

# High-Temperature Series for Scalar-Field Lattice Models: Generation and Analysis

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An implementation of the free-embedding scheme for high-temperature series generation on the body-centered cubic family of lattices in arbitrary dimension  $d$  is described. Series to order 21 in inverse temperature are tabulated for several scalar field models, both for the magnetic susceptibility and for the second moment of the spin correlation function. The critical behavior of a family of 3-dimensional "double Gaussian" models, which interpolate continuously between the spin-1/2 Ising model and the Gaussian model, is analyzed in detail away from the Gaussian model limit using confluent inhomogeneous second-order differential approximants. With our best estimate of the correction-to-scaling exponent,  $\theta = 0.52 \pm 0.03$ , the leading exponents for the susceptibility and correlation length for this family are consistent with universality and are given by  $\gamma = 1.237 \pm 0.002$  and  $\nu = 0.630 \pm 0.0015$ , respectively, and  $\eta = 2 - \gamma/\nu = 0.0359 \pm 0.0007$ .

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**KEY WORDS:** Ising model; series generation; series analysis; critical exponents; universality.

## 1. INTRODUCTION AND SUMMARY OF RESULTS

Estimates of critical exponents deduced from high-temperature series on 3-dimensional lattices have been puzzling for a number of years. Contrary to the expectations of renormalization-group theory, there has been evidence both for the failure of hyperscaling<sup>(1)</sup> and the absence of universality. The latter is suggested by a discrepancy between the "classical" estimates of the susceptibility exponent  $\gamma = 1.250 \pm 0.003$ <sup>(2)</sup> and the correlation length exponent  $\nu = 0.638 \pm_{-0.001}^{+0.002}$ <sup>(3)</sup> and the most recent space

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continuum  $\phi^4$ -model estimates.<sup>(4)</sup> These are  $\gamma = 1.241 \pm 0.002$  and  $\nu = 0.6300 \pm 0.0015$ , based on Borel resummation of coupling constant perturbation expansions, and  $\gamma = 1.2390 \pm 0.0025$  and  $\nu = 0.6310 \pm 0.0015$ , based on Borel resummation of  $\epsilon$ -expansion series supplemented by exact results in two dimensions. However, the numerical arguments for or against hyperscaling and universality appear to depend on the method used to analyze series expansions of limited length. Each method inevitably builds in particular “function biases” and, as a consequence, yields analysis-dependent results.<sup>3</sup> It is therefore hoped that with longer series, less function-biased analyses might be undertaken which will either confirm, say, the absence of universality or resolve the apparent discrepancies and show how they arose from certain biases.

Although the prospects for extending these series for general 3-dimensional lattices are not encouraging, a great simplification in the high-temperature series generation process is possible for the body-centered cubic (bcc) lattice.<sup>(5)</sup> Exploiting this simplification, Nickel reported new 21-term spin-1/2 Ising series for the susceptibility and correlation length at Cargèse in 1980.<sup>(9)</sup> Also reported was a preliminary analysis of these and corresponding higher-spin- $S$  series which showed that the “classical” exponent estimates were seriously in error and that the new estimates appeared to be consistent with universality. Since then, series for other models have been derived and many more analyses<sup>(10-21)</sup> of these bcc series have been reported; ref. 21 contains a recent discussion. Here we finally (!) report the details of this series derivation, tabulate series coefficients for models we hope will be of general interest, and present an analysis which in preliminary stages was reported at Stat Phys XIV,<sup>(22)</sup> Rutgers,<sup>(23)</sup> and APS<sup>(24)</sup> meetings.

Our analysis is based on confluent inhomogeneous second-order differential approximants which, by allowing for a correction-to-scaling term in a simple form and an analytic background, can (potentially) yield an unbiased test of universality. However, in practice we can only obtain the high precision of about three decimal places for  $\gamma$  and  $\nu$  and not quite two decimal places for the correction-to-scaling exponent  $\theta$  by comparing different models and “forcing” universality by a best-fit procedure. As opposed to other methods of series analysis which usually focus on a single thermodynamic quantity, our approach uses both susceptibility and correlation-length series and makes use of several internal consistency checks to help reduce the effects of function bias. Our best estimates of the critical exponents are consistent with (1) a common correction-to-scaling

<sup>3</sup> See, for example, the discussion of hyperscaling in ref. 5, or compare the analyses by Gaunt and Sykes<sup>(6)</sup> and Zinn-Justin.<sup>(7)</sup> A review of early work has been compiled by Gaunt.<sup>(8)</sup>

exponent  $\theta$  for a family of models; (2) the same critical temperature for both the susceptibility and correlation length series for a given model; (3) a common value of  $y^*$ , i.e., the model parameter at which the leading correction-to-scaling vanishes; and (4) universality of the subdominant amplitude ratio. The use of confluent approximants is essential to our method; Guttman<sup>(20)</sup> also carried out a differential approximant analysis without explicitly including a confluent singularity in each approximant and obtained rather different results. Inhomogeneous approximants have been found to be particularly important in reducing the overall scatter of the critical exponent estimates, especially for the  $\xi^2$  series. Such inhomogeneous approximants automatically incorporate an analytic background and remove spurious effects of the leading terms in a series. The effect of the inhomogeneous term on critical exponent estimates is a reduction of about 0.002 in both  $\gamma$  and  $2\nu$ . Our results are, within error limits, consistent with other analyses that are also unbiased in their exponent choices and that explicitly depend on model comparisons.<sup>(13)</sup> A common conclusion is that for the spin-1/2 Ising model, the correction-to-scaling term, though small, *cannot* be neglected. On the other hand, our conclusion is similar to that reached by Zinn-Justin<sup>(10)</sup> and is worth stressing; namely, that even with the long series now available, any analysis based solely on the spin-1/2 series *cannot predict* the presence of a correction-to-scaling term.<sup>4</sup>

A summary of this paper in somewhat more detail is as follows. As mentioned in ref. 5, the evaluation of graph embedding constants, which for most lattices is the most time-consuming part of the series calculation, becomes almost trivial on the family<sup>5</sup> of  $d$ -dimensional lattices for which the interactions couple fields bilinearly on lattice sites separated by any of the  $2^d$  vector displacements  $(\pm 1, \pm 1, \dots, \pm 1)$ . Another consequence of this factorization is that the high-temperature susceptibility series can be written as

$$\chi(K) = \sum_{n=0}^{\infty} \frac{1}{n!} K^n \sum_{\sum im_i = n+1} \left( \prod_{i=1}^m (\mu_{2i})^{m_i} \right) \times \sum_g [E_g(\{m_i\})]^d W_g(\{m_i\}) \quad (1.1)$$

<sup>4</sup> Both Mellin transform<sup>(11)</sup> and 5-point fits<sup>(16)</sup> fail to find significant corrections for the spin-1/2 case. The trend of the  $D \log$  Padé estimates<sup>(9)</sup> is suggestive of a correction, but of course each approximant specifically excludes such a term. Finally, for spin 1/2, second-order differential approximants<sup>(22)</sup> fit just as easily with  $\theta \equiv \gamma$ , i.e., an analytic background, as with  $\theta \approx 0.5$ .

<sup>5</sup> This "bcc family" includes a pair of sites ( $d=0$ ), the linear chain ( $d=1$ ), the simple quadratic lattice ( $d=2$ ), the bcc ( $d=3$ ), and higher-dimensional generalizations. The basis for the simplification is a factorizability described in Section 2, which reduces the  $d$ -dimensional embedding calculation to that in one dimension.

and the second moment of the 2-point correlations as

$$M_2(K) = \sum_{n=0}^{\infty} \frac{1}{n!} K^n \sum_{\sum m_i = n+1} \left[ \prod_{i=1}^{\infty} (\mu_{2i})^{m_i} \right] \times \sum_g [E_g(\{m_i\})]^{d-1} F_g(\{m_i\}) W_g(\{m_i\}) \quad (1.2)$$

where  $K$  is the inverse temperature and  $\{\mu_{2i}\}$ , the cumulant moments of the single-site field distribution [see Eqs. (2.1) and (2.6)], are the physical model-dependent parameters; the dimension  $d$  appears only as an exponent, while the remaining quantities are integer constants that can be given a graphical interpretation. In particular, the  $m_i$  are the number of vertices of order  $2i$  in 2-rooted graphs of type  $g$ ;  $E_g(\{m_i\})$  is a one-dimensional embedding constant or zeroth moment in root separation, while  $F_g(\{m_i\})$  is the second moment in root separation.  $W_g(\{m_i\})$  is a sum of symmetry-related weight factors of all graphs with the same embedding constant moments  $E_g$  and  $F_g$ . A few technical details of the computer program that determines these integer constants through order  $n=21$  are also described in Section 2.

The data for  $\chi$  and  $M_2$  for the order  $K^{21}$  calculation comprise nearly 100,000 entries of the constants  $E_g$ ,  $F_g$ , and  $W_g$  and can be conveniently transferred only via magnetic tape. To make these results more directly accessible, we specialize the general scalar models, characterized by the set of cumulant moments  $\{\mu_{2i}\}$ , to models in which the single-site field distribution is parametrized by a single variable  $y$ . The series for  $\chi$  and  $M_2$  can then be written as

$$\chi(K, y) = \sum K^n A_n(y), \quad M_2(K, y) = \sum K^n B_n(y) \quad (1.3)$$

Furthermore, a number of physically interesting models exist for which the  $A_n(y)$  and  $B_n(y)$  are expressible as polynomials of order approximately  $n$ . Such models, which include spin- $S$  Ising, Blume-Capel,<sup>(25)</sup> Klauder,<sup>(26)</sup> and double-Gaussian<sup>(23)</sup> or range,<sup>(27)</sup> are described in Section 3 and a few representative tables of coefficients of double power series in  $K$  and  $y$  are listed in the Appendix. Readers interested in other models should contact the authors.

With the much longer series now available one can reexamine the previous Ising model critical exponent estimates using a number of methods ranging from such commonly used approaches as the ratio and  $D \log$  Padé to the more recently developed second-order differential approximants<sup>(28)</sup> and (two-variable) partial differential approximants.<sup>(18, 29)</sup> Each method has its relative merits. For example, the conventional  $D \log$  Padé is easy to

apply and directly separates the effects of unphysical singularities from the critical singularities of physical interest. Unfortunately, the method assumes the absence of correction-to-scaling terms discussed by Wegner,<sup>(30)</sup> and this can lead to systematic errors in the leading critical exponent estimates. Exponents from  $D \log$  Padé approximants<sup>(9)</sup> to 21-term spin- $S$  Ising series are spin dependent and taken at face value suggest the absence of universality. On the other hand, the two-variable partial differential approximant method<sup>(13)</sup> as applied to the double-Gaussian and Klauder series assumes the presence of a single correction-to-scaling term in the scaling form predicted by renormalization-group theory.<sup>(30)</sup> Since this method uses all the information in each two-variable series simultaneously, it will probably yield the best possible exponent estimates if the renormalization-group hypothesis is correct and if higher-order corrections are sufficiently small. Of course, it is conceivable that the observed scatter in those estimates<sup>(13)</sup> is a response to model-dependent exponents, and thus in a sense the method is not a test of universality. The partial differential approximant method of ref. 18 is based on the same scaling assumption, but uses more limited information, namely two single-variable series  $\chi(K)$  and  $\partial\chi(K)/\partial y$  for a given model parameter  $y$ . Exponent estimates have also been made<sup>(19)</sup> using inhomogeneous first-order differential approximants and determining, self-consistently, a value  $y^*$  at which the leading nonanalytic corrections-to-scaling in  $\chi$  vanish. Although not a test of universality, the resulting exponents have been used to check the validity of hyperscaling.

In the present paper we concentrate on analysis of the double-Gaussian series by single-variable confluent inhomogeneous second-order differential approximants. This simple generalization of the  $D \log$  Padé method assumes that a single correction-to-scaling term is important. Also, as described in Section 4,  $\chi$ ,  $M_2$ , and the correlation length squared  $\xi^2 \propto M_2/\chi$  are assumed to have critical behavior

$$F(K) \sim \begin{cases} A_F \left(1 - \frac{K}{K_c}\right)^{-\gamma_F} \left[ 1 + a_F \left(1 - \frac{K}{K_c}\right)^{\theta_F} \right] + B_F, & K \approx K_c \\ C_F \left(1 + \frac{K}{K_c}\right)^{1-a_F} + D_F, & K \approx -K_c \end{cases} \quad (1.4)$$

in the neighborhood of the ferromagnetic and antiferromagnetic critical points  $K = \pm K_c$ .<sup>6</sup>

<sup>6</sup> The second-order inhomogeneous differential approximants exhibit critical behavior of the form (1.4), in which the coefficients  $A_F$ ,  $a_F$ , and  $B_F$  ( $C_F$  and  $D_F$ ) are regular functions of  $K$  at  $K_c$  ( $-K_c$ ). While it is not likely that the background term  $B_F$  contains the leading corrections beyond the  $(1 - K/K_c)^{\theta}$  term, its inclusion tends to give more stable estimates for  $\gamma_F$  and  $\theta_F$ . This background term may also be the best polynomial approximation to additional important but slowly varying confluent corrections.

In principle one could determine without bias, other than the implicit function bias of a given method, estimates of  $K_c$ ,  $\gamma_F$ , and  $\theta_F$  for many different models and then reasonably decide whether universality is satisfied; i.e., whether the  $\gamma_F$  are model independent and the  $\theta_F$  are both model and function independent. We find, not too surprisingly,<sup>(31)</sup> that such double exponential fitting is very unstable and that even longer series will be needed before one can hope to succeed in verifying universality with this naive approach. Thus, instead, we have adopted the procedure of fixing  $\theta_F$  at a few discrete values and determining only  $K_c$  and  $\gamma_F$ . We find that there is a “best” value for  $\theta_F = \theta \approx 0.52 \pm 0.03$ , for which the exponents  $\gamma_F$  are most constant over a wide range of  $\gamma$  parameter values in the double-Gaussian model. In this limited sense we do verify universality and find  $\gamma_\chi \equiv \gamma = 1.237 \pm 0.002$ ,  $\gamma_{\xi^2} \equiv 2\nu = 1.260 \pm 0.003$ , and  $\eta \equiv 2 - \gamma/\nu = 0.0359 \pm 0.0007$ . It is not clear how much function bias remains in these results. While slightly lower than some estimates, our present exponents are consistent, within error bounds, with other analyses of the double-Gaussian model; e.g.,  $\gamma = 1.2385 \pm 0.0015$  from ref. 13,  $\gamma = 1.237 \pm 0.003$  from ref. 14,  $\gamma = 1.2378 \pm 0.0012$  from ref. 18 (we have doubled those authors’ one-standard-deviation error estimates), and  $\gamma = 1.2395 \pm 0.0004$  from ref. 19. Similarly, our results for  $\nu$  are also consistent with other analyses; e.g.,  $\nu = 0.632 \pm 0.001$  from ref. 13,  $\nu = 0.630 \pm 0.003$  from ref. 14, and  $\nu = 0.6312 \pm 0.0006$  from ref. 18. Our value  $1 - \alpha_\chi = 0.89 \pm 0.02$  is consistent with the hyperscaling relation  $3\nu = 2 - \alpha$ , but is too uncertain to be considered a significant test. By comparison, the inhomogeneous differential approximants of ref. 19 yield  $1 - \alpha_\chi = 0.895 \pm 0.007$ , for which the hyperscaling relation is satisfied to a precision of  $\pm 0.01$ .

