $\{\gamma_n\}$ ,  $\{2\nu_n\}$  for the fcc lattice continue to indicate  $d=3$  exponents with the same consistency as for  $R=1$ , while for the sc lattice there is considerable curvature toward the  $R=1$  values.

We have also applied the “ $T_c$  renormalization” method to the transformed series and used then Park's method with  $x_c = 1$  [cf. Eq. (2.20)]. Although one might expect faster convergence because  $x_c$  is now known, the estimates  $\{2\nu_n\}$  are not qualitatively different from those obtained by using Park's method on the transformed series (cf. Figs. 10 and 11).

It is interesting to compare the results of the above analysis using Park's method with those for the spherical model. Comparing Figs. 6 and 12 we see that for a given  $R$  the estimates  $\{\gamma_n\}$  are more erratic for the spherical model than for the Ising model. For  $R \ll 1$  this may be due to the fact that the  $d=2$  Ising model displays a phase transition while the  $d=2$  spherical model does not (although it does have a singularity at  $T=0$ ). For  $R \gg 1$  there is also no reason to expect a similarity between  $\{\gamma_n\}_{\text{Ising}}$  and  $\{\gamma_n\}_{\text{spherical}}$  because the expres-

TABLE III. Estimates (in units of  $10^{-2}$ ) for the critical-point exponent  $\gamma$  from PA's to  $(d/dx)\ln\bar{\chi}(x)$  for the fcc Ising model for various values of the parameter  $R$ . For  $0.08 \lesssim R$  the estimates are consistent and indicate  $\gamma(R) \cong \gamma(R=1) \cong 1.25$ .

$\gamma$ : Ising, fcc, $R=0.01$								$\gamma$ : Ising, fcc, $R=0.02$									
	$N$	1	2	3	4	5	6	7		$N$	1	2	3	4	5	6	7
(a)	$D$								(b)	$D$							
	2	153	171	141	134	138	141	130		2	147	157	131	125	128	130	123
	3	175	160	131	137	145	139			3	159	150	123	127	132	128	
	4	134	141	140	140	138				4	128	131	130	129	128		
	5	147	140	140	140					5	133	130	129	130			
	6	167	140	140						6	97	129	130				
	7	139	130							7	129	125					
	8	136								8	127						
$\gamma$ : Ising, fcc, $R=0.04$								$\gamma$ : Ising, fcc, $R=0.08$									
	$N$	1	2	3	4	5	6	7		$N$	1	2	3	4	5	6	7
(c)	$D$								(d)	$D$							
	2	139	142	123	121	123	125	123		2	130	131	121	122	124	126	125
	3	142	140	120	122	128	124			3	131	130	122	121	127	125	
	4	122	124	124	125	124				4	121	123	124	125	124		
	5	125	124	124	124					5	124	125	132	125			
	6	123	124	124						6	124	123	125				
	7	124	124							7	140	125					
	8	124								8	125						
$\gamma$ : Ising, fcc, $R=0.20$								$\gamma$ : Ising, fcc, $R=0.60$									
	$N$	1	2	3	4	5	6	7		$N$	1	2	3	4	5	6	7
(e)	$D$								(f)	$D$							
	2	123	126	125	125	125	125	125		2	122	126	125	125	125	125	125
	3	126	125	125	126	125	125			3	126	125	122	125	125	125	
	4	124	125	125	125	125				4	125	124	125	125	125		
	5	125	125	125	125					5	125	125	125	125			
	6	125	125	125						6	125	125	125				
	7	125	125							7	125	125					
	8	124								8	125						
$\gamma$ : Ising, fcc, $R=1.00$								$\gamma$ : Ising, fcc, $R=\frac{5}{3}$									
	$N$	1	2	3	4	5	6	7		$N$	1	2	3	4	5	6	7
(g)	$D$								(h)	$D$							
	2	126	126	126	124	125	125	125		2	121	126	125	125	125	125	125
	3	126	126	125	125	125	125			3	126	125	118	124	125	125	
	4	126	125	125	124	125				4	125	119	125	125	125		
	5	124	125	125	125					5	125	125	125	125			
	6	125	125	125						6	125	125	125				
	7	125	125							7	125	130					
	8	125								8	125						
$\gamma$ : Ising, fcc, $R=5.00$								$\gamma$ : Ising, fcc, $R=100.00$									
	$N$	1	2	3	4	5	6	7		$N$	1	2	3	4	5	6	7
(i)	$D$								(j)	$D$							
	2	122	126	126	125	125	125	125		2	121	126	126	125	125	125	125
	3	126	126	121	125	125	125			3	127	126	126	125	125	125	
	4	125	124	125	125	124				4	126	119	125	124	125		
	5	125	125	125	125					5	125	125	125	125			
	6	125	125	125						6	125	125	125				
	7	125	125							7	125	125					
	8	125								8	125						

TABLE IV. Estimates (in units of  $10^{-2}$ ) for the critical-point exponent  $2\nu$  from PA's to  $(d/dx)\ln[\chi^{-1}\mu_2(x)/\bar{\chi}(x)]$  for the fcc Ising lattice for various values of the parameter  $R$ . For  $0.08 \lesssim R$  the estimates are consistent and indicate  $2\nu(R) \cong 2\nu(R=1) \cong 1.28$ . Although the cause for the apparent 2% difference in the PA estimates for  $2\nu$  between the sc and fcc lattices is not clear, the difference is probably spurious because it does not appear when other techniques of analysis are used.