There is now little indication of an absence of universality or of a significant discrepancy between high-temperature series and field-theoretic results. Although earlier continuum  $\phi^4$ -model estimates,<sup>(4)</sup>  $\gamma = 1.241 \pm 0.002$  and  $\eta = 0.031 \pm 0.004$ , were only marginally in agreement with the lattice results, the latest estimates<sup>(4)</sup> derived from  $\varepsilon$ -expansions and exact results,  $\gamma = 1.2390 \pm 0.0025$  and  $\eta = 2 - \gamma/\nu = 0.0365 \pm 0.003$ , are now consistent, within error limits. Additional support for universality is provided by studies of leading amplitude ratios.<sup>(19)</sup> Possible evidence for a lack of universality is that the correction-to-scaling amplitude ratio  $a_{\xi^2}/a_\chi$  is weakly model dependent and near its maximum value  $a_{\xi^2}/a_\chi \approx 1.7$  at the spin-1/2 Ising limit. This ratio is some 25% larger than the value of  $\approx 1.3$  estimated<sup>(32)</sup> for the continuum model; however, given the latest continuum model results, the value 1.3 is now suspect. Both the large magnitude and model dependence of  $a_{\xi^2}/a_\chi$  are consistent with those found by Nickel and Dixon<sup>(14)</sup> based on Roskie’s<sup>(12)</sup> quadratic mapping. The

estimate  $a_{\xi^2}/a_\chi \approx 1.42 \pm 0.14$ , obtained by Zinn-Justin<sup>(10)</sup> by a modified ratio method, is somewhat lower.

Overall, however, we believe that the analyses based on these new high-temperature series favor universality. The series are probably still too short to capture the true asymptotic behavior of the *correction-to-scaling* terms, especially since, as already mentioned, these cannot yet be predicted for the spin-1/2 Ising model treated in isolation. In view of this, we discuss in Section 5 considerations important for an extension of the present calculation to generate additional series terms.

## 2. SERIES GENERATION

The models considered in this paper are defined by the bcc family partition functions

$$Z = \prod_i \left[ \int d\phi_i f(\phi_i^2) \exp(h_i \phi_i) \right] \exp \left( K \sum_{nn} \phi_i \phi_j \right) \quad (2.1)$$

where the sites  $\mathbf{r}_i$  are either all even ( $2l, 2m, \dots$ ) or all odd ( $2l+1, 2m+1, \dots$ ) integer translations from the origin. The interaction couples “nearest” neighbor scalar fields  $\phi_i, \phi_j$  on sites separated by  $(\pm 1, \pm 1, \dots, \pm 1)$ . The 2-point correlation function in zero magnetic field  $h_i$  is

$$\langle \phi_i \phi_j \rangle = \frac{\partial^2}{\partial h_i \partial h_j} \ln Z \Big|_{\{h_i=0\}} \quad (2.2)$$

and its Fourier transform is the propagator or  $\mathbf{q}$ -dependent susceptibility

$$G(\mathbf{q}, K) = \chi_{\mathbf{q}} = \sum_j \langle \phi_i \phi_j \rangle \exp[i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)] \quad (2.3)$$

Of particular interest is the uniform susceptibility  $\chi = \chi_{\mathbf{q}=0}$  and the second moment of the spin correlations

$$M_2 = - \frac{\partial^2 \chi_{\mathbf{q}}}{\partial q_x^2} \Big|_{\mathbf{q}=0} = \sum_j (x_i - x_j)^2 \langle \phi_i \phi_j \rangle \quad (2.4)$$

from which one can define the correlation length  $\xi$  via

$$\xi^2 = M_2/2\chi \quad (2.5)$$

Different models are distinguished by the single-site field distribution

function  $f(\phi^2)$  or equivalently by its cumulant moments  $\mu_{2n}$ , which are determined from the generating function,

$$\exp \left[ \sum_n \frac{\mu_{2n}}{(2n)!} h^{2n} \right] = \int d\phi f(\phi^2) e^{h\phi} \quad (2.6)$$

A number of explicit choices for  $f(\phi^2)$  are discussed in Section 3.

The coefficients of the expansion of  $\chi_q$  in powers of  $K$  can be represented as a graphical sum. Each graph consists of vertices (lattice sites) connected by bonds [“nearest” neighbor vectors  $(\pm 1, \pm 1, \dots, \pm 1)$ ], each of which is associated with a factor  $K$ . For the zero-magnetic-field expansion considered here, the number of bonds leaving each vertex, which is the order of the vertex, must be even. For this particular counting purpose an “external” bond is considered to be associated with each *root vertex*  $i$  and  $j$  in the average  $\langle \phi_i \phi_j \rangle$  in (2.2). Also, for the free embedding scheme employed here, multiple bonds between pairs of vertices are allowed and distinct vertices in a graph are *not* restricted to correspond to distinct sites on the lattice. For a complete description of this scheme we refer the reader to the excellent article by Wortis.<sup>(33)</sup>

The numerical contribution of a particular graph is the product of a number of factors. Besides the factor  $K^n$  associated with the  $n$  internal bonds in the graph, a cumulant average  $\mu_{2m}$  is associated with each vertex of order  $2m$ . Dividing these factors is the symmetry number of the graph, which is the number of distinct ways the internal bonds and vertices can be labeled and leave the graph topologically unchanged. Finally, one must multiply by the embedding constant, which is the total number of ways the vertices of the graph can be identified with lattice sites.

For example, the graphs shown in Figs. 1a and 1b contribute to  $\chi_q$  the values

$$\chi_{[1a]} = K^{18} \mu_2^6 \mu_6^3 \mu_8 \left( \frac{1}{3! 5!} \right) \left( \frac{1}{2} \right) \sum_{\mathbf{r}_2, \dots, \mathbf{r}_{10}} V_{13} V_{14} \cdots \exp[i\mathbf{q} \cdot (\mathbf{r}_1 - \mathbf{r}_2)] \quad (2.7a)$$

$$\chi_{[1b]} = K^{18} \mu_2^3 \mu_4^5 \mu_6^2 \left( \frac{1}{3!} \right)^3 \left( \frac{1}{2} \right) \sum_{\mathbf{r}_2, \dots, \mathbf{r}_{10}} V_{13} V_{37} \cdots \exp[i\mathbf{q} \cdot (\mathbf{r}_1 - \mathbf{r}_2)] \quad (2.7b)$$

where the  $V_{ij}$  are the “nearest” neighbor interactions, that is,  $V_{ij} = 1$  if  $\mathbf{r}_i - \mathbf{r}_j = (\pm 1, \dots, \pm 1)$  and zero otherwise. The  $3!$  and  $5!$  in Eq. (2.7) correspond to the possible permutations of the multiple bonds. The factor  $1/2$  in (2.7a) is the result of the vertex pair  $7, 8 \rightarrow 9, 10$  relabeling symmetry, while in (2.7b) it is the  $4 \rightarrow 6$  relabeling.

The presence of multiple bonds does not affect the lattice site sums, since  $V_{ij}^2 = V_{ij}$ . Furthermore, since all site locations are unrestricted, site



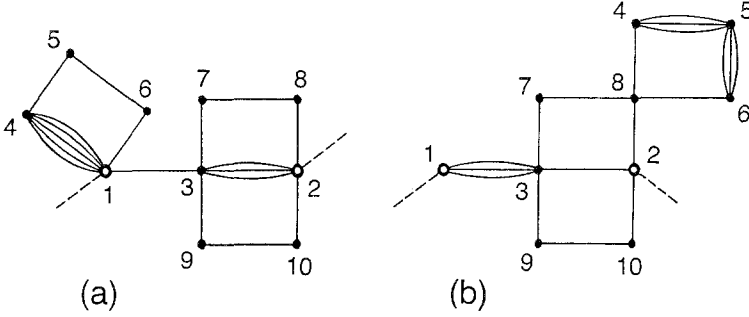


Fig. 1. Two order- $K^{18}$  contributions to  $\chi$ . The open circles labeled 1 and 2 are the roots, each solid line is a “nearest” neighbor bond associated with a factor  $K$ , and the dashed lines are the fictitious external bonds. All vertices are necessarily of even valence; all loops are of even length.

sums can also be evaluated simply in Fourier space. Using the inverse transform  $V_{ij} = \int d^d q V_{\mathbf{q}} \exp[-i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)] (2\pi)^d$ , where

$$V_{\mathbf{q}} = 2^d \cos q_x \cos q_y \cdots \quad (2.8)$$

is the Fourier transform of the “nearest” neighbor interaction  $V_{ij}$ , we obtain for the sums in both (2.7a) and (2.7b) the same three-loop integral

$$\begin{aligned} \sum_{\mathbf{r}_2, \dots, \mathbf{r}_{10}} (\dots) &= V_{\mathbf{q}} \int \frac{d^d q_1}{(2\pi)^d} \int \frac{d^d q_2}{(2\pi)^d} V_{\mathbf{q}_1}^3 V_{\mathbf{q}_2}^3 V_{\mathbf{q}_1 - \mathbf{q}_2 + \mathbf{q}} \\ &\times \int \frac{d^d q_3}{(2\pi)^d} V_{\mathbf{q}_3}^4 \end{aligned} \quad (2.9)$$

The form for  $V_{\mathbf{q}}$  in Eq. (2.8) is special to the bcc family; because of its factorizability, the expression (2.9) can be rewritten as a product  $\prod_x E_{q_x}$  of  $d$  one-dimensional embedding constants, of the form

$$\begin{aligned} E_{q_x} &= 2 \cos q_x \int_0^{2\pi} \frac{dq_1}{2\pi} \int_0^{2\pi} \frac{dq_2}{2\pi} (2 \cos q_1)^3 (2 \cos q_2)^3 \\ &\times 2 \cos(q_1 - q_2 + q_x) \int_0^{2\pi} \frac{dq_3}{2\pi} (2 \cos q_3)^4 \\ &= 108 + 108 \cos 2q_x \end{aligned} \quad (2.10)$$

where  $q_x$  is one of the components of  $\mathbf{q}$ . The evaluation of such one-dimensional embedding constants is usually most easily carried out in position space, but in any case is no longer the most time-consuming part of the graph calculation. This is the crucial feature that has made the present order- $K^{21}$  calculation possible.

Quite generally, the contribution of a particular graph to  $\chi_q$  is of the two possible forms

$$\chi_{[g]} = \frac{1}{n!} K^n \prod_m (\mu_{2m})^{c_m} \prod_\alpha \left( \sum_k e_k \left\{ \begin{array}{l} \cos 2kq_\alpha \\ \cos(2k+1)q_\alpha \end{array} \right\} \right) w \quad (2.11)$$

A complete description of this contribution is contained in the two linear and integer arrays  $c_m$  and  $e_k$  and the weight  $w$ , which, because of the factor  $n!$ , is also an integer. Graphs which are described by the same characteristic arrays  $c_m$  and  $e_k$  can be combined by adding together their respective weights  $w$ . This leads to a very considerable reduction of the number of tabular entries. Further reduction is possible if we specialize to the uniform susceptibility or the second moment; the array  $e_k$  can then be combined into the single number  $E_g$  as in (1.1) or the pair  $E_g$  and  $F_g$  as in (1.2). This reduction in storage requirements is the second most important feature that has made possible the present calculation.

In the remainder of this section we will describe a few technical details of the graph generation program. We have used the 2-point renormalization scheme as outlined by Wortis,<sup>(33)</sup> with one basic difference: that we never explicitly specify the field distribution function  $f(\phi^2)$  and hence the moments  $\{\mu_{2m}\}$ . Instead, the equivalent information is always stored in arrays like  $c_m$  in (2.11) which specify the number of vertices of various orders.

The program divides roughly into five parts. First, a table of elementary 2-rooted, 2-irreducible graphs is generated. Second, the bonds in these graphs are replaced in all possible ways by 2-rooted, 1-irreducible segments to produce a table of elementary 2-rooted, 1-irreducible contributions. Third, another program segment generates 2-rooted nodal and ladder contributions which, when combined with the elementary contributions, yields a table of all 2-rooted, 1-irreducible contributions. Fourth, the two roots are collapsed to a single root to generate vertex insertions. These are self-consistently iterated to generate a complete table of 1-rooted contributions with bare vertices. Fifth, the 1-root contributions are used as replacements for the vertices in the 2-rooted, 1-irreducible table to generate all 2-rooted contributions with bare vertices. These last two tables constitute the information from which  $\chi$  and  $M_2$  can be obtained via (1.1) and (1.2).

The description of the entire program would be too long and not particularly instructive. Instead, we outline below the third segment to give a flavor of the data-handling techniques we have employed. Some additional remarks may be found in Section 5, where we discuss the prospects for a higher-order calculation.

Assume that a table of low-order elementary, nodal, and ladder con-

tributions exists. A particular entry contains the following information elements: (1) order  $n$ ; (2) type: elementary, nodal, or ladder; (3) whether the embedding constant array represents an expansion in  $\cos 2kq$  or  $\cos(2k+1)q$  [cf. Eq. (2.11)]; (4) whether the roots are of odd order or even order; (5) orders  $v_L$  and  $v_R$  of the two roots; (6) array in which element  $c_m$  is the number of vertices exclusive of the roots of order  $2m$ ; (7) number of elements in embedding constant array  $e_k$ ; (8) greatest common factor  $f$  of the array elements  $e_k$ ; and (9) pointer to another table giving location of the reduced array  $e_k/f$ . For ladder entries the following additional information is stored: (10) pointer to the same table giving location of the most recently added rung; and (11) the number of times  $l$  this particular rung is present in the ladder. The final piece of information is the weight  $w$ , which, because it is an integer of order  $n!$ , is stored in four 32-bit words as an IBM quadruple-precision real. All the remaining information is packed into additional sets of four 32-bit words.

This packing onto a fixed length of 32 bytes/entry considerably simplifies the data handling. The variable-length entries are restricted entirely to the table of reduced embedding constant arrays  $e_k/f$ , but it is a relatively short table and its handling is not a problem. Note also that packing leads in some cases to greater efficiency in the use of the data. For example, the entire array  $c_m$  fits in a single 32-bit word and the addition of two arrays  $c_m$  and  $c'_m$  becomes the addition of two single words. Since addition is the only operation performed on the  $c_m$  arrays in this particular program segment, those arrays need never be unpacked.