$2\nu$ : Ising, fcc, $R=0.01$							$2\nu$ : Ising, fcc, $R=0.02$							
	$N$	1	2	3	4	5	6	$N$	1	2	3	4	5	6
(a)	$D$							(b)	$D$					
	2	156	179	161	126	161	159	2	151	164	148	156	145	143
	3	185	172	146	159	154		3	166	159	125	143	131	
	4	81	162	166	155			4	120	145	150	137		
	5	158	170	162				5	143	156	146			
	6	158	159					6	145	144				
	7	159						7	144					
$2\nu$ : Ising, fcc, $R=0.04$							$2\nu$ : Ising, fcc, $R=0.08$							
	$N$	1	2	3	4	5	6	$N$	1	2	3	4	5	6
(c)	$D$							(d)	$D$					
	2	143	148	138	140	134	133	2	134	136	132	131	130	130
	3	149	145	121	133	119		3	136	134	126	130	131	
	4	131	132	138	130			4	130	128	131	129		
	5	132	130	134				5	119	130	130			
	6	135	134					6	130	130				
	7	134						7	130					
$2\nu$ : Ising, fcc, $R=0.20$							$2\nu$ : Ising, fcc, $R=0.60$							
	$N$	1	2	3	4	5	6	$N$	1	2	3	4	5	6
(e)	$D$							(f)	$D$					
	2	125	129	129	129	129	129	2	0	128	128	128	128	128
	3	129	129	129	129	129		3	128	128	128	128	128	
	4	129	129	129	129			4	128	128	125	128		
	5	129	129	129				5	128	128	128			
	6	129	129					6	128	120				
	7	129						7	124					
$2\nu$ : Ising, fcc, $R=1.00$							$2\nu$ : Ising, fcc, $R=\frac{5}{3}$							
	$N$	1	2	3	4	5	6	$N$	1	2	3	4	5	6
(g)	$D$							(h)	$D$					
	2	130	129	128	128	128	128	2	0	128	128	128	128	128
	3	129	127	128	128	128		3	128	128	128	128	128	
	4	128	128	128	128			4	128	128	128	128		
	5	128	128	126				5	128	128	128			
	6	128	128					6	128	128				
	7	118						7	128					
$2\nu$ : Ising, fcc, $R=5.00$							$2\nu$ : Ising, fcc, $R=100.00$							
	$N$	1	2	3	4	5	6	$N$	1	2	3	4	5	6
(i)	$D$							(j)	$D$					
	2	122	127	128	128	128	128	2	121	127	128	128	128	128
	3	127	129	128	128	128		3	127	130	128	128	128	
	4	128	128	128	128			4	129	128	128	128		
	5	128	128	128				5	128	128	128			
	6	128	128					6	128	128				
	7	128						7	128					

sions for the values of  $\chi$  are totally different for the two models:

$$\chi_{d=1}^{\text{Ising}} \propto (1/T) e^{2J/k_B T}, \quad (3.4)$$

$$\chi_{d=1}^{\text{spherical}} \propto \frac{1}{[1 + (2J/k_B T)^{-2}]^{1/2}}. \quad (3.5)$$

### C. Other Tests; Conclusions about $\gamma(R)$ and $\nu(R)$

For the sake of completeness we have applied the ratio test to the original series with an  $x_c$  estimated from the Park's and PA analysis. We have also tested for the asymptotic nature of the series

TABLE V. Estimates for the critical-point exponent  $\gamma$  (in units of  $10^{-2}$ ) for the spherical model on the sc lattice from PA's to  $(d/dx)\ln\bar{\chi}(x)$ . For  $R=1$ , the estimates  $\gamma_{N,D} \cong 2.00$  for  $N+D \gtrsim 11$  while for  $R=0.2$ ,  $\gamma_{N,D} \cong 2.00$  for  $N+D \gtrsim 15$ ; this illustrates the fact that longer series are needed to obtain reliable estimates for  $\gamma$  when  $R$  differs appreciably from 1.

$\gamma$ : spherical model, sc lattice, $R=1.00$																		
$N$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
(a) $D$																		
1	119	169	132	198	154	199	167	201	178	201	185	201	190	201	194	201	196	200
2	137	146	154	169	175	180	183	187	189	192	193	195	196	197	197	198	198	
3	147	0	0	181	187	223	201	199	198	200	199	200	200	200	200	200		
4	156	0	129	185	176	203	198	198	199	200	200	200	200	200	200	200		
5	179	186	188	191	196	199	198	198	199	200	200	199	200	200				
6	184	188	186	199	205	199	199	199	200	200	200	201	200					
7	186	0	229	204	200	199	200	200	200	200	200	200	200					
8	189	221	196	183	199	199	200	200	200	200	200	200						
9	192	203	181	194	200	200	200	200	200	200								
10	194	198	199	199	200	200	200	200	200									
11	196	200	199	198	200	200	200	200										
12	197	199	200	200	200	200	200											
13	198	201	200	200	200	201												
14	198	200	200	200	200													
15	199	200	200	200														
16	199	200	200															
17	199	200																
18	199																	
$\gamma$ : spherical model, sc lattice, $R=0.20$																		
$N$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
(b) $D$																		
1	143	242	227	120	129	121	108	247	206	279	278	179	182	160	152	211	204	228
2	165	229	243	128	125	141	119	213	231	278	279	182	179	147	159	204	209	
3	291	186	172	122	133	124	126	278	420	244	233	156	120	173	171	173		
4	348	174	194	104	120	126	122	341	285	235	251	137	153	171	173			
5	136	143	118	173	149	193	166	196	182	200	187	203	193	201				
6	0	138	139	152	159	171	177	187	190	193	195	196	197					
7	139	139	138	0	177	200	209	197	197	200	200	198						
8	139	139	133	166	187	210	203	197	197	200	200							
9	236	316	0	232	197	198	198	199	199	198								
10	259	211	0	170	198	198	198	199	199									
11	195	292	346	216	198	198	197	198										
12	191	340	308	175	199	200	198											
13	191	192	119	213	199	199												
14	192	191	192	192	198													
15	0	0	166	203														
16	171	176	180															
17	191	190																
18	190																	