The rules for generating a new graph  $C$  from two graphs  $A$  and  $B$  are simple. A ladder  $C$  can be generated from all possible  $A$  and  $B$  that have the same information element 3, except that, to avoid overcounting, both may not simultaneously be ladders themselves. Also, again to avoid overcounting, the rungs are added in a particular order; if  $B$  is considered as the new rung to be added to  $A$ , it may not come from any table location beyond that of the previously added rung (see information element 10). If it comes from the same location,  $l$  is incremented by unity; otherwise,  $l$  is set equal unity (see information element 11). Then

$$\begin{aligned} n(C) &= n(A) + n(B) \\ v_{L,R}(C) &= v_{L,R}(A) + v_{L,R}(B) \\ c_m(C) &= c_m(A) + c_m(B) \\ e_k(C) &= e_k(A) \cdot e_k(B) \\ w(C) &= \binom{n(C)}{n(A)} w(A) w(B)/l \end{aligned}$$

The binomial coefficient in the expression for the new weight arises because of our decision to include a factor of  $n!$  in (2.11); dividing the weight by  $l$  generates the correct  $l!$  symmetry factor associated with  $l$  identical rungs in the ladder. Similarly, a nodal contribution  $C$  can be generated from all  $A$  and  $B$  that have the same information element 4, except that both may not be nodal. Now

$$\begin{aligned} n(C) &= n(A) + n(B), & v_L(C) &= v_L(A), & v_R(C) &= v_R(B) \\ c_m(C) &= c_m(A) + c_m(B) + \delta_{2m, v_R(A) + v_L(B)} \\ w(C) &= \binom{n(C)}{n(A)} w(A) w(B) \end{aligned}$$

The new embedding constant  $e_k(C)$  is a convolution of the two arrays,  $e_k(A)$  and  $e_k(B)$ ; that is, the new array in Fourier space representation is a simple product of the old arrays.

As new contributions are generated, a search is initiated through the embedding constant array table for the reduced array  $e_k/f$ . If such an entry is found, the pointer to this old entry is recorded as information element 9; otherwise, a new entry is made and a new pointer is generated first. A search based on the  $B$ -tree algorithm described by Knuth<sup>(34)</sup> is then initiated through the table of ladder or nodal graphs. If an entry is found whose four 32-bit word descriptor is identical to the descriptor of the new contribution, the new weight  $w$  is added to the already stored weight. Otherwise, a new entry is established. Note that what is stored in this 2-rooted, 1-irreducible table of elementary, ladder, and nodal contributions is not necessarily individual graphs, but, rather, sums of graphs whose description elements 1–11 given above are the same. Even with this very significant packing, the cumulative number of entries in the table through order  $K^{21}$  is nearly 3,000,000 and requires three 40-megabyte tapes for storage.

We conclude by reviewing the most important features of the present calculation. First, it is not important that free embedding counts are larger than the counts in either the weak or the strong embedding scheme. What is crucial, and yet was not recognized in the Wortis article,<sup>(33)</sup> is that for the bcc family of lattices the free embedding count factorizes and each graph embedding constant reduces to a one-dimensional calculation. Also, each graph that contributes in dimension  $d=3$ , say, also contributes in any other dimension  $d$ . Thus, the known  $d=1$  and  $d=2$  results serve as complete sum rule checks not available in the weak and strong embedding schemes. Second, although renormalization in the free embedding scheme replaces graphical complexity by algebraic complexity, it was recognized by

Wortis and co-workers<sup>(33,35)</sup> that a significant advantage can still be gained by renormalization. That is, if the complete description of a graph as contained, say, in the adjacency matrix<sup>(33)</sup> is replaced by the limited algebraic information as given in 1–11 above, then many graphs may combine into a single algebraic entry. Savings in both handling time and storage increase dramatically with the order of the calculation.

At the 1-point and 2-point renormalization level used here, only elementary 2-rooted, 2-irreducible graphs need be generated and stored as graphs. For orders 7, 9, 11, 13, 15, 17, 19, and 21 the cumulative total number of elementary graphs required is approximately 1, 1, 6, 26, 145, 917, 6931, and 60,237. Extrapolation suggests that about  $7 \times 10^6$  graphs would be required for an order- $K^{25}$  calculation: such a list is quite manageable in terms of storage requirements. However, to generate this list is nontrivial by present techniques and will be discussed briefly in Section 5. We now believe this is a more fundamental barrier to any extension of the series for  $\chi$  and  $M_2$  than the problem of sorting and storing the 1-irreducible contributions as stated at Cargese.<sup>(9)</sup>

### 3. MODELS

The models discussed in this paper are distinguished by the scalar-field distribution function  $f(\phi^2)$  in (2.1). In all our work below we choose the width of this distribution so that the second (cumulant) moment is unity; i.e.,

$$\mu_2 = \int d\phi \phi^2 f(\phi^2) / \int d\phi f(\phi^2) = 1 \quad (3.1)$$

With this normalization our definitions of certain models differ from the conventional ones by a rescaling of the inverse temperature parameter  $K$ .

#### 3.1. Spin- $S$ Ising Model

Of the many possible simple scalar models, probably the best known is the spin- $S$  Ising model in which 3-dimensional quantum spins interact via the anisotropic coupling  $JS_i^z S_j^z$ . This model is equivalent to the scalar model (2.1) with the choice

$$f(\phi^2) = \sum_{m=-S}^S \delta(\phi + 2m\sqrt{y}), \quad y = \frac{3}{4S(S+1)} \quad (3.2)$$

From the logarithmic derivative of the generating function (2.6) we easily derive

$$\mu_{2n} = \frac{d^{2n-1}}{dh^{2n-1}} [(2S+1)\sqrt{y} \coth[(2S+1)\sqrt{y}h] - \sqrt{y} \coth \sqrt{y}h]_{h=0} \quad (3.3)$$

which, by use of  $(2S+1)^2 = 1 + 3/y$  and the known expansion for  $\coth x$ , we can also rewrite entirely in terms of the parameter  $y$  as

$$\mu_{2n} = [(3+y)^n - y^n] \frac{4^n B_{2n}}{2n} \quad (3.4)$$

where the  $B_{2n}$  are the Bernoulli numbers. Because of the particular polynomial form of the moments in (3.4), the expressions (1.1) and (1.2) for  $\chi$  and  $M_2$  reduce to the double power series of essentially triangular form

$$\begin{aligned} \chi(K, y) &= A_0^0 + \sum_{n=1} K^n \sum_{m=1}^n \frac{A_n^m}{m!} y^{m-1} \\ M_2(K, y) &= \sum_{n=1} K^n \sum_{m=1}^n \frac{B_n^m}{m!} y^{m-1} \end{aligned} \quad (3.5)$$

Because the coefficients  $A_n^m$  and  $B_n^m$  for the spin- $S$  models are not integers (though they could be expressed as rational fractions), they will not be presented here. Readers interested in these tables should consult the authors. However, the single variable series for  $S=1/2, 1, 2$ , and  $\infty$  in dimensions 2 and 3 are given in the Appendix (Table I).

### 3.2. Blume-Capel Model

Another simple model that has been discussed in the literature and is useful for the study of tricritical behavior in addition to ordinary critical behavior is the Blume-Capel, or 3-state, model.<sup>(25)</sup> The distribution function with our normalization (3.1) is

$$f(\phi^2) = \delta(\phi + \sqrt{y}) + 2(y-1)\delta(\phi) + \delta(\phi - \sqrt{y}) \quad (3.6)$$

and its cumulant moments are given by

$$\mu_{2n} = \frac{d^{2n-1}}{dh^{2n-1}} \left[ \frac{\sqrt{y} \sinh \sqrt{y} h}{y-1 + \cosh \sqrt{y} h} \right]_{h=0} \quad (3.7)$$

Explicit power series division in (3.7) shows that the  $\mu_{2n}$  for  $n > 1$  can be generated recursively from the relation

$$\mu_{2n} = y^{n-1} - \sum_{m=1}^{n-1} y^{n-1-m} \binom{2n-1}{2m-1} \mu_{2m} \quad (3.8)$$

Because the  $\mu_{2n}$  in (3.8) are of the same polynomial form as in (3.4), the Blume–Capel  $\chi$  and  $M_2$  series are also expressible in the triangular form (3.5). The coefficients  $A_n^m$  and  $B_n^m$  for this model in both  $d=2$  and  $d=3$  are listed in the Appendix (Table II). Except for the  $A_0^0=1$  entry in the tables for  $\chi$ ,  $m$  varies from 1 to  $n$  for fixed  $n$  in each block of  $n$  values. Two checks are possible in that  $y=1$  is the  $S=1/2$  model,  $y=3/2$  is  $S=1$ . The value  $y=2$  yields the  $l=2$  “loop model” mentioned most recently by Zinn-Justin.<sup>(7)</sup> In the neighborhood of some critical value  $K=K_c(y)$ ,  $y=y_c > 2$ , the model is expected to display tricritical behavior. In the future one might attempt both to locate this point and deduce the expected logarithmic corrections that modify the classical (mean field) behavior in  $d=3$ . However for the present we believe it is more useful to deal with simpler models in which the mean-field point is purely Gaussian and its location is exactly known.

### 3.3. Ising-Gaussian Interpolation Models

One simple model that can interpolate between  $S=1/2$  Ising and Gaussian behavior is a model of classical, fixed-length,  $y$ -dimensional spins, again coupled anisotropically via  $JS_i^z S_j^z$ . In this case the equivalent scalar distribution is

$$f(\phi^2) = \begin{cases} (y - \phi^2)^{(y-3)/2}, & |\phi| < \sqrt{y} \\ 0, & |\phi| > \sqrt{y} \end{cases} \quad (3.9)$$

which in the limit  $y \rightarrow 1$  becomes the  $S=1/2$  Ising distribution and in the limit  $y \rightarrow \infty$  becomes the Gaussian  $f \propto \exp(-\phi^2/2)$ . In the interval  $1 < y < \infty$ , the model passes through the  $S=\infty$  Ising point at  $y=3$ . However, the power moments of the distribution,  $m_{2n} \equiv \int f(\phi^2) \phi^{2n} d\phi$ , which can be determined recursively from

$$m_{2n+2} = \frac{y(2n+1)}{y+2n} m_{2n} \quad (3.10)$$

are not polynomials in  $y$  and thus a simple triangular expansion as in (3.5) is not possible. Similarly, the  $\phi^4$  model<sup>(1)</sup> defined by  $f(\phi^2) \propto \exp[\alpha\phi^2 - \beta(\alpha)\phi^4]$ ,  $\beta(\alpha) > 0$ , does not have a triangular expansion.

We have not bothered to tabulate single variable series for these models, but have instead concentrated on two other models which do have triangular expansions similar to (3.5). These models, the Klauder<sup>(26)</sup> and double-Gaussian,<sup>(23)</sup> or range,<sup>(27)</sup> also allow interpolation between  $S = 1/2$  Ising and Gaussian. A possible limitation is that they are not defined for temperatures below some critical value, i.e.,  $K > K^*(y)$ . However, as this temperature is below the interesting second-order phase transition line  $K = K_c(y)$ , we feel they are useful nonetheless and hope that our work will trigger further investigations into their properties.

### 3.4. Klauder Model

The Klauder model<sup>(26)</sup> is defined by the distribution

$$f(\phi^2) = |\phi|^{y/(1-y)} e^{-\phi^2/2(1-y)} \quad (3.11)$$

provided that

$$K < K^*(y) = \frac{1}{2^d(1-y)} \quad (3.12)$$

On the interval  $0 \leq y \leq 1$  the model interpolates between Gaussian and  $S = 1/2$  Ising. Since the moments satisfy the recursion relations

$$m_{2n+2} = (2n+1-2ny)m_{2n} \quad (3.13)$$

the cumulant moments  $\mu_{2n}$  are again polynomials of order  $n-1$  as in (3.4). It is, however, convenient to rewrite the expansion for  $\chi$  and  $M_2$  for the model as

$$\begin{aligned} \chi(K, y) &= A_0^0 + \sum_{n=1}^{\infty} \frac{2^n}{n!} K^n \sum_{m=1}^n A_n^m y^{m-1} \\ M_2(K, y) &= \sum_{n=1}^{\infty} \frac{2^n}{n!} K^n \sum_{m=1}^n B_n^m y^{m-1} \end{aligned} \quad (3.14)$$

For  $d=3$  the coefficients  $A_n^m$  and  $B_n^m$  are integers and are listed in Table III of the Appendix with precisely the same ordering as used for the Blume-Capel model series.

Some properties of the Klauder model in the vicinity of the Gaussian line  $y=0$  can be determined fairly directly, as we illustrate below specifically for  $d=3$ . Note that at  $y=0$  all  $\mu_{2n}$  for  $n > 1$  vanish and the propagator (2.3) is given by the free-field expression

$$G_0(\mathbf{q}, K) = (1 - 8K \cos q_x \cos q_y \cos q_z)^{-1} \quad (3.15)$$



Corrections to this result can be derived systematically if we treat  $y$  as a small parameter. To obtain a complete description near the critical point the full machinery of renormalized perturbation theory should be used, but here we will only evaluate the leading  $y$  dependence of the critical line  $K_c(y)$ , for which lowest order elementary perturbation theory is adequate. For small  $y$  the cumulant moments are given by

$$\mu_{2n+2} \approx (-2)^n n! y, \quad n \geq 0 \quad (3.16)$$

Then the propagator to leading order in  $y$  is modified by a self-energy which is a sum of terms, each corresponding to a single vertex insert of order greater than two. Attached to the vertex of order  $2n+2$  are  $n$  closed loops with symmetry factor  $2^n n!$ . Each loop contributes a factor given by the momentum integral

$$I(K) = \int \frac{d^3 q}{(2\pi)^3} [G_0(\mathbf{q}, K) - 1] \quad (3.17)$$

and so the complete self-energy contribution is

$$\sum_{n=1}^{\infty} \frac{\mu_{2n+2}}{2^n n!} [I(K)]^n = -\frac{yI(K)}{1+I(K)} \quad (3.18)$$

The susceptibility is

$$G(\mathbf{q}, K) \approx \left( 1 - 8K \cos q_x \cos q_y \cos q_z + \frac{yI(K)}{1+I(K)} \right)^{-1} \quad (3.19)$$

and the critical  $K_c(y)$  is determined by the divergence of  $G(0, K)$ . To leading order in  $y$ ,

$$8K_c(y) \approx 1 + \frac{yI(1/8)}{1+I(1/8)} \quad (3.20)$$

Numerically,  $I(1/8) = (4/\pi^2) K^2(1/2) - 1 \approx 0.3982\dots$ , where here  $K(m)$  is the complete elliptic integral.<sup>(36)</sup> Note that the instability line as given by (3.12) is, to leading order in  $y$ ,

$$8K^*(y) \approx 1 + y \quad (3.21)$$

and thus for  $y > 0$ ,  $K_c < K^*$ . For  $y < 0$ ,  $K_c > K^*$  and Ising-like critical behavior *cannot* be observed in this regime. It is for this reason that we believe the model is not useful for the purpose originally envisioned by Klauder.<sup>(26)</sup>

### 3.5. Double-Gaussian Model

The second very useful model with a triangular expansion is the double-Gaussian model defined by

$$f(\phi^2) = \exp \left[ -\frac{(\phi + \sqrt{y})^2}{2(1-y)} \right] + \exp \left[ -\frac{(\phi - \sqrt{y})^2}{2(1-y)} \right] \quad (3.22)$$

provided the restriction (3.12) is again fulfilled. Also,<sup>7</sup> just as for the Klauder model, this model interpolates between Gaussian and  $S=1/2$  Ising as  $y$  varies between 0 and 1. However, somewhat surprisingly, this model has an analytic continuation to the regime  $y > 1$ , which can be interpreted physically and which we call the range model. The cumulant moments for the double-Gaussian model are simply related to the  $S=1/2$  Ising moments  $\mu_{2n}^{(I)} = (4^n - 1)4^n B_{2n}/(2n)$ , given in (3.4),

$$\mu_{2n} = \begin{cases} \mu_2^{(I)} = 1, & n = 1 \\ y^n \mu_{2n}^{(I)}, & n > 1 \end{cases} \quad (3.23)$$

and the expressions (1.1) and (1.2) for  $\chi$  and  $M_2$  can therefore be written

$$\begin{aligned} \chi(K, y) &= A_0^0 + \sum_{n=1} K^n \left( A_n^0 + \sum_{m=1}^n \frac{A_n^m}{m!} y^{m+1} \right) \\ M_2(K, y) &= \sum_{n=1} K^n \left( B_n^0 + \sum_{m=1}^n \frac{B_n^m}{m!} y^{m+1} \right) \end{aligned} \quad (3.24)$$

The integer coefficients  $A_n^m$  and  $B_n^m$  are listed in Table IV of the Appendix for  $d=3$ . Within each block of  $n+1$  entries,  $m$  varies from 0 to  $n$ . Note that a 3-way sum rule check is possible between Blume-Capel, Klauder, and double-Gaussian tables by setting  $y=1$ .

An analysis similar to that described for the Klauder model can be used to determine the leading behavior of the critical line  $K_c(y)$ . In this case, (3.23) shows directly that the leading self-energy corrections involve only the fourth-order vertex insert at order  $y^2$  and the sixth-order vertex insert at order  $y^3$ . We find

$$G(\mathbf{q}, K) \approx \{1 - 8K \cos q_x \cos q_y \cos q_z + y^2 I(K) - 2y^3 [I(K)]^2\}^{-1} \quad (3.25)$$

<sup>7</sup> One can show that both models are members of a class of one-parameter models with triangular expansions for the series coefficients, all of which interpolate continuously between Ising and Gaussian limits. The moment generating functions  $G(h) = \int f(\phi^2) \exp(-h\phi) d\phi$  for this class satisfy the second-order differential equation  $G'' - (1+\lambda)(1-y)hG' - [1 - \lambda(1-y)^2 h^2]G = 0$ , with  $0 \leq \lambda \leq 1$ . The value  $\lambda=0$  corresponds to the Klauder model and  $\lambda=1$  to the double-Gaussian model.

which diverges at  $\mathbf{q} = 0$  when  $K = K_c(y)$ , where

$$8K_c(y) \approx 1 + y^2 I(\frac{1}{8}) - 2y^3 [I(\frac{1}{8})]^2 \quad (3.26)$$

Again, for  $y > 0$ ,  $K_c < K^*$ , and so it is consistent to identify  $K_c(y)$  as the critical line.

### 3.6. Range Model

As observed by Baker and Bishop,<sup>(27)</sup> the partition function (2.1) in uniform magnetic field  $h_i = h$  with the double-Gaussian distribution (3.22) can be written in the Ising-like form of a sum over discrete “spin” values:

$$\begin{aligned} Z_{\text{DG}}(K, y, h) &= \sum_{\{s_i = \pm 1\}} \prod_i \int d\phi_i \exp \left\{ K \sum_{nn} \phi_i \phi_j - \sum_i \frac{(\phi_i - s_i \sqrt{y})^2}{2(1-y)} + h \sum_i \phi_i \right\} \quad (3.27) \end{aligned}$$

or

$$\begin{aligned} Z_{\text{DG}}(K, y, h) &= Z_1(y) \sum_{\{s_i = \pm 1\}} \prod_i \int d\phi_i \exp \left\{ -\frac{1}{2} \sum_{ij} \phi_i M_{ij} \phi_j \right. \\ &\quad \left. + \sum_i \phi_i \left( h + \frac{s_i \sqrt{y}}{1-y} \right) \right\} \quad (3.28) \end{aligned}$$

where

$$M_{ij} = \int \frac{d^d q}{(2\pi)^d} M_{\mathbf{q}} \exp[i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)], \quad M_{\mathbf{q}} = \frac{1}{1-y} - KV_{\mathbf{q}} \quad (3.29)$$

with  $V_{\mathbf{q}}$  the “nearest” neighbor interaction (2.8). The prefactor  $Z_1(y)$  in (3.28) does not depend on the field  $h$  and hence will not enter into the calculation of the susceptibility to be discussed below. The integration over the Gaussian field variables  $\phi_i$  is accomplished by first shifting  $\phi_i$  to  $\phi_i + \sum_j M_{ij}^{-1} [h + s_j y^{1/2}/(1-y)]$ , where the inverse matrix  $M_{ij}^{-1}$  is

$$\begin{aligned} M_{ij}^{-1} &= \int \frac{d^d q}{(2\pi)^d} M_{\mathbf{q}}^{-1} \{ \exp[i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)] \} \\ &= (1-y) \delta_{ij} + K(1-y)^2 \\ &\quad \times \int \frac{d^d q}{(2\pi)^d} \frac{V_{\mathbf{q}}}{1 - K(1-y)V_{\mathbf{q}}} \exp[i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)] \quad (3.30) \end{aligned}$$

We obtain

$$Z_{\text{DG}}(K, y, h) = Z_2 \sum_{\{s_i = \pm 1\}} \exp \left\{ \frac{1}{2} \sum_{ij} \left( h + \frac{s_i \sqrt{y}}{1-y} \right) \right. \\ \left. \times M_{ij}^{-1} \left( h + \frac{s_i \sqrt{y}}{1-y} \right) \right\} \quad (3.31)$$

and the argument of the exponential in (3.31) can be simplified, with the use of the result  $\sum_j M_{ij}^{-1} = (1-y)/[1-2^d K(1-y)]$ , to

$$\left\{ \frac{y}{2(1-y)^2} \sum_{ij} s_i M_{ij}^{-1} s_j + h \sqrt{y} \sum_i \frac{s_i}{1-2^d K(1-y)} \right. \\ \left. + \frac{1}{2} \frac{Nh^2(1-y)}{1+2^d K(1-y)} \right\} \quad (3.32)$$

where  $N$  is the number of sites in the lattice. Note also that the diagonal term  $(1-y)\delta_{ij}$  in (3.30) will contribute a constant to the quadratic  $s_i M_{ij}^{-1} s_j$ , which can be absorbed into the prefactor in (3.31) and change it to  $Z_3(K, y)$ .

Let us now define an  $S=1/2$  Ising model with the ‘‘long’’-range interaction  $K'J_{ij}(\rho)$ , where

$$J_{ij}(\rho) = \int \frac{d^d q}{(2\pi)^d} \frac{V_{\mathbf{q}}}{1-\rho V_{\mathbf{q}}} \exp[i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)] \quad (3.33)$$

Provided  $|\rho| < 2^{-d}$ , the interactions are exponentially damped with distance; in the coordinate direction  $x$ , say,  $J_{ij} \sim e^{-x_{ij}/\lambda}$ , where the range  $\lambda$  is the solution of  $\cosh(1/\lambda) = 2^{-d}/|\rho|$ . For  $K' > 0$ , which we consider here, the ‘‘nearest’’ neighbor interaction is always ferromagnetic, as indeed are all interactions between a spin at the origin and a spin on the odd lattice sites  $(2l+1, 2m+1, \dots)$ . However, the interactions between spins at the origin and even lattice sites  $(2l, 2m, \dots)$  are only ferromagnetic for  $\rho > 0$ ; for  $\rho < 0$  these interactions inhibit ferromagnetic ordering. But since the total interaction  $\sum_j J_{ij} = 2^d/(1-2^d \rho)$  is always ferromagnetic, the model is only an example of a *partially frustrated* ferromagnet in the regime  $\rho < 0$ . The partition function for this model, which we call the range model, is defined as

$$Z_{\text{R}}(K', \rho, h') = \sum_{\{s_i = \pm 1\}} \exp \left\{ \frac{1}{2} K' \sum_{ij} s_i J_{ij}(\rho) s_j + h' \sum_i s_i \right\} \quad (3.34)$$

and on comparing (3.34) with (3.31) and (3.32) we find

$$\ln Z_{\text{DG}}(K, y, h) = \ln Z_{\text{R}}(Ky, K(1-y), \sqrt{y} h/[1-2^d K(1-y)]) \\ + \frac{1}{2} Nh^2(1-y)/[1-2^d K(1-y)] + \ln Z_3(K, y) \quad (3.35)$$

That is, except for some trivial additive functions, the double-Gaussian and range model free energies are equal, provided we make the parameter identifications

$$K' = Ky, \quad \rho = K(1 - y), \quad h' = \frac{\sqrt{y} h}{1 - 2^d K(1 - y)} \quad (3.36)$$

By differentiating (3.35) twice with respect to field, we find

$$\chi_{\text{DG}} = \frac{y}{[1 - 2^d K(1 - y)]^2} \chi_{\text{R}} + \frac{1 - y}{1 - 2^d K(1 - y)} \quad (3.37)$$

which implies that  $\chi_{\text{R}}$  has the expansion

$$\chi_{\text{R}}(K, y) = 1 + \sum_{n=1} K^n \sum_{m=1}^n \frac{R_n^m}{m!} y^m \quad (3.38)$$

The coefficients  $R_n^m$  are given in terms of the coefficients  $A_n^m$  of the double-Gaussian expansion (3.24) by

$$\begin{aligned} R_n^m = & 2^{dn} \delta_{m1} + A_n^m - 2^{d+1}(A_{n-1}^m - mA_{n-1}^{m-1}) \\ & + 2^{2d}[A_{n-2}^m - 2mA_{n-2}^{m-1} + m(m-1)A_{n-2}^{m-2}] \end{aligned} \quad (3.39)$$

with the proviso that the  $A_l^k$  on the right-hand side are set to zero whenever  $l < 1$  or  $k < 1$  or  $k > l$ .

As stressed above, the range model analytically continues the double-Gaussian model to the region  $y > 1$  provided that  $(y-1)K < 2^{-d}$ . No analysis of the series (3.38) have been performed to date, but an estimate of the critical line  $K_c(y)$  has been obtained for  $d=3$  by a crude least-squares fit to double-Gaussian model approximants in the range  $0.5 < y \leq 1$ . Our approximation is

$$K_c^{-1}(y) \approx 8 - 3.05602y^2 + 2.96137y^3 - 2.5771y^4 + 1.274y^5 - 0.248y^6 \quad (3.40)$$

The coefficients of  $y^2$  and  $y^3$  were not fixed in the fit and yet are within 4% and 14%, respectively of the exact values given in (3.26). The estimate (3.40) intersects the model boundary  $K^{-1} = 8(y-1)$  at  $y \approx 1.6$ , and thus critical behavior over the wide range  $1 < y \leq 1.6$  remains to be explored by single-variable series analysis. On the other hand, since Chen *et al.*<sup>(13)</sup> could clearly identify only a single Ising-like multicritical point in the range  $0 < y < 1.8$  for the double-Gaussian model, universality of critical exponents is to be expected.

#### 4. DOUBLE-GAUSSIAN SERIES ANALYSIS

The analysis described in this section is based on the method of confluent inhomogeneous second-order differential equations discussed by Rehr *et al.*<sup>(28)</sup> Its utility lies in the fact that it may lead to a significant test of the universality hypothesis. As discussed in Sec. 1, the method biases the unknown functions of interest to have the appropriate leading critical behavior (1.4) which, although not of the scaling form discussed by Wegner,<sup>(30)</sup> should be adequate, provided higher order terms in  $(K_c - K)^{n\theta}$  and other corrections proportional to  $(K_c - K)^{\theta_n}$ ,  $\theta_n > \theta$ , are small or can be incorporated into the analytical factors  $A_F(K)$  and  $a_F(K)$  or an "effective" background  $B_F(K)$ .

We have analyzed in detail the three-dimensional double-Gaussian model discussed in Sec. 3, which we believe is typical of models that interpolate between spin-1/2 Ising and Gaussian limits. Of course, we investigate the model only at a discrete set of parameter values. These are chosen so that the width of each Gaussian in the distribution (3.22) is an integer multiple of 0.05, i.e.,

$$\omega \equiv \sqrt{1 - y} = 0.05n \quad (4.1)$$

We could only successfully determine approximants with the critical behavior (1.4) in the range  $0 \leq \omega \leq 0.70$ ; presumably for larger  $\omega$  the higher order terms  $(K_c - K)^{n\theta}$  or other confluent corrections are so large that the fact that (1.4) is not of scaling form is significant. If  $\theta = 0.5$  exactly, (1.4) would *in principle* contain such terms. Also, because the double exponential fitting problem is so unstable, we limited ourselves to the biased problem in which  $\theta_F = \theta$  is fixed in (1.4). If a common  $\theta$  can be found for which the  $\gamma_F$  are independent of  $\omega$ , then, in a limited sense, we will have verified one aspect of universality.

The approximations to  $\chi$ ,  $M_2$ , and  $\xi^2 \propto M_2/\chi$  which have the confluent asymptotic critical behavior (1.4) are determined as the solutions of the second-order differential equation

$$[Q_2(K) D_2 + Q_1(K) D_1 + Q_0(K)] F(K) = P(K) \quad (4.2)$$

where the  $Q_i(K)$  and  $P(K)$  are polynomials in  $K$  with  $Q_1(K)$  and  $Q_2(K)$  forced to take the factorizable form

$$Q_1(K) = (K_c - K) \dot{Q}_1(K) \quad Q_2(K) = (K_c - K)^2 (K_c + K) \dot{Q}_2(K) \quad (4.3)$$

The  $D_i$  in Eq. (4.2) are differential operators in  $K$  of order  $i$ , and the coefficients in the polynomials  $Q_i(K)$  and  $P(K)$  are fit so that (4.2) is satisfied

as a power series to some order  $K^N$ . In addition to the Rehr *et al.*<sup>(28)</sup> choice for the differential operators

$$D_1 = K \frac{d}{dK} \quad D_2 = D_1^2 \quad (4.4)$$

we have used others, such as

$$D_1 = \frac{d}{dK} \quad D_2 = \begin{cases} D_1^2 \\ K D_1^2 \end{cases} \quad (4.5)$$

Finally, we have restricted our choice of approximants to those in which the degrees of the  $Q_i(K)$  are roughly comparable. The essential difference between our differential approximants and those of Guttmann<sup>(20)</sup> is the inclusion of the constraints in Eq. (4.3). Without these constraints, the solution of Eq. (4.2) generally consists of a single power-law singularity together with analytic factors and background terms, i.e., a solution which ignores non-analytic confluent singularities.