using the test described in Sec. II F. All of these tests are consistent with the conclusions of Secs. III A and III B that for  $0.2 \lesssim R \lesssim 5$  (sc) and  $0.08 \lesssim R$  (fcc) we have enough coefficients to see true asymptotic behavior and that for these values of  $R$  the exponents  $\gamma$  and  $\nu$  maintain their  $R=1$  values. For values of  $R$  for which we do not have enough coefficients to see asymptotic behavior we have no direct evidence for invariance of  $\gamma$  and  $\nu$ . However, from the way in which the estimates  $\{\gamma_n\}$  and  $\{\nu_n\}$  are bending toward the  $R=1$  values, it seems likely that  $\gamma(R) = \gamma(R=1)$ ,  $\nu(R) = \nu(R=1)$  for all finite  $R$ , as predicted by the universality hypothesis.

The appearance of marked curvature in the series analysis estimates of critical properties for Hamiltonians which depend on a parameter has also been noted by other authors.<sup>16,75</sup>

#### D. Critical Temperatures

In Fig. 13 and Table IV we present estimates for  $T_c(R)/T_c^{\text{mft}}(R)$ , where  $T_c^{\text{mft}}(R)$  is the mean field theory (mft) value of  $T_c$  and where  $T_c(R)$  has been estimated from PA and Park's method analysis. We note (i) that  $T_c(R)/T_c^{\text{mft}}(R) < 1$  for all  $R$ , consistent with Fisher's<sup>76</sup> exact result that  $T_c^{\text{mft}}$  is an upper bound on the exact  $T_c$ , and (ii) that the mft esti-

mates become worse as the effective coordination number decreases, i.e., as the lattices become "less three dimensional."

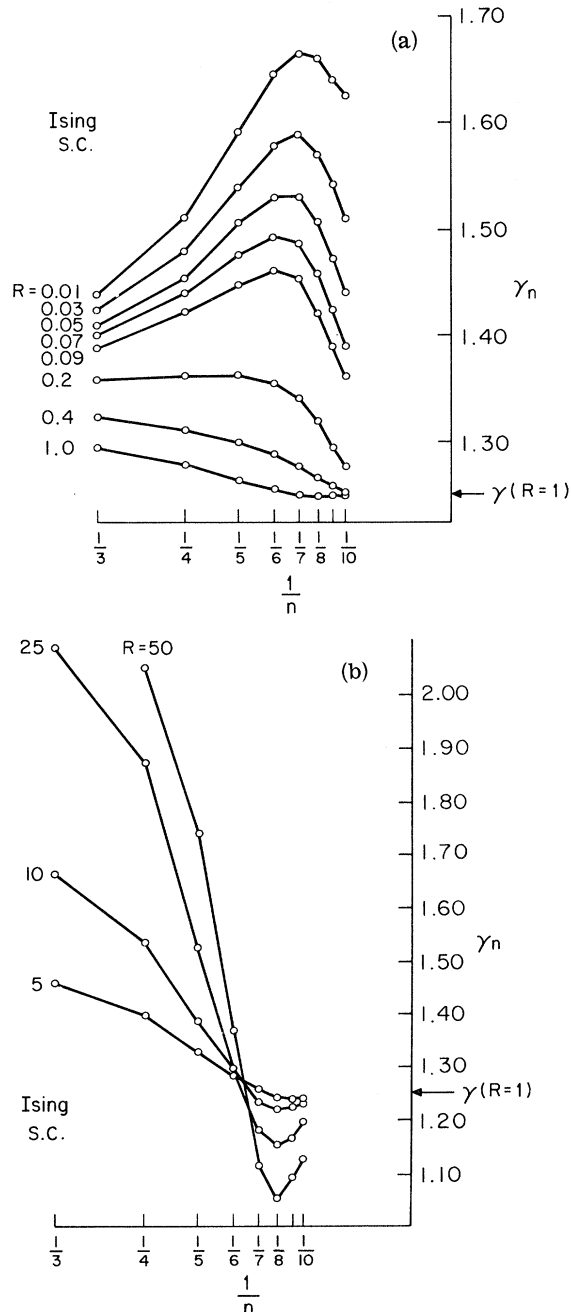


FIG. 6. Estimates for  $\gamma$  for the sc Ising lattice from Park's method applied to series which have been transformed to reduce the effects of antiferromagnetic singularities. We note that the transformation has eliminated all trace of the oscillations present in the estimates from Park's method applied to the untransformed series (cf. Fig. 5). The absence of the oscillations allows one to clearly observe the marked curvature in the estimates for exponents when  $R \ll 1$  (sc, fcc) and  $R \gg 1$  (sc).

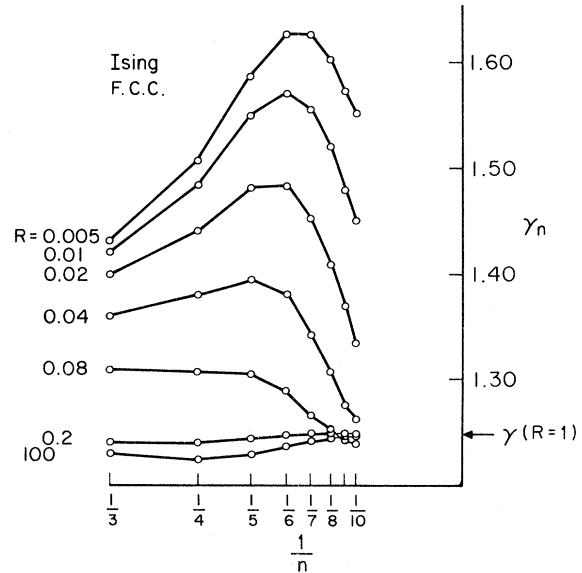


FIG. 7. Estimates for  $\gamma$  for the fcc Ising lattice. Details described in caption to Fig. 6.