The numerical procedure for determining the critical constants in (1.4) is straightforward. For fixed  $K_c$  in (4.3) the remaining coefficients in  $Q_i$  and  $P$  are obtained from the solution of a set of linear equations. Solutions in which the function  $\hat{Q}_2(K)$  has zeros in the disk  $|K| < K_c$  or near  $K_c$  are considered “defective” and ignored. Knowledge of the polynomials  $Q_i(K)$  suffices to determine  $\gamma_F$  and  $\theta_F$  directly as the solutions of a quadratic indicial equation.<sup>(28)</sup> As already observed for the spin- $S$  Ising model,<sup>(9)</sup> very reproducible correlations between  $\gamma_F$  and  $\theta_F$  are found as  $K_c$  is varied. To fix  $\theta_F = \theta$  and hence determine our *biased*  $\gamma_F$  estimates, we employ a Newton–Raphson search which starts with  $K_c$  near the critical line given by (3.40). Occasionally, no real solution to this nonlinear problem can be found. For  $\theta$  in the neighborhood of 0.5 most final estimates of  $K_c$  at order  $K^{21}$  lie within  $5 \times 10^{-6}$  of the value (3.40) for  $0 \leq \omega \leq 0.70$ . The dispersion in these estimates is much smaller at about  $\pm 2 \times 10^{-6}$ . The use of several different choices of differential operators  $D_i$  has proved to be important. For reasons we do not understand, for some parameter ranges many approximants can be found for some particular choices of  $D_i$ , but not for others. The amplitudes  $A_F$  and  $a_F$  in (1.4) can be obtained by integrating the differential equation (4.2) numerically, starting with the known initial conditions at  $K=0$ . A simpler and faster procedure,<sup>(28)</sup> which we have adopted here, is to use the differential equation (4.2) to generate two power series representations of  $F(K)$ , one about  $K=0$ , the other about  $K=K_c$ . The expansion about  $K=0$  agrees with the known series through the order used (e.g., 21) and thereafter simply extends this series to higher order, while the expansion about  $K=K_c$  depends linearly on the two unknown

amplitudes  $A_F$  and  $A_F a_F$ . These series can be used directly to evaluate the function in the interval  $0 < K < K_c$  and matching  $F$  and  $dF/dK$  at some conveniently chosen intermediate  $K$  then determines  $A_F$  and  $a_F$ .

We have included in Table V of the Appendix 50-term series obtained from two representative differential approximants to the 21-term spin-1/2 Ising model susceptibility series:  $xd/dx[9, 6, 9; \phi]$  and  $d/dx[7, 6, 7; 1]$ . We hope these series will prove useful in tests of other methods of confluent singularity analysis. The series coefficients satisfy 9-term recurrence rela-

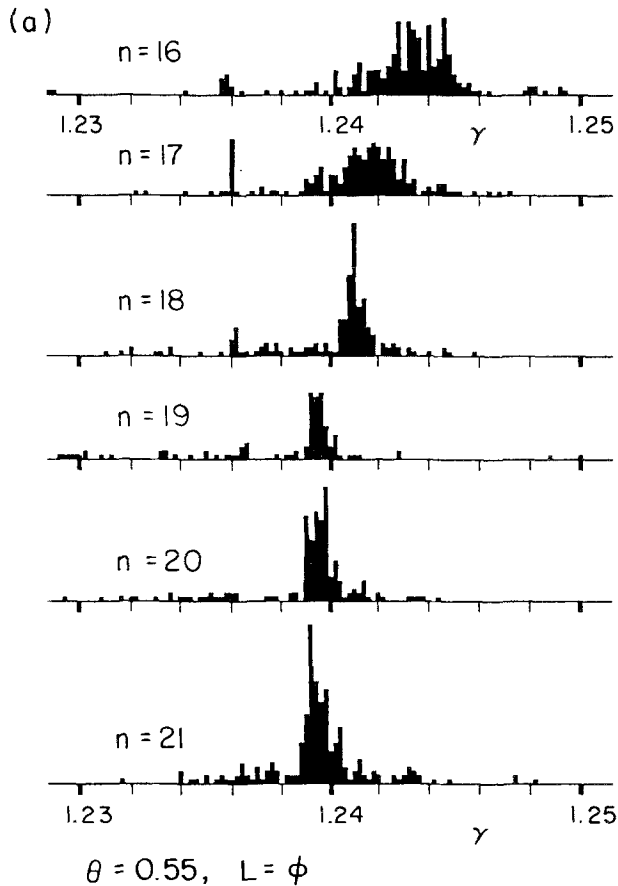


Fig. 2. (a) Number of homogeneous approximants to  $\chi(\omega)$  yielding a particular  $\gamma$  with a resolution  $2 \times 10^{-4}$ , with a fixed correction-to-scaling exponent  $\theta = 0.55$ . Results, cumulative over  $\omega = 0, 0.05, \dots, 0.70$ , show overall convergence with order; (b) As in (a), but showing instead estimates of  $1 - \alpha$  within a resolution  $2 \times 10^{-3}$  from the antiferromagnetic singularity in  $\chi$ ; (c) Again, estimates of  $\gamma$  from  $\chi$ . Here  $\theta = 0.50$  and  $n = 21$  are fixed. The order of the inhomogeneous term  $P_L$  in (4.2) varies from  $L = \phi$  ( $P_L$  null) through  $L = 2$  as indicated.



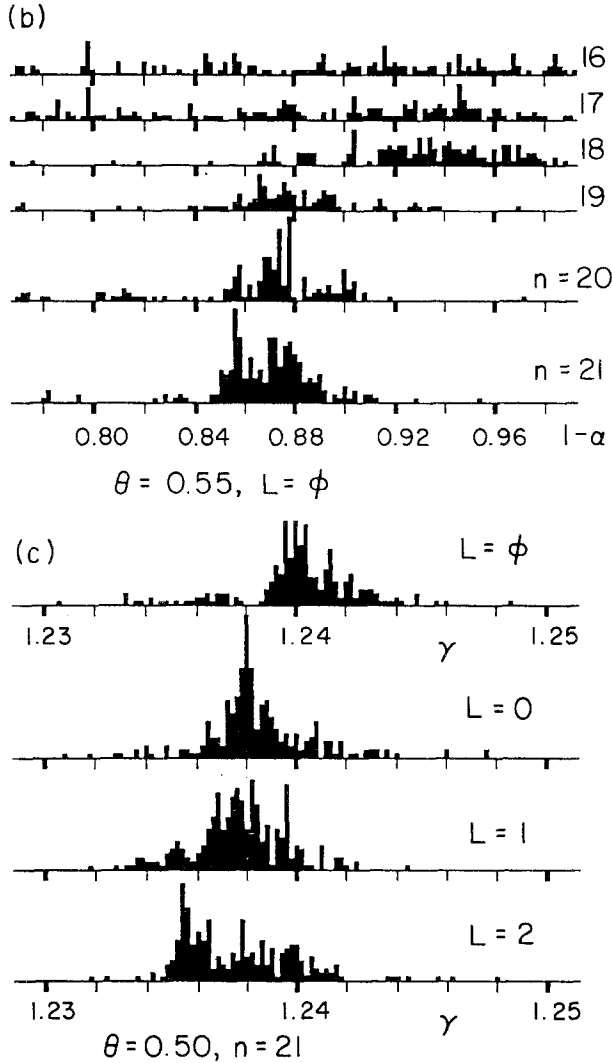


Fig. 2. (Continued)

tions of the form  $\sum_{ij} Q(i, j)(n-j)^i c(n-j) = P(n)$ , from which additional terms can be calculated.

Two important trends are apparent when all the data for  $0 \leq \omega \leq 0.70$  are combined into a single output. The first is convergence with order; in Figs. 2a and 2b we show histograms of the number of biased *homogeneous* ( $L = \phi$ ) differential approximant estimates for  $\gamma$  and  $1 - \alpha$  with  $\theta = 0.55$

based on  $\chi$  series to order  $K^n$ ,  $n = 16, 17, \dots, 21$ . We note that even forcing a correction-to-scaling term, as we have done by using (4.2), does not guarantee converged estimates if the series length is too short. Consistency suggests that only the  $n = 19, 20$ , and  $21$  estimates for  $\gamma$  represent the asymptotic value. It is interesting but probably coincidental that also no significant estimate of  $1 - \alpha$  can be made until  $n \geq 19$ . The second important trend results from allowing for a nonvanishing polynomial  $P(K)$  in (4.2). In Fig. 2c we show biased estimates  $\gamma$  with  $\theta = 0.50$ , with  $P$  ranging from null ( $L = \phi$ ) to finite order  $L = 0, 1, 2$ . There is a significant drop in the estimate of  $\gamma$  in going from  $L = \phi$  to 0 or 1, while at  $l = 2$  the dispersion in the estimates begins to increase. Since we have no *a priori* reason for believing the background  $B_F$  in (1.4) should be zero and hence  $P$  null, and because they tend to reduce the scatter and improve overall consistency, we base most of our quantitative estimates in the following on  $L = 1$  inhomogeneous differential approximants.

Detailed results explicitly showing variations with  $\omega$  are displayed in Figs. 3–6. Figures 3 and 4 are histograms of the number of biased estimates of  $\gamma$  for each value of  $\omega$  separately; Fig. 3 illustrates convergence with order, while Fig. 4 illustrates the effect of inhomogeneous terms in the differential equation (4.2). In both figures we also show the effect of changes in  $\theta$  between 0.50 and 0.55 at order  $K^{21}$ . We find that  $\gamma$  correlates positively with  $\theta$  for small  $\omega$  and anticorrelates with  $\theta$  for large  $\omega$ , in qualitative agreement with the spin- $S$  Ising results.<sup>(9)</sup> Our “best” approximants are those obtained with the polynomial  $P$  of order  $L = 1$ ; those based on the operator choice (4.5) are shown in Figs. 4c and 4d for  $\theta = 0.50$  and 0.55. From this and additional data based on the choice (4.4) we conclude that universality is best satisfied with

$$\gamma = 1.237 \pm 0.002, \quad \theta_\chi = 0.52 \pm 0.03 \quad (4.6)$$

The error bars are subjective, but, we believe, reasonable. In particular, the very distinct downward trend of  $\gamma$  with increasing  $\omega$  shown in Fig. 4d makes any value  $\theta > 0.55$  unreasonable if universality is assumed. On the other hand,  $\theta$  slightly smaller than 0.50 is probably not excluded by the data shown in Fig. 4c, especially if the estimates for  $\omega \geq 0.60$  are excluded as unreliable. Such exclusion might be reasonable, since the amplitude  $a_\chi$  is large in this regime and the form (1.4) is likely first to become inadequate there. Finally, the estimate (4.6) is lower than our preliminary spin- $S$  estimate  $\gamma = 1.239 \pm 0.002$  almost certainly because of our present reliance on inhomogeneous approximants. Figure 5 shows histograms of biased estimates of  $2\nu$  determined from  $M_2/\chi = 2\xi^2$  approximants. Again, from the

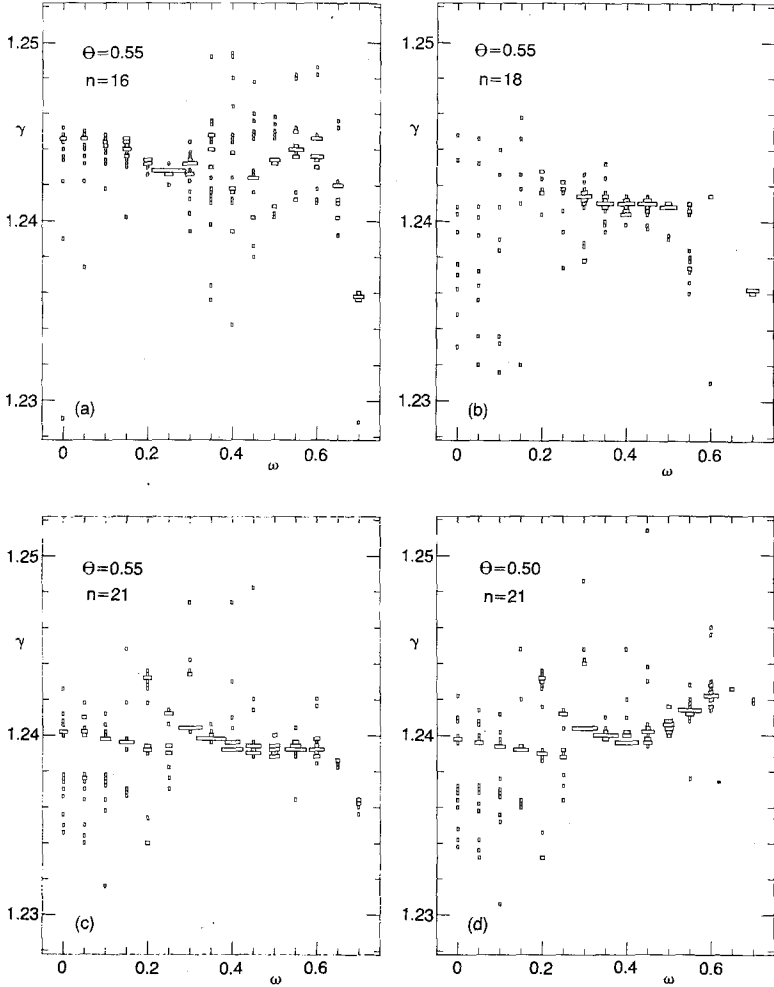


Fig. 3. Histograms, centered on discrete  $\omega$ , of the number of homogeneous approximants to  $\chi(\omega)$  yielding a particular  $\gamma$  with resolution  $2 \times 10^{-4}$ . For each  $\omega$ , about 25 approximants with the choice (4.5) are sought; of those that are found, only the nondefective are plotted. This number may be small, as, for example, in (b), where for  $\omega=0, 0.05, \dots$  only 10, 10, 8, 6, 7, ... estimates are available. Plots (a), (b), and (c) show variations with order  $n$  with fixed  $\theta=0.55$  and are a detailed breakdown of some of the cumulative results in Fig. 2a. The result of changing to  $\theta=0.50$  with  $n=21$  is shown in (d). The equivalent cumulative result is shown in Fig. 2c.

$L = 1$  data shown in Figs. 5c and 5d and from additional data based on (4.4), we conclude that universality is best satisfied with

$$2\nu = 1.260 \pm 0.003, \quad \theta_{\xi^2} = 0.51 \pm 0.03 \quad (4.7)$$

The consistency between  $\theta_{\xi^2}$  and  $\theta_\chi$  is noteworthy.

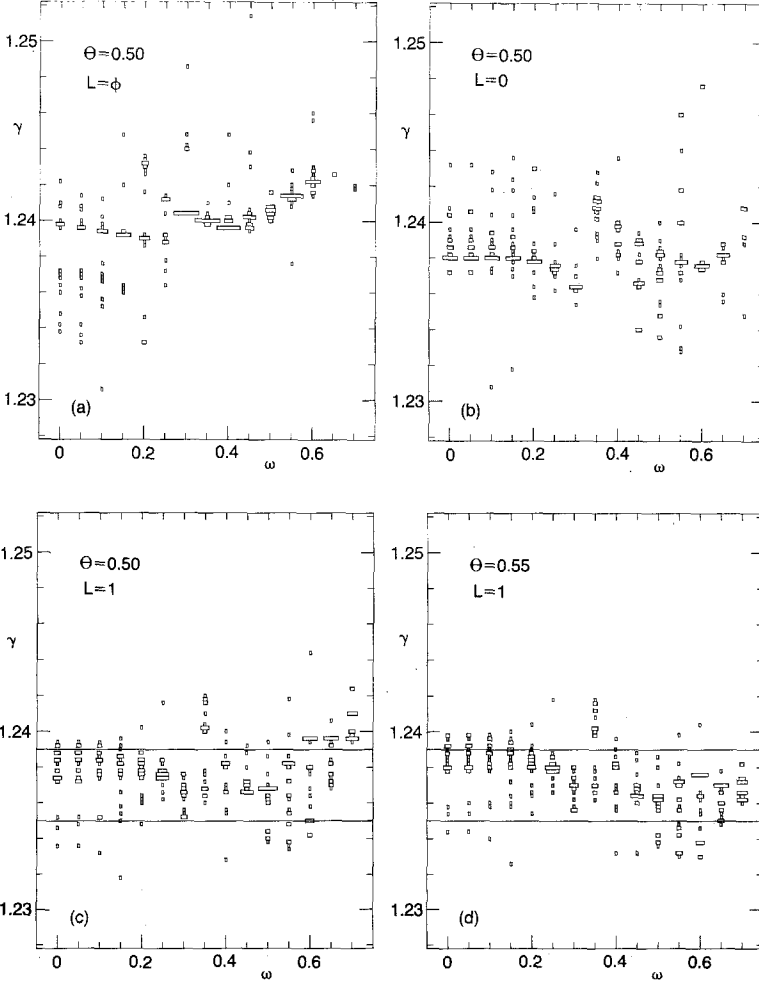


Fig. 4. Histograms of  $\gamma$  estimates similar to Fig. 3, but with  $n = 21$  fixed and a possible inhomogeneous term  $P_L$  in (4.2). Plots (a), (b), and (c) show variation with order  $L$  with fixed  $\theta = 0.50$  and are a detailed breakdown of some cumulative results in Fig. 2c. The result of changing to  $\theta = 0.55$  with  $L = 1$  is shown in (d). The solid horizontal lines in (c) and (d) indicate the bounds in our estimate  $\gamma = 1.237 \pm 0.002$ .

Finally, Fig. 6 shows histograms of  $1 - \alpha$  based on both  $\chi$  and  $M_2/\chi$  series. A correction-to-scaling term is *not* built into the antiferromagnetic singular point in (1.4) and hence the substantial deviations from universal behavior are not surprising. From the low- $\omega$  regime we conclude that

$$\alpha = 0.11 \pm 0.02 \quad (4.8)$$

which agrees with the value given by the hyperscaling relation,  $\alpha = 2 - 3\nu$ , using the estimate (4.7); however, the precision is not sufficient for a

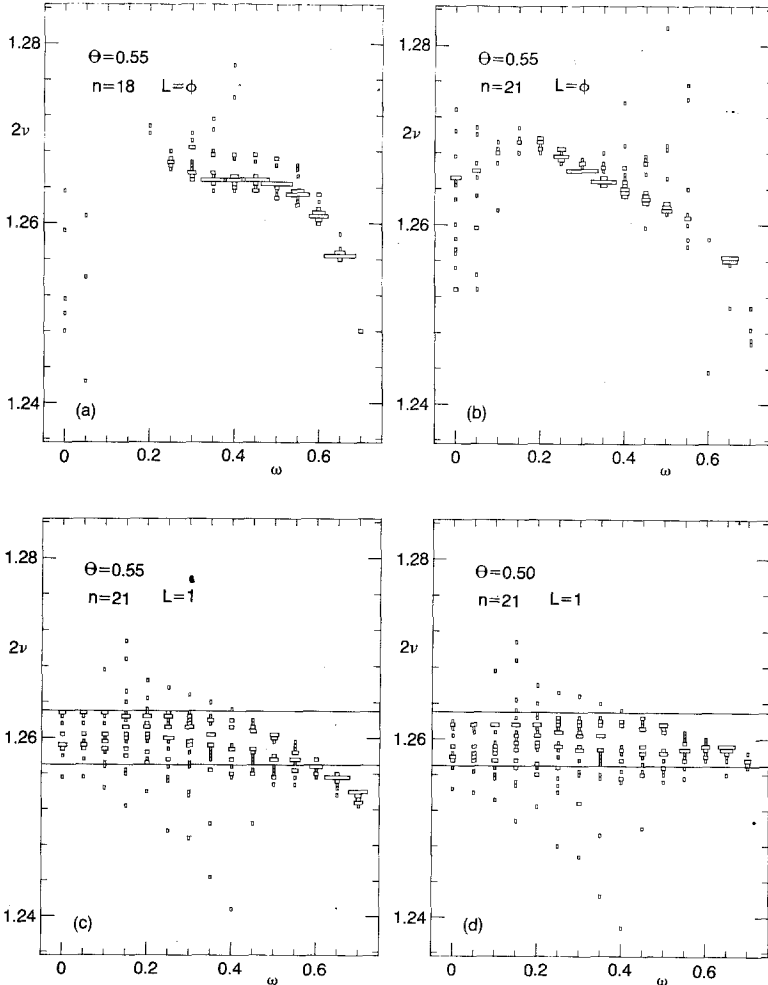


Fig. 5. Histograms of  $2\nu$  estimates based on approximants to  $\xi^2$  with the choice (4.5). Plots (a)–(d) show variations with  $n$ ,  $L$ , and  $\theta$  as labeled. Resolution in  $2\nu$  is  $4 \times 10^{-4}$ . The solid horizontal lines in (c) and (d) indicate the bounds in our estimate  $2\nu = 1.260 \pm 0.003$ .

definitive test. At the particular value  $\omega=0.31$  (i.e.,  $y^*=0.90$ ) our approximants yield  $1-\alpha_\chi=0.895 \pm 0.01$ , in good agreement with the estimate of ref. 19. While the hyperscaling relation  $\alpha=2-3\nu$  is satisfied better at this value of  $\omega$ , drawing conclusions about the validity of hyperscaling based on a single series estimate may be misleading.

From (4.6) and (4.7) we deduce  $\eta=2-\gamma/\nu=0.036 \pm 0.006$ , if we assume that the errors in  $\gamma$  and  $\nu$  are uncorrelated. However, this is not

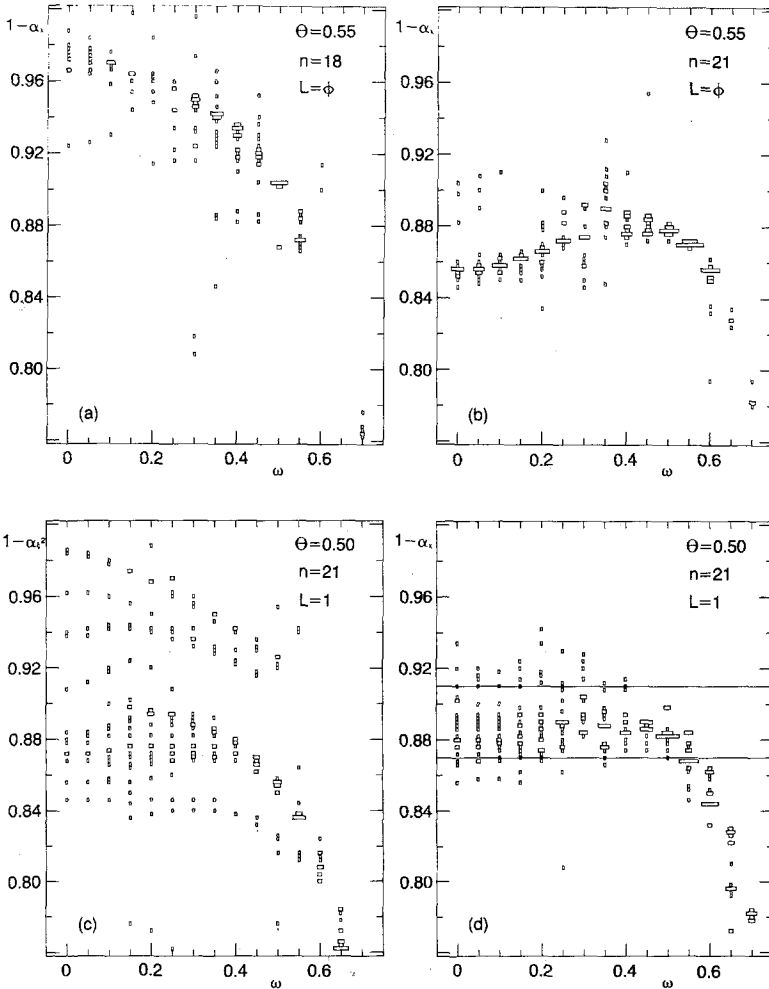


Fig. 6. Histograms of  $1-\alpha$  estimates from  $\chi$  or  $\xi^2$  series as labeled. Resolution in  $1-\alpha$  is  $2 \times 10^{-3}$ . Plots (a) and (b) are a detailed breakdown of some cumulative results shown in Fig. 2b. The solid horizontal lines in (d) indicate the bounds in our estimate  $\alpha = 0.11 \pm 0.02$ .

realistic, since we observe strong linear correlation with nearly equal slopes between the pairs  $\gamma$  and  $K_c$ , and  $2\nu$  and  $K_c$ . If we impose the obvious constraint that  $\chi$  and  $M_2/\chi$  have the same  $K_c$ , we find  $2\nu - \gamma = 0.0226 \pm 0.0004$  and hence

$$\eta = 0.0359 \pm 0.0007 \quad (4.9)$$

This value is consistent with the latest field-theoretic results from ref. 4,  $\eta \approx 0.0365 \pm 0.003$ , and marginally consistent with the series estimate from ref. 18,  $\eta \approx 0.0375(10)$  (again doubling those authors' one-standard-deviation error estimates). Note that our best estimates of  $\gamma$  and  $2\nu$  in Eqs. (4.6) and (4.7) are also consistent with this constraint on  $K_c$ ; with  $\gamma = 1.237$  we obtain  $2\nu = 1.2596 \pm 0.0004$ ; and with  $2\nu = 1.260$  we obtain  $\gamma = 1.2374 \pm 0.004$ .

Precise and meaningful values for the correction-to-scaling amplitudes cannot be given without first specifying the critical exponents. We show in Figs. 7a and 7b the very nearly linear correlations between  $a_\chi$  and  $\gamma$ , and

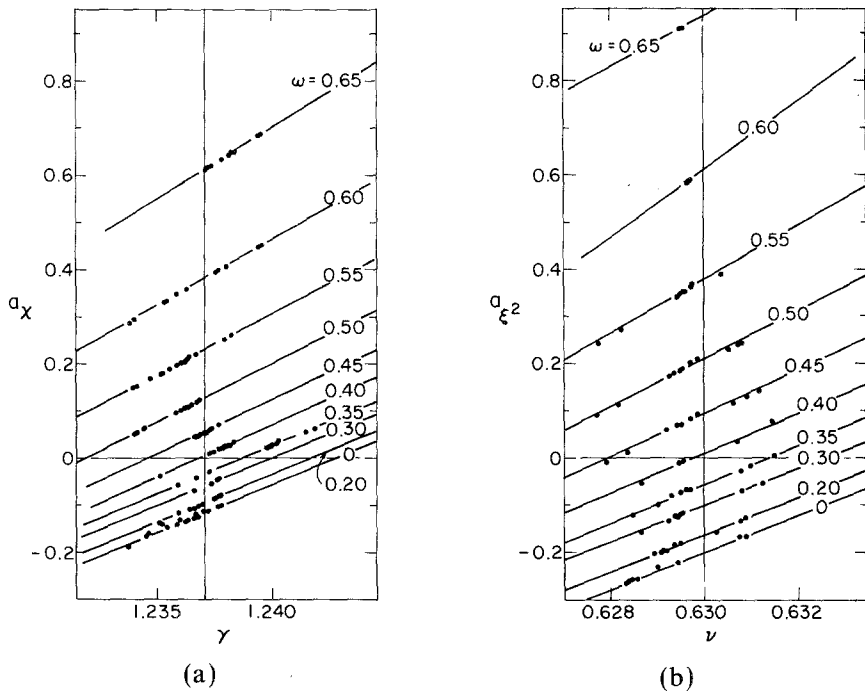


Fig. 7. Correction-to-scaling amplitudes. (a) Correlation plot  $a_\chi$  versus  $\gamma$  from  $\chi$  approximants with the choice (4.4) and  $\theta = 0.50$ ; (b) correlation plot of  $a_\chi^2$  versus  $2\nu$  from  $\xi^2$  approximants with the choice (4.4) and  $\theta = 0.50$ .