#### IV. SUMMARY

We have calculated series expansions for  $\mathcal{K}_{l \text{ anis}}$  for the two-spin correlation function for both the Ising model ( $D=1$ ) and the exactly soluble spherical model ( $D=\infty$ ). To the best of our knowledge the present work is the first treatment of  $\mathcal{K}_{l \text{ anis}}$  using high-temperature series-expansion techniques.

A detailed analysis of the series for the Ising model indicated that the exponents  $\gamma$  and  $\nu$  are constant over a wide range of the parameter  $R \equiv J_z/J_{xy}$  [ $0.2 \lesssim R \lesssim 5$  (sc),  $0.08 \lesssim R$  (fcc)]. Outside of this range of  $R$  we have evidence that we do not have enough coefficients to see the true asymptotic behavior of the series. From the curvature of the series in the nonasymptotic region, however, it appears quite likely that  $\gamma(R) = \gamma(R=1)$  and  $\nu(R) = \nu(R=1)$  for all finite  $R$  as predicted by the universality hypothesis. The series for  $\overline{C}_H$  were not regular enough to allow for predictions concerning the exponent  $\alpha$ .

#### ACKNOWLEDGMENTS

We are grateful to M. H. Lee, K. Matsuno, and most especially S. Milošević for helpful discussions. We also wish to thank M. Ferer, M. A. Moore, and M. Wortis for providing us with a computer program that they used for isotropic nearest-neighbor lattices.

#### APPENDIX A: SPHERICAL MODEL

The spherical model<sup>34</sup> is defined by the Hamiltonian

$$\mathcal{H}_{\text{spherical}} \equiv -\frac{1}{2} \sum_{i,j} J_{ij} \sigma_i \sigma_j - H \sum_i \sigma_i, \quad (\text{A1})$$



where  $H$  is an external field. The spins  $\sigma_i$  can take on the values  $-\infty < \sigma_i < \infty$ , with the restriction

$$\sum_{i=1}^N \sigma_i^2 = N, \quad (\text{A2})$$

where  $N$  is the number of sites on the lattice.

The zero-field correlation function for a  $d$ -dimensional hypercubical lattice with arbitrary exchange constants,  $J_{\vec{l}} \equiv J_{i,j}$  with  $\vec{l} \equiv \vec{r}_i - \vec{r}_j$ , is given by<sup>77</sup>

$$C_2(\vec{r}) = \frac{1}{x} \frac{1}{(2\pi)^d} \int_0^{2\pi} \dots \int_0^{2\pi} d\vec{\omega} \frac{\cos(\vec{r} \cdot \vec{\omega})}{z_s S(0) - S(\vec{\omega})}, \quad (\text{A3})$$

with  $x \equiv 1/k_B T$ . Here  $\vec{\omega} \equiv (\omega_1, \omega_2, \dots, \omega_d)$  and  $\vec{r} \equiv (r_1, r_2, \dots, r_d)$  denote  $d$ -dimensional vectors. The quantity  $z_s$  is defined implicitly by the equation

$$x = \frac{1}{(2\pi)^d} \int_0^{2\pi} \dots \int_0^{2\pi} d\vec{\omega} \frac{\cos(\vec{r} \cdot \vec{\omega})}{z_s S(0) - S(\vec{\omega})} \quad (\text{A4})$$

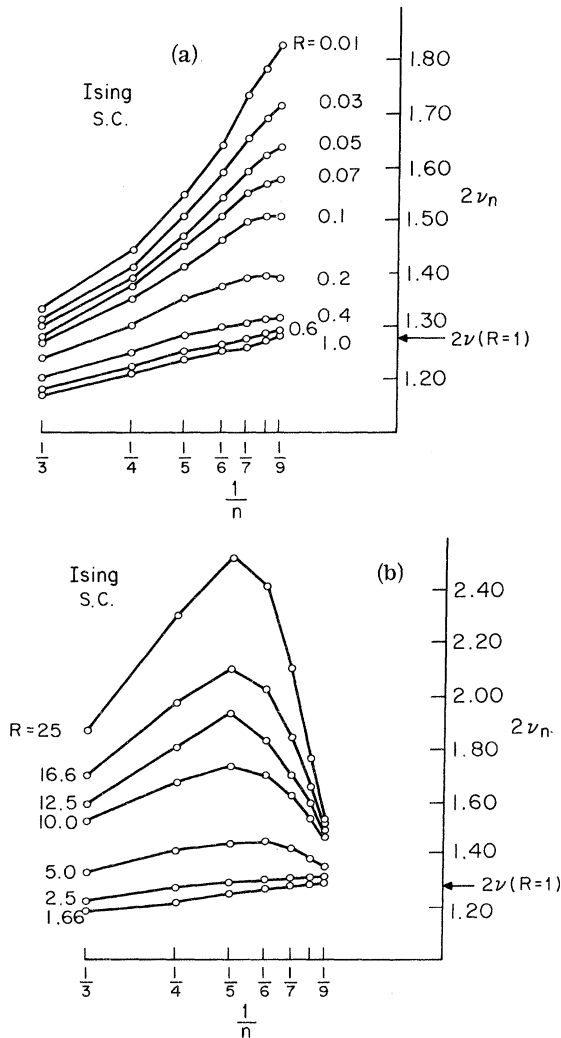


FIG. 8. Estimates for  $2\nu$  for the sc Ising lattice. Details described in caption to Fig. 6.

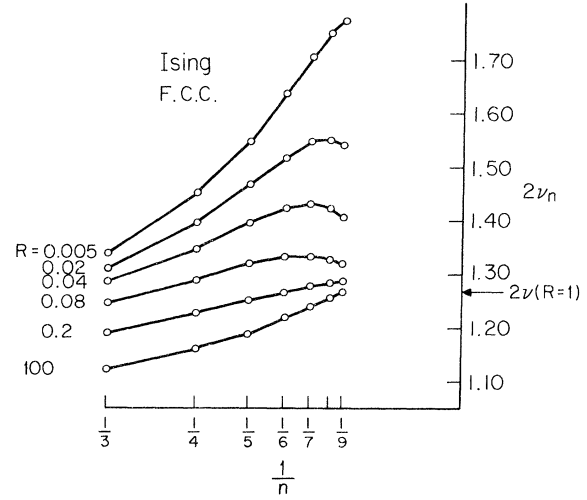


FIG. 9. Estimates for  $2\nu$  for the fcc Ising lattice. Details described in caption to Fig. 6.

and  $S(\omega)$  is defined by

$$S(\vec{\omega}) \equiv \sum_{\vec{l}} J_{\vec{l}} \cos(\vec{\omega} \cdot \vec{l}). \quad (\text{A5})$$

Following Joyce,<sup>78</sup> who treated long-range forces, it is easy to show that the predictions of universality in Sec. IA apply for the exponent  $\gamma$ .

To verify the universality predictions for the exponent  $\nu$  it will be useful to prove a relation among

TABLE VI. Estimates for  $T_c(R)/T_c^{\text{mft}}(R)$ . Confidence limits on  $T_c(R)$  are such that the errors in these estimates are in the last significant figure. The superscript mft denotes mean field theory.

fcc		sc	
$R$	$\frac{T_c(R)}{T_c^{\text{mft}}(R)}$	$R$	$\frac{T_c(R)}{T_c^{\text{mft}}(R)}$
0.0	0.5673	0.0	0.5673
0.005	0.602	0.01	0.587
0.01	0.620	0.02	0.602
0.02	0.653	0.04	0.617
0.04	0.6859	0.06	0.635
0.08	0.7323	0.08	0.648
0.2	0.7464	0.1	0.6575
0.6	0.8129	0.2	0.6948
1.0	0.8162	0.4	0.7279
1.67	0.8142	0.6	0.7434
5.0	0.8040	0.8	0.7500
100.0	0.7949	1.0	0.7518
$\infty$	0.7868	1.25	0.7497
		1.67	0.7413
		2.5	0.7168
		5.0	0.648
		10.0	0.560
		25.0	0.449
		50.0	0.379
		$\infty$	0.0

the even moments.

$$\mu_{2m} \equiv \sum_{\vec{r}} C_2(\vec{r}) |\vec{r}|^{2m}, \quad m=0, 1, 2, \dots \quad (A6)$$

The relation we derive will also (i) allow us to express  $\mu_2$  in terms of  $\bar{\chi}$  so that an independent analysis of the second-moment spherical-model series becomes unnecessary and (ii) allow us to explain the origin of nonphysical singularities which arise when high-order moments ( $\mu_t, t > 2$ ) for the Ising, planar, and Heisenberg models are analyzed.

In order to prove the relation between moments we first note the formal identities

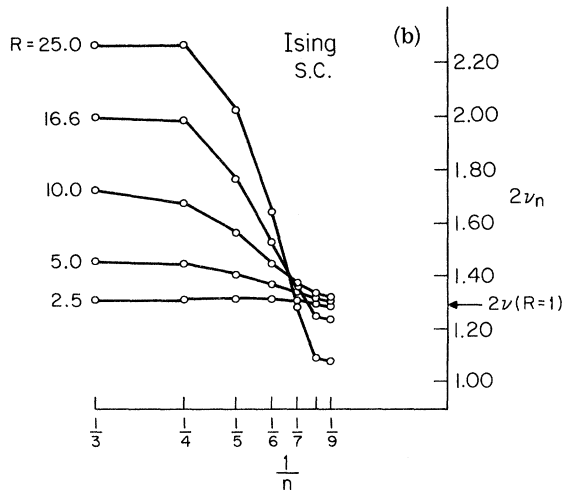
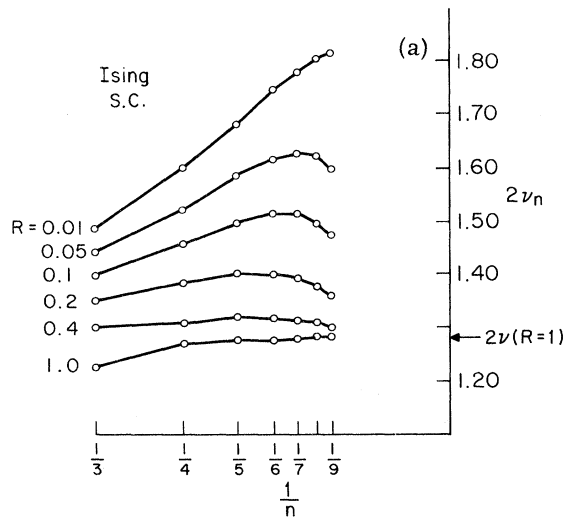


FIG. 10. Estimates for  $2\nu$  for the sc Ising lattice from the " $T_c$  renormalization" method applied to transformed series. Even though  $x_c$  is known in this method the estimates do not seem to be converging any faster than the estimates obtained from Park's method. In particular we again note the curvature for  $R \ll 1$  (sc, fcc) and  $R \gg 1$  (sc).