$a_{\xi^2}$  and  $2\nu$ , obtained from our inhomogeneous approximants with  $L=1$  and  $\theta=0.50$ . Thus, with the central values in (4.6) and (4.7) we find that the leading correction to scaling vanishes consistently for  $\chi$  and  $M_2/\chi$  at  $\omega = \omega^*$ ,  $y = y^*$  with

$$\omega^* = 0.39, \quad y^* = 0.85 \quad (4.10)$$

With the Chen *et al.*<sup>(13)</sup> central estimate of  $y^* = 0.87$  we obtain from Fig. 7 the value  $\gamma \approx 1.2383$ , consistent with their result (1.2385), and predict  $\nu \approx 0.6311$ . Similarly, with  $y^* = 0.90$  of ref. 19, we obtain  $\gamma \approx 1.2395$  and  $\nu \approx 0.6322$ , which are again consistent with their estimates. Note, however, that with these higher values for the exponents  $\gamma$  and  $\nu$ ,  $\eta \approx 0.0379$  and  $0.0396$ , respectively, which is no longer consistent with the value in (4.9), obtained by demanding  $K_c$  equality. The consistency of our results gives us additional confidence in the validity of our estimates. If we were to make the now *unreasonable* assumption that corrections to scaling vanish for the spin-1/2 Ising model, we would find  $\gamma \approx 1.243$ , in agreement with the analysis by Ferer and Velgakis<sup>(16)</sup> based on a 5-fit method or Guttman<sup>(20)</sup> based on nonconfluent differential approximants; similarly, we would find  $\nu \approx 0.635$ . Again, with our own central estimates  $\gamma = 1.237$ ,  $2\nu = 1.260$ , and  $\theta = 0.52$ , we obtain from Fig. 8 the spin-1/2 Ising estimates of the correction-to-scaling amplitudes

$$a_\chi = -0.13, \quad a_{\xi^2} = -0.22 \quad (4.11)$$

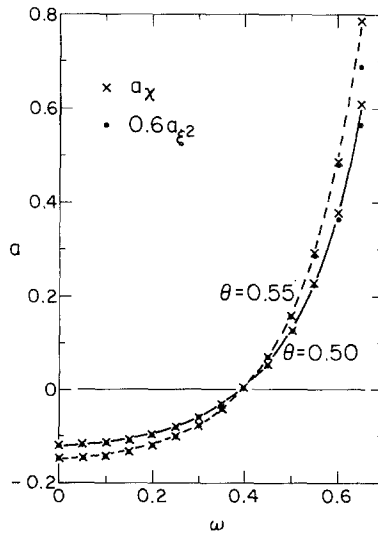


Fig. 8. Correction-to-scaling amplitudes. Estimates of  $a_\chi$  ( $\times$ ) and  $0.60a_{\xi^2}$  ( $\bullet$ ) versus  $\omega$  from Fig. 7 assuming  $\gamma = 1.237$ ,  $2\nu = 1.260$ , and  $\theta = 0.50$  (solid line); and from a similar plot assuming  $\gamma = 1.237$ ,  $2\nu = 1.260$ , and  $\theta = 0.55$  (dashed line).



and

$$\frac{a_{\xi^2}}{a_\chi} = 1.70 \quad (4.12)$$

This same ratio estimate applies to within a few percent for all  $\omega \leq 0.5$ , as can be seen from our plot of  $a_\chi$  and  $0.60a_{\xi^2}$  versus  $\omega$  in Fig. 8. For  $\omega \geq 0.5$  this ratio drops considerably and could conceivably agree with the continuum  $\phi^4$  model estimate<sup>(32)</sup> of  $1.30 \pm 0.10$  in the neighborhood of the Gaussian point. As discussed in Section 1, this model dependence of the amplitude ratio is one of the indications we have for a possible absence of universality. However, given the latest continuum model estimates,<sup>(4)</sup> the value 1.30 may well be suspect.

Of course it is worth recalling from Fig. 2 that systematic trends in many of our estimates are apparent through order  $K^{19}$ . It is only because of the apparent stability of estimates based on 19-, 20-, and 21-term series and the internal consistency of results for  $\chi$  and  $\xi^2$  over a range of  $\omega$  that we can have any confidence at all in our estimates. Also, the low- $\omega$  regime, and in particular the spin-1/2 Ising limit, remains notoriously difficult to analyze. Even at order  $K^{21}$ , the estimates for  $\gamma$  are typically bimodally distributed, as can be seen in Fig. 4. Finally, there is still a fairly large uncertainty in the value of  $\theta$  and in the correction-to-scaling amplitude ratios. Thus, there is still very considerable justification for attempting to obtain even longer series.

## 5. EXTENSION OF SERIES

In the conclusion of the preceding section we discussed how the question of universality is not fully resolved and why there is justification for attempting to extend the available series even further. Extension by two orders in  $K$  is unlikely to lead to any significant change in these conclusions; extension by five or more orders in  $K$  is almost certainly impossible with the techniques and computer resources now available. Thus, the discussion below assumes as a reasonable goal the extension of the series to order  $K^{25}$ . At this order the array  $c_m$  used in the program segment described in Section 3 can still be packed onto a single 32-bit word, and the graph weights  $w$  can probably still be handled exactly as integers with the IBM quadruple-precision facility. Thus, large sections of the present program still can be employed without major modification.

Two features of the present program, however, must almost certainly be modified or at least receive serious attention. The first feature is apparent when we estimate the storage requirements for a naive extension

of the calculation by the program segment described in Section 3. The number of entries of 2-rooted, 1-irreducible contributions in each order  $n$  for  $n = 1, 3, 5, \dots, 19$ , and 21 are 1, 2, 5, 19, 81, 353, 1619, 7704, 38,353, 204,854, and 1,055,792. Extrapolation suggests  $6 \times 10^6$  and  $35 \times 10^6$  entries at orders 23 and 25. At 32 bytes/entry the order-25 list would require some thirty 40-megabyte tapes for storage. However, as discussed in Section 3, each entry contains the information necessary to obtain the complete embedding constant array  $e_k$ . If we restrict ourselves *a priori* to calculations of  $\chi$  and  $M_2$  only, then the complete arrays  $e_k$  at high order are not required and a very considerable increase in packing density should be possible.

The second feature, which we believe will be the more difficult to modify significantly, is the time required for the generation of the elementary 2-rooted, 2-irreducible graphs. Our present program generates these graphs recursively by using the slightly modified Heap rules<sup>(37)</sup>: (1) Join any two existing vertices with a new bond, provided the vertices are not already linked by a bond; (2) insert a second-order vertex on any existing bond and join it to an existing vertex with a new bond, provided again that the vertices are not already linked by a bond; and (3) insert two second-order vertices on distinct existing bonds and join these by a new bond. The modifications we have introduced are for the purpose of excluding graphs with multiple bonds.

Finally, we use as the starting graph for this process the 2-rooted elementary graph shown in Fig. 9a and supplement the three Heap rules with the following: (4) Do not join the two root vertices with a new bond. We can prove that this algorithm will generate all elementary graphs by showing that for any elementary graph other than the starting graph, at least one bond can be removed which will leave the resulting graph elementary. For example, for the graph shown in Fig. 9b, any one of the four

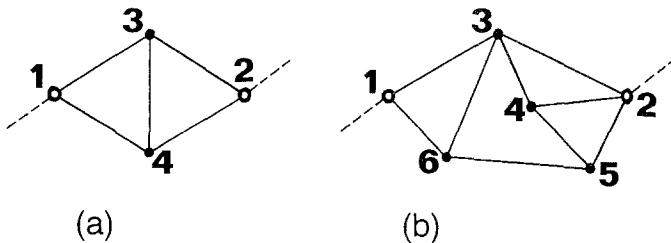


Fig. 9. Two elementary 2-rooted, 2-irreducible graphs with vertex assignments obtained from the algorithm described in the text. Each edge will eventually be replaced by a “nearest” neighbor bond or a 2-rooted, 1-irreducible segment in the bond renormalization section of the graph generating program.

bonds joining vertices 2–3, 2–4, 2–5, or 3–6 can be removed. Of course, this also shows that the graph in Fig. 9b will be generated four separate times on application of the Heap rules to lower-order graphs. Since for a general high-order graph almost all bonds can be so removed, the Heap rules are very inefficient, because of duplication. To obtain the  $7 \times 10^6$  graphs estimated in Section 3 for an order- $K^{25}$  calculation, probably in excess of  $10^8$  graphs must first be generated. We believe that to make an order- $K^{25}$  calculation feasible, a more efficient algorithm to replace the Heap rules is required, and we hope some reader will be interested in this challenging theoretical design problem. Ideally, all duplication should be avoided by such a new algorithm; if this is not possible, one will still require an efficient algorithm for uniquely identifying each graph so that a tabular search can be initiated.

The algorithm we used for graph identification is probably adequate and is easily described. We begin as our step 1 by labeling the roots 1 and 2 in both possible ways. Internal vertices are labeled 3, 4,... in subsequent steps. Now in general, at the completion of step  $n - 1$ , where  $n = 2, 3, \dots$ , distinct labelings of the first  $n$  vertices will have been kept in store as possible candidates for further testing. To accomplish this testing at step  $n$ , we first scan through the labeled vertices in the first member of our candidate list in search for the largest vertex which is connected to as yet unlabeled ones. Having found this largest, say  $m \leq n$ , we proceed to assign  $n + 1$  in turn to every unlabeled vertex that is connected to it. For each assignment we form the integer string  $mlk\dots$  of labeled vertices that are connected to  $n + 1$  with the convention  $m > l > k > \dots$ . Then, of all possible labelings at this step, we keep in a temporary list those that maximize in turn  $l$ , then  $k, \dots$ . Since the strings to be tested will in general be of varying length, we need to imagine for this maximization that each string  $mlk\dots$  is supplemented on the right with trailing zeros. As an example, the possible strings at  $n = 4$  are, in order,  $4321 > 432 > 431 > 43 > 421 > 42 > 41 > 4 > 321 > 32 > 31 > 3$ ; the remaining  $21 > 2 > 1$  never occur.

Having found the maximal string and associated (temporary) labelings for the first member in our candidate list, we proceed through the rest in a similar fashion. Either we find a smaller string, in which case the new vertex assignment is discarded, or we find a string greater than or equal to the previous maximal. If greater, all preceding temporary lists are discarded, but in both this and the equals case the new labeling is incorporated as part of our (temporary) list. On testing completion this list becomes the possible candidate list for step  $n + 1$ . Note that the discard process makes the algorithm relatively efficient; each list length is the symmetry number of the partially labeled graph and this typically is quite small.

When the labeling is finally complete, we use as the unique graph

identifier the composite integer string formed from the individual strings generated at  $n = 2, 3, \dots$  and listed from left to right with a single 0 between string segments. As an example, the algorithm generates the unique strings 210321 and 210320420531 for the graphs in Fig. 9. Furthermore, it shows that the corresponding labeling in Fig. 9b is unique, whereas the labeling in Fig. 9a is only one of four symmetry equivalent ones—essential information for the subsequent bond renormalization segment of our program.

Given the integer strings generated as described above, graph comparisons are easily made by an individual integer-by-integer comparison or, equivalently, by number comparison where each graph is the single number that is the string in a system with an appropriate radix. For a list of *all* elementary graphs of  $\leq 25$  bonds, a radix  $\geq 17$  is necessary, but in fact, such a complete list is not required and radix 16 is both adequate and convenient for packing all strings on at most five 32-bit words.

The elementary list reduction comes from the fact that for a calculation of zero-field  $\chi$  and  $M_2$  on the bcc lattice family, every elementary graph must, after bond renormalization, contain only even-order internal vertices and even loops so that it can be embedded on a linear chain or a pair of nearest-neighbor sites. For example, the even-order vertex requirement can be achieved by doubling bond 3–4 in Fig. 9a and bonds 1–6 and 4–5 in Fig. 9b. The even-loop requirement can be achieved by the insertion of a second-order vertex on bond 3–4 in Fig. 9a and on bonds 1–3 and 2–4 in Fig. 9b. Other doublings and insertions may also work, but in any case the graphs in Fig. 9 cannot contribute at orders lower than the “true” orders defined by the addition of these minimal doublings and insertions to the direct bond counts, i.e.,  $5 + 1 + 1 = 7$  and  $9 + 2 + 2 = 13$ . These “true” orders are the ones used for the graph counts given in Section 3, but the Heap rules were not completely successfully supplemented to avoid redundancy by generating graphs of too high “true” order.

In summary, we believe the derivation of an efficient algorithm to replace the Heap rules for graph generation represents a challenging theoretical problem whose solution would be of great practical use in making possible the extension of the series now available.

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## APPENDIX

Spin- $S$ , Blume–Capel, Klauder, and double-Gaussian series coefficients (Tables I–IV) and representative differential approximants (Table V).





Table II

	---	BLUME - CAPEL	MODEL	---
1		7490801/32		98166157/64
4		26066973/16		781452453/64
10		605732763/64		11255253387/128
10		1295186835/4		3488222931/64
10		512620022/8		2766659557/32
10		559897/16		4276335657853/48
10		1633671/8		3989983050753/48
22		3947691/4		65784360281619/40
24		17629131/4		58862844279897/8
24		240596608203/2		100308028052911/4
4		74013625/4		97559553870681/2
4		212011305/4		6674500591488239/120
43		2412862115/12		1518230646659619/40
43		410907970		11682064659619/40
50		202727066		301381148329/8
50		259440336/4		961500749488/5
4		43566090		30675328677/5
4		3931650		786430
4		122860/7		4
88		22002		45502945/16
106		196395/2		95829355/4
309		285642		839525769/8
72		3520379/4		939525769/8
72		2170848		3374500098163/48
184		1520933/6		3374500098163/48
429		2370539/3		41203948627481/192
64		642666/5		464762874838351/80
2232		16143104/12		82530244082099/4
4		1076961565/2		4296858003746351/48
4		1806192488		33233308137073/2
460/3		19871/2		6032563385422811/5
4		188221/4		1010388122241267/4
761/2		209692		181829911785160
968		794713		154753340761716
2075		363623/4		752702568948
2075		157226292		152824400215/7
2146		43812622/35		8388600/7
216		131064/5		4
216		9377997		4
4		15187948/5		4
4		401391		4
2893/4		15350/3		4
9447/4		8104693/64		4
25251/4		50791079/64		26377013/32
3353/2		728716237/64		50149469/8
11889/2		3081513/32		675740459/16
475		3459341747/32		977978991/4
4		232731127/8		26737593005/64
2699/2		202630/2		372595220785/8
62713/4		3502971/8		471164145530/3
42578200		1995953		2194478114045/4
1200610		12655921/2		2301482749320
7540		20203666		21926973828425/4
93755/6		17771333/3		7213343899995
680		216417880/3		13273128793973/24
		46578200		7007891950932/3
		10612700		675783751017/12
		1200610		15168442538/3
		7540		331128
		93755/6		4
		680		4



Table II. (Continued)