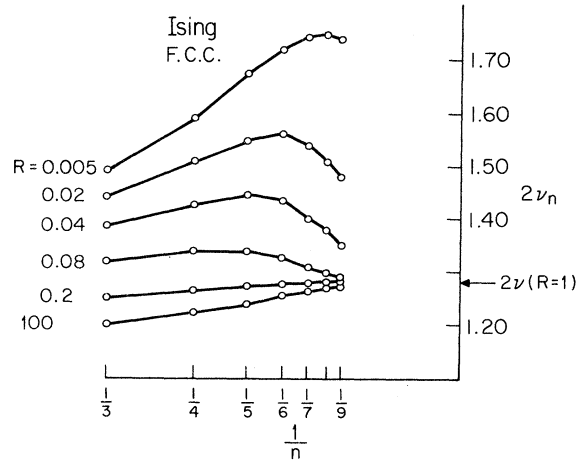


FIG. 11. Estimates for  $2\nu$  for the fcc Ising lattice. Details described in caption to Fig. 10.

$$\begin{aligned} & \sum_{\vec{r}} (r_1^2 + r_2^2 + \dots + r_d^2)^m \cos(\vec{r} \cdot \vec{\omega}) \\ &= (-1)^m \left( \frac{\partial^2}{\partial \omega_1^2} + \dots + \frac{\partial^2}{\partial \omega_d^2} \right)^m \sum_{\vec{r}} \cos(\vec{r} \cdot \vec{\omega}) \\ &= (-1)^m \left( \frac{\partial^2}{\partial \omega_1^2} + \dots + \frac{\partial^2}{\partial \omega_d^2} \right)^m \delta(\vec{\omega} = 0). \end{aligned} \quad (A7)$$

We then have from Eqs. (A3), (A6), and (A7)

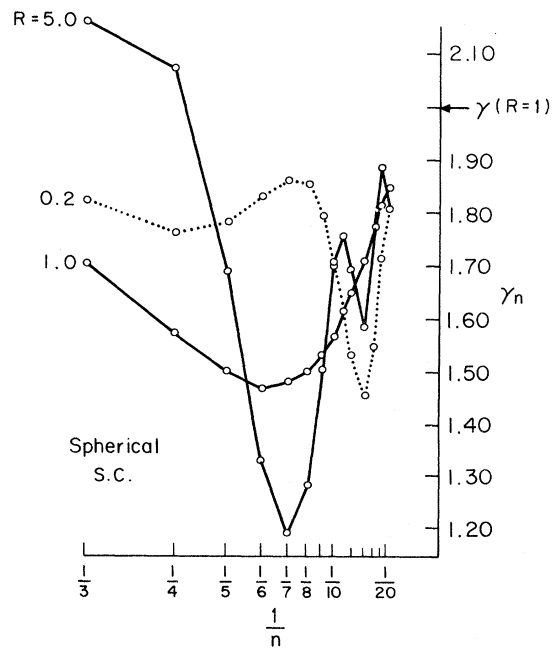


FIG. 12. Estimates for  $\gamma$  for the spherical model on the sc lattice from Park's method applied to transformed series.

TABLE VII. Susceptibility series for the spherical model, sc lattice, for selected values of  $J_{xy}$  and  $J_z$ .

	$J_{xy}=1.00, J_z=0.01$	$J_{xy}=1.00, J_z=0.20$	$J_{xy}=1.00, J_z=0.40$
$n=0$	0.1000000000D 01	0.1000000000D 01	0.1000000000D 01
1	0.4020000000D 01	0.4400000000D 01	0.4800000000D 01
2	0.1216020000D 02	0.1528000000D 02	0.1872000000D 02
3	0.3280320000D 02	0.4928000000D 02	0.6912000000D 02
4	0.7922403198D 02	0.1498528000D 03	0.2443968000D 03
5	0.1711748160D 03	0.4378880000D 03	0.8432640000D 03
6	0.3385337318D 03	0.1253775616D 04	0.2859746304D 04
7	0.6091592832D 03	0.3542528000D 04	0.9584640000D 04
8	0.9998897100D 03	0.9921427994D 04	0.3179061734D 05
9	0.1534427358D 04	0.2763909632D 05	0.1046139494D 06
10	0.2243783441D 04	0.7650986435D 05	0.3417115044D 06
11	0.3388609881D 04	0.2105867878D 06	0.1109379318D 07
12	0.5791530898D 04	0.5763413278D 06	0.3582365962D 07
13	0.1097586219D 05	0.1568823815D 07	0.1151506712D 08
14	0.2186994819D 05	0.4251365918D 07	0.3686555329D 08
15	0.4085154346D 05	0.1147696605D 08	0.1176123136D 09
16	0.6640637063D 05	0.3088440349D 08	0.3740422746D 09
17	0.9360080998D 05	0.8288911223D 08	0.1186241918D 10
18	0.1063265566D 06	0.2219148598D 09	0.3752510581D 10
19	0.1130962659D 06	0.5927849552D 09	0.1184329183D 11
20	0.2118234666D 06	0.1580113429D 10	0.3730027619D 11
	$J_{xy}=1.00, J_z=0.60$	$J_{xy}=1.00, J_z=0.80$	$J_{xy}=1.00, J_z=1.00$
$n=0$	0.1000000000D 01	0.1000000000D 01	0.1000000000D 01
1	0.5200000000D 01	0.5600000000D 01	0.6000000000D 01
2	0.2232000000D 02	0.2608000000D 02	0.3000000000D 02
3	0.9152000000D 02	0.1164800000D 03	0.1440000000D 03
4	0.3610528000D 03	0.5011648000D 03	0.6660000000D 03
5	0.1396096000D 04	0.2116352000D 04	0.3024000000D 04
6	0.5301915904D 04	0.8772668416D 04	0.1347600000D 05
7	0.1989478400D 05	0.3592601600D 05	0.5932800000D 05
8	0.7384612795D 05	0.1455264743D 06	0.2583540000D 06
9	0.2718650522D 06	0.5846665933D 06	0.1115856000D 07
10	0.9935476916D 06	0.2331879934D 07	0.4784508000D 07
11	0.3609360835D 07	0.9245542154D 07	0.2039385600D 08
12	0.1304322086D 08	0.3646527156D 08	0.8647354800D 08
13	0.4692395194D 08	0.1431831018D 09	0.3650348160D 09
14	0.1681414460D 09	0.5599865979D 09	0.1534827960D 10
15	0.6004033476D 09	0.2182507920D 10	0.6431000832D 10
16	0.2137234234D 10	0.8479648201D 10	0.2686222845D 11
17	0.7586655783D 10	0.3285431461D 11	0.1118919705D 12
18	0.2686279532D 11	0.1269732505D 12	0.4649022634D 12
19	0.9489885444D 11	0.4896025363D 12	0.1927243552D 13
20	0.3345536949D 12	0.1883962215D 13	0.7972767769D 13

$$\mu_{2m} = \frac{(-1)^m}{x} \left[ \left( \frac{\partial^2}{\partial \omega_1^2} + \dots + \frac{\partial^2}{\partial \omega_d^2} \right)^m \frac{1}{z_s S(\vec{0}) - S(\vec{\omega})} \right]_{\vec{\omega}=\vec{0}}. \quad (\text{A8})$$

This is the relation we shall need below.

For  $m=0$  and  $m=1$  we have, respectively,

$$\mu_0 = \bar{\chi} = \frac{1}{x} \frac{1}{z_s S(\vec{0}) - S(\vec{0})}, \quad (\text{A9})$$

$$\mu_2 = \frac{1}{x} \sum_{\vec{1}} J_{\vec{1}} |\vec{1}|^2 \frac{1}{[z_s S(\vec{0}) - S(\vec{0})]^2} = \text{const} \times \bar{\chi}^2. \quad (\text{A10})$$

Thus with  $\mu_2 \sim (x_c - x)^{-\gamma-2\nu}$  we find that all universality predictions for  $\gamma$  also hold for  $\nu$ .<sup>79</sup>

From (A10) it is also clear that in using the spherical model as a test for series-expansion techniques it is necessary only to investigate  $\bar{\chi}$  and not  $\mu_2$ . For example, use of Park's method, Eq. (2.19) on the series for  $\bar{\chi}$  and  $\mu_2/\bar{\chi}$  would yield

$$\gamma_n = 2\nu_n \quad (\text{A11})$$

identically for all  $n$ .

TABLE VII. (Continued)

	$J_{xy}=0.20, J_z=1.00$	$J_{xy}=0.10, J_z=1.00$	$J_{xy}=0.02, J_z=1.00$
$n=0$	0.1000000000D 01	0.1000000000D 01	0.1000000000D 01
1	0.2800000000D 01	0.2400000000D 01	0.2080000000D 01
2	0.5680000000D 01	0.3720000000D 01	0.2324800000D 01
3	0.9856000000D 01	0.4032000000D 01	0.6722560000D 00
4	0.1668160000D 02	0.3927600000D 01	-0.4424314126D -01
5	0.2920960000D 02	0.5616000000D 01	0.1773291520D 00
6	0.5013529600D 02	0.8532624000D 01	0.3538011514D 01
7	0.8136540160D 02	0.7374643200D 01	0.4424314126D -01
8	0.1304916429D 03	0.2813127480D 01	-0.8807007336D 01
9	0.2166363996D 03	0.9238339008D 01	0.1050653311D -01
10	0.3575965512D 03	0.2603923006D 02	0.2500537812D 02
11	0.5600355785D 03	0.1123437745D 02	0.2421616551D -02
12	0.8682408620D 03	-0.3590524881D 02	-0.7548059316D 02
13	0.1417101314D 04	0.1336741287D 02	0.5458708962D -03
14	0.2316483209D 04	0.1670060458D 03	0.2381846907D 03
15	0.3527943262D 04	0.1564591416D 02	0.1210169916D -03
16	0.5295303090D 04	-0.4799452845D 03	-0.7761945761D 03
17	0.8671618397D 04	0.1807791666D 02	0.2648018136D -04
18	0.1433245557D 05	0.1673950167D 04	0.2592224104D 04
19	0.2109637650D 05	0.2067189144D 02	0.5732845938D -05
20	0.3018589857D 05	-0.5587456344D 04	-0.8825608726D 04

Finally we consider higher moments. Analysis of the Ising, planar, Heisenberg, and spherical-model series indicated a first order *zero* on the negative real  $x$  axis. Padé approximant analysis indicated that in addition to this zero there was a physical singularity on the positive real axis but at a greater distance from the origin. For example  $\mu_4$  had the form

$$\mu_4(x) \sim (x - x_0)(x - x_c)^{-\lambda}, \quad (\text{A12})$$

with  $x_c > -x_0 > 0$ . Furthermore  $\lambda \hat{=} \gamma + 4\nu$  as predicted by scaling.<sup>12</sup> We feel that the presence of the nonphysical zero can be understood by examining the exact solution for the spherical-model moments.

Consider  $\mu_4$  for the spherical model. From Eq. (A8) we find

$$\begin{aligned} \mu_4(x) &= (1/x) [B_2(x\bar{\chi})^2 + B_3(x\bar{\chi})^3] \\ &= x B_3 \bar{\chi}^3 [B_2/B_3 \bar{\chi}(x) + x], \end{aligned} \quad (\text{A13})$$

with  $B_2$  and  $B_3$  constants. Now if  $\bar{\chi}(x)$  were a constant then  $\mu_4$  would clearly have a first-order zero at  $B_2/(B_3\bar{\chi})$ . Under a very reasonable assumption this will also be true with the real  $\bar{\chi}(x)$ . Specifically assume that

$$g(x) \equiv B_2/B_3 \bar{\chi}(x) \quad (\text{A.14})$$

is analytic for  $x \leq x_0$  (Ref. 80) where  $x_0$  is defined implicitly by

$$g(x_0) + x_0 = 0. \quad (\text{A.15})$$

We can then write

$$\begin{aligned} \mu_4(x) &= B_3 \bar{\chi}^3 (x - x_0) \left( 1 + \frac{g(x) - g(x_0)}{x - x_0} \right) \\ &\equiv B_3 \bar{\chi}^3 (x - x_0) A(x), \end{aligned} \quad (\text{A.16})$$

with  $A(x)$  analytic for  $x \leq |x_0|$ .

Thus  $\mu_4$  has a first order zero at  $x = x_0$ . Similar considerations for higher-order moments of the spherical model also indicate the presence of non-physical first-order zeros.

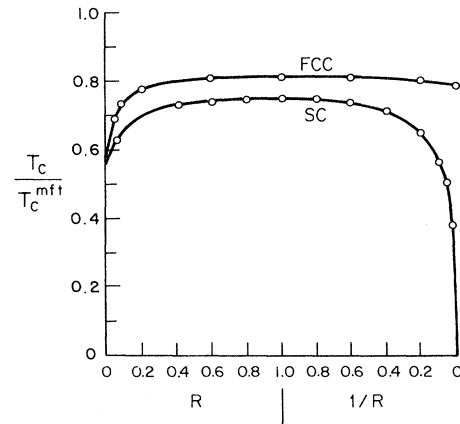


FIG. 13.  $T_c/T_c^{\text{mft}}$  vs  $R$  or  $(1/R)$  for the sc and fcc lattices. The confidence limits on  $T_c$  are smaller than the size at the points in the figure.

Although we do not have exact solutions for moments for the Ising, planar, and Heisenberg models, we feel that the origin of the observed zero for these models is qualitatively the same as that for the spherical model.

#### APPENDIX B: SELECTED SERIES FOR THE SPHERICAL MODEL

The susceptibility series for selected values of  $J_{xy}$  and  $J_z$  for the sc spherical model is given in Table VII.

- \*Work forms a portion of a Ph. D. thesis submitted to the MIT Physics Department by G. P. A preliminary report appeared in G. Paul and H. E. Stanley, Phys. Letters **37A**, 347 (1971). For the values of the exact series coefficients, the reader should order document NAPS 01750 from Asis-National Auxiliary Publications Service, c/o CCM information Corporation, 866 Third Ave., New York, N. Y. 10022, remitting \$2.00 for each microfilm or \$5.00 for each photocopy.
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## Transport Measurements on the Ferromagnetic Phase of $PdCo$ Alloys\*

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(Received 12 October 1971)

The electrical resistivity of the five  $PdCo$  alloys, ranging in concentration from 2 to 7.5 at.% Co, has been measured over the temperature interval 1.4-77 K. At temperature  $T$ , well below the magnetic ordering temperature  $T_c$ , the incremental resistivity of the alloy  $\Delta\rho(T) = \rho_{\text{alloy}}(T) - \rho_{Pd}(T)$  can be expressed in the form  $\Delta\rho(T) = A + BT^2$ .  $A$  is found to vary linearly with concentration  $c$ , having the value  $1.27 \pm 0.03 \mu\Omega \text{ cm/at.\% Co}$ , while  $B \propto c^n$ , and  $n = -0.75 \pm 0.05$ . On the basis of a localized "s-d" model, an expression for  $\Delta\rho(T)$  at temperature  $T \ll T_c$  is derived; its application to the present data yields  $|V|$  (the "potential" integral) =  $0.44 \pm 0.01 \text{ eV}$ , while the coefficient of the  $T^2$  term involves the s-electron-local-moment exchange coupling  $|J_{s\text{-local}}|$ , the "giant-moment" spin  $S$ , and the Fermi wave vector  $k_F$ . Using saturation-magnetization measurements in conjunction with ferromagnetic-resonance data enables estimates of  $S$  to be made; by combining the present data with previous measurements on  $PdCo$  by Schwaller and Wucher,  $|J_{s\text{-local}}|$  is evaluated;  $k_F$  is obtained by using an effective-mass treatment of the s band. These estimates enable values of the acoustic spin-wave stiffness  $D$  to be extracted from the experimental data.  $D$  is found to satisfy the equation  $D = D_0 c^n$ , with  $D_0 \approx 11 \text{ K } \text{\AA}^2$  and  $n = 1.00 \pm 0.05$ , in the range 2-7.5 at.% Co.

### INTRODUCTION

The properties of the ferromagnetic phase of dilute transition-metal alloys, typified by the giant-moment systems  $PdFe$  and  $PdCo$ , have received much attention over the past few years; the former system perhaps more than the latter. Initial measurements by Veal and Rayne<sup>1</sup> on the  $PdFe$  system revealed at temperatures  $T \ll T_c$  (where  $T_c$  is the Curie temperature) a  $T^{3/2}$  contribution to the specific heat. Similar subsequent measurements by several investigators confirmed this, both in the  $PdFe$ <sup>2,3</sup> and the  $PdCo$ <sup>4</sup>

systems. This contribution to the specific heat was attributed to the presence of energetically low-lying spin-wave-like excitations in the exchange-coupled impurity-moment-d-band system of the alloy. Later magnetization<sup>3,5</sup> and NMR<sup>6</sup> measurements also established a  $T^{3/2}$  contribution to the magnetization in the low-temperature regime; this result reinforced the above conclusions regarding excitations from the ordered ground state. Confirmatory evidence for this assignment was also furnished by low-temperature neutron-scattering measurements on  $PdFe$  alloys<sup>7</sup>; these were successfully analyzed in terms of