	---	BLUME - CAPEL MODEL	---
	SECOND	MOMENT ...	DIMENSION = 2
4	178660	17744287/4	1368871009/32
32	530728	40816689/2	3976013565/16
1329130	161367009/2	163332787113/8	79079099931/64
2369760	266383686	356725665013/16	124492918339/4
2706550	753628320	4883336204939/20	168332787113/8
1617756	1705206360	15711599782989/20	356725665013/16
1485628/3	8110405930/3	1664255871243/2	4883336204939/20
176032/3	2660274320	4529168436273/8	15711599782989/20
8192/5	172269340	228573028224	1664255871243/2
0	7845676940	736404073187/14	228573028224
0	409877	630373905/4	4530041163
1688	1386114	92520	530373905/4
1476	7963707/2	0	92520
693	8732010	0	4010720
72	58867067/4	131072/7	4410720
4	12820608	0	178666959/2
4098907/6	4098907/6	30553801/32	54673073
1659120	1659120	23555452529/8	178666959/2
2232	2232	13779547979	54673073
4	4	1409434201033/24	23555452529/8
4710	4710	888891089931/4	1409434201033/24
6329	6329	2930812775079/4	888891089931/4
5128	5128	629357430718/3	2930812775079/4
1376	1376	6072872532820	629357430718/3
512/3	512/3	18087264680	6072872532820
0	0	156474085443/10	12266031846045/3
24953/2	24953/2	80583345768	3478978104120
21768	21768	2382897751	80583345768
27373	27373	295440480	2382897751
14400	14400	103004022/7	295440480
316	316	131064/5	103004022/7
216	216	4	1559833760/3
475936	475936	40622615/2	1559833760/3
16384/3	16384/3	219556409/2	2097152/9
0	0	203591513/4	0
67656	67656	2041237599	5924274569/32
1151716	1151716	7260905045	9785528855/8
103728	103728	22098159162	110388724015/16
47376	47376	55740428090	1382256735623/4
8332	8332	101786286960	101647314858205/64
316	316	62925117236/5	5270665661685/8
401236068	401236068	326793162604/4	232176593299385/96
1380310757/3	1380310757/3	42584408916	22968609446810/3
194679	194679	10759263984	326793162604/4
1650937/4	1650937/4	401441050405675	42584408916
552504	552504	528855572552629/24	10759263984
1239845/3	1239845/3	65536	401441050405675
148430	148430	229014304/5	528855572552629/24
4875/2	4875/2	15306997615315/12	65536
680	680	1831563790	229014304/5
4	4	331128	15306997615315/12
1523305685/4	1523305685/4	48388600/7	1831563790
5339390595/2	5339390595/2	0	331128
31848321405/2	31848321405/2	12454029621/16	48388600/7
170015221731/2	170015221731/2	5770518816	0
1673999758995/4	1673999758995/4	2321938300399/64	12454029621/16
1524801137959/4	1524801137959/4	164291150672/8	5770518816
26082497186695/124	26082497186695/124	51756085054601/48	2321938300399/64
8917189303285/3	8917189303285/3	140714437202869/8	164291150672/8
1923868911376632	1923868911376632	270696029735504/64	51756085054601/48
3235723113218420	3235723113218420	24735091299332951/80	140714437202869/8
371514921952020	371514921952020	3535219967364707/4	270696029735504/64
4281900418502458/15	4281900418502458/15	90358716353553439/48	24735091299332951/80
701437435314826/5	701437435314826/5	5674903204686177/2	3535219967364707/4
40286844056921	40286844056921	4113594479208602021/140	90358716353553439/48
6262462049872	6262462049872	1027864329647271/5	5674903204686177/2
154630666232/5	154630666232/5	3696369718094163/4	4113594479208602021/140
31506016832/5	31506016832/5	344292718467784	1027864329647271/5
4194306/5	4194306/5	1300891804300	3696369718094163/4
0	0	158103255255/7	344292718467784
0	0	8388600/7	1300891804300

Table II. (Continued)

	---	BLUME - CAPEL	MODEL	---	
	SUSCEPTIBILITY	...	DIMENSION	...	
1	179333501/2	848834064671/8		337999003449551/16	8344803905052165/2
	3153337853/2	27070949867/8		531620371248509/8	4263030842869092520/8
8	40247745/2	1032573675309/2	3	318919219370902/32	28257374633441855759/32
	191154122	815463495928		562596476154111	75867513385283154571/32
52	123748280	1076018103370		862296748168428	7480273919979931017/16
	44904249	11816158121010		44484613530388579/4	196791063979450360115/24
8	2383982/3	294827528782/3		8626109963903631/10	15004898711398592565/12
	1038908/3	294827528782/3		447284913349581	15966990961846740417/10
2014	35757/2	140550166566/3		603021405991131/4	1620667344364490499
		24065400180		2059114497803/7	9925269728132163365/8
1114		1442417371534		2359114497803/7	3462662550690203/15
236		18879400180		3391198185/2	37887213739298521/60
8	527680859	46677780		431760	36207134222333669/4
	1032347656	573352/7		8	639119567467226
9304	1482986070			3938596883481155/32	781144065246212/5
3642	1653359784			13170487348599931/32	3671899894098/5
336	2734012901/2	9946065922907/16		33215390767973152/32	18350036/5
	411253033	2613521796937/8		20625845283386509/48	8
8	614753033	2613521796937/8		72280183780377	388338599549927333/16
	83342368/3	53707652117449/6		125694393362941837/12	764804320957752945/8
72820	7502556/5	10404750632045		4674617359949561/4	9108937168177295323/32
70358	10416	7022054413056		44269791584783095/12	2949695951832283507/4
41032		808593314076		1727490377941045	41298860052028355653/24
9764		11726849825		4295070878831400/21	14546135993539350667/4
2152/3		726849825		11939797973230/3	663573721023601643705/96
8	6189112937/2	5195932892/35		2179397973230/3	11617195600918020876
	6668756859	611632/5		17820227540/3	67086221732855646803/40
434759	4253592635/4			5174952/9	1182517029596292571/6
390816	4095941617/2			8	1278668082683185338
189154	19097051029/2			444006784773347758699/70	1278668082683185338
158272	24976408141/6			10801329035639378599/5	94803921375124831/2
24836	2999361514/3			8	59755281629478064
1008	577815484/5			2867967100303733/4	3636443008060896
	4744294			2539584381229660	69818071889016
547651/2	71636/3			3433336937893377/8	18254175958707
701181/2	8			13131650363321339/2	5592403
6635847/2				106782090418337/16	8
189154				892051955251855/8	
59154	7267169703/4			453173392506209595/48	
6269348702	74737670896			38639865925035210/3	
70173	94924832884436			14230129071474798	
2218	106774945636			119611549885805260	
8	32410877947			72227467172517000	
	109689359482			2992445131320100	
15231633	197042233948/3			96785738715606187/12	
23755006	70466166512/3			38562588512441664/3	
52934779/2	4643970632			6291669393730/3	
20058744	425181760			902959329346/3	
2918600/3	14135268			617336670548/3	
543395/3	8			15495264	
9920/3				8	

Table II. (Continued)

	--- BLUME - CAPEL MODEL ---	
	SECOND MOMENT ... DIMENSION = 3	
128	1812419584	2081899004403572123
0	2333092304	13376121318636147265/2
1356	1229156256	32098932113620167156/2
112	483890196	11795282647352872443/2
	108868344	18757528200353871627/2
12160	38979400/3	14651612421375757859/12
2560	1760320/3	6845858966159925852/5
256	32768/5	101980977062212364/6
0		5805405583666684240
98728	12072564/23	2436044288313576128
35628	17659802/60	2161257489991682860/3
6114	18257446782	700326050827897788/5
336	13685522472	16095352265677230
3	14354738981/2	901268637561376
8	14354738981/2	1785782184032
752856	1408333129/3	630614903
401968	45994160	16777216/5
151840	9503868/5	0
14	10416	
2088/3	0	
0	793886884/32	
5493959	131374195816	
3913312	155829388960	
1711662	139617303008	
360000	27757363320/3	
38748	41925993432	
1008	598273844/3	
	16759160	
	41259160	
	65536/3	
38835920	0	
34791768	870867136353894	
20241000	1074686290620894	
6672864	383352789008456	
1173600	2065695244151/4	
83520	95421167374	
2048	50854018315104	
	214201647277584	
	107091088548	
	60572891619254	
	8282395/5	
	10322368914912	
267866325	302852013344/7	
290061102	18929449696/3	
4238833003/2	638861768	
96123672	262144	
81212290/3	458028608	
3810420	16749390	
251105	35280	
9920/3	8	
	13516561548199	
	328093616201037	
	178933715491607/2	
	870867136353894	
	1074686290620894	
	383352789008456	
	50854018315104	
	214201647277584	
	107091088548	
	60572891619254	
	8282395/5	
	10322368914912	
	302852013344/7	
	458028608	
	262144	
	175139775458344446/3	
	988261860884305/6	
	36827277600	
	21448887068	
	1542664	
	8	
	5356037371029579	
	30217313556966121/2	
	126759733320392203/4	
	526877335886840342	
	101718387886418015/12	
	219249039031239549/2	
	236044594825480611/2	
	306284026467316504/3	
	306284026467316504/3	
	93611233240051140	
	35260065157587560/3	
	2743003528515840	
	273174532907646/7	
	86325346009364/3	
	2510228440900/3	
	15598337600/3	
	8388608/9	
	0	
	33464450075837594	
	10094749688759136	
	181598836467620433/8	
	86487629266653383/2	
	22928881709240203155/32	
	411168717938059935/4	
	60166393973973873635/48	
	378995651567772650/4	
	10236962434946836	
	10236962434946836	
	28341091138750100	
	234744445207679467/12	
	75139775458344446/3	
	988261860884305/6	
	36827277600	
	21448887068	
	1542664	
	8	
	2064258124308175901/16	
	35181408019481084397/8	
	358933317818464196235/32	
	198103370401167049531/4	
	138357716229301241693/24	
	33073245209616050843/32	
	473900783024915317220/32	
	6847616196256556544331/40	
	15080977238295986187/40	
	627864871052441785939/6	
	5542899078963708354	
	30594004347427722583/14	
	21219325746093316787/2	
	1803434329910770	
	5013434329910770	
	80852066866296	
	18700049436190/7	
	5592400	
	8	

Table III

1	SUSCEPTIBILITY	MODEL	--- KLAUDER	--- DIMENSION = 2	255 10826256125828464640000
2	3715891200	14282329123020800	46620662575398912000	-2508323137535627525000	-192423354718348970695687500
8	-15588516100	-69478336303037800	-182088730346539521750	15068982237200414120319250	10665892237200414120319250
-2	15697622430	20672646059613645	18736503108497706672208	-256028425812095951884070	256028425812095951884070
48	-11892097614	-1562623650914609489	1670003719753943670256084	302592827642786699848430242	302592827642786699848430242
-24	5434843048	18363963576582882	-554285637591973351320	2735164512339098137243248480	2735164512339098137243248480
384	-1514152556	-1134716377438914	-5980020693160063378424	19330787979286857465737276	19330787979286857465737276
-318	245180054	4523163204820783	12608056136330378424	107581859265802782193095240	107581859265802782193095240
76	711456	-15232904324133928	-19080429425925753920	-475113556787127289244391016	-475113556787127289244391016
3840	81749606400	4247484735714436	4049344785785840	16604416970731022268518408	16604416970731022268518408
-4440	-28934449200	-3772815360	-3382622208000	-4257919084469501753780152	-4257919084469501753780152
1718	452110350375	-7257600	1678343852714360832000	162925932746594487733584	162925932746594487733584
-224	404293119846	4628973690624000	-11260925079619375660500	181893679714069395744	181893679714069395744
8	2822819219	55798687093966519	35466781284962398843590	-145605833784369421440	-145605833784369421440
46080	17950890408	-829246050414243295.5	92700915866768119829276	-17233391218825712640	-17233391218825712640
-70380	-2415998008	82948926880955691.5	68833018580422671185628	71686639898103251968	71686639898103251968
40158	173499776	-584971695998572974.5	-39171000529076374969056	7342962846105600	7342962846105600
-9918	-4963200	29804254038737294.5	17167399418290867407504	-2633637888000	-2633637888000
960	28800	29427939354374448.5	-57860004471901100009964	107145471537284795514880000	107145471537284795514880000
-24	1961990536600	29427939354374448.5	14853685919547471808	-97214157284795514880000	-97214157284795514880000
605120	-7802021096100	75343490977426192	-284857335651209728536	3372087949054483316293460375	3372087949054483316293460375
-120120	1407701283550	75343490977426192	3761444462096453328	-8206004743949853755449672900	-8206004743949853755449672900
916491	9663069099550	-55011892342872	-218424007647210294	14049700999197882234919317900	14049700999197882234919317900
-327702	-4278032936622	2242694153704	-6389688112473600	-17931468972939822766616895108	-17931468972939822766616895108
55145	1259741047224	-28689292800	435588837862400	17644337478016366060139180715	17644337478016366060139180715
-3840	-240823400136	50803200	-2926266243200	-8424768391028709568228018220	-8424768391028709568228018220
72	28110117840	-1751115360	6377066031457116160000	4162243028266783428319055904	4162243028266783428319055904
10321920	416332880	-1128200	45797715903513298734000	1586669275693694423278412912	1586669275693694423278412912
-2575920	-34870285038595875900	-1128200	-55039227634293394608275	330532612974792812822196	330532612974792812822196
11017588	3176830863659745116	51011750393600	48137930375748143501592270	-25426037530586527929259280	-25426037530586527929259280
-2890340	-2251541185656400	18316448212957609228	-52049166274422770316612656	3755446984924057983377296	3755446984924057983377296
383820	450132649775235	-7994103026467732572	42771857181558254826430250	-40460599827311438229760	-40460599827311438229760
21408	-53345759340312	25880040094466395964	-2718327161315586428249660	29850834873786681894912	29850834873786681894912
-288	-217302832717740	103746852054413184	1347717510832454887480844	-13515673020445332920	-13515673020445332920
185794560	78674484241229	-11900436822031936	-522189485133426054841984	29630170233175321600	29630170233175321600
-501250680	-19411026117032	8461334404913792	157346214912984676453760	-95957418188664000	-95957418188664000
34343575	319693952668	-308889334725640	63592699527922593104	2633637888000	2633637888000
-34343575	-319693952668	3261652600	-19594816316624584701260		
124522332	16764883736	-406422600	38647340547253873408		
-24722336	-321615360	1036800	96436519744463040		
2577496	11036800		-5101837332488000		
-110976			2633637888000		

Table III. (Continued)

	---	KLAUDER	MODEL	---
	SECOND	MOMENT	...	DIMENSION = 2
2	7925512637871781504000			5102165312251656282800000
	-3931081655000927427000			-31780842488777954952800000
	912670388647254919350			32866403845261103253191200
	1209422661619459109848			-278531714121991542331272160
	-9383719910647232320680			221796648562362915376983136
16	74837527693748800			-164182329635467917826034880
	128516453419146660			-98204896379147816369740528
144	-43897168344			4608788134440330304562169440
-24	11541877408			-17273367300729489598943568
-2	-2970973696			51593719863414424323161344
1536	60901984			-12176258295240903569739776
-576	-562176			22339596365238306792602
64	66448631606400			-333321774999103322112
0	559575957568			-215160452665071089920
	-208764198144			8958790392524060545024
	-2438000640			-17732555959803863040
	8992456720000			596993116686633600
19200	-2333922820000			
-12120	26784304031455			30210189348858494976000
2678	741381823643			-162458870474641769028000
-224	-200588718352			410972594526859849468600
	34905187416			-647219369466265217847640
57680	-3705165000			708281717850373291751472
-85040	2118942206			-3959306162262588230352
-492800	-492800			16340337947125270541600
704	23543886643200			59677078809025192241152
0	-6902679369600			-1689769410497939206016
4515840	9322980572360			36656380009728156938656
-5498640	-7283758875360			-597077378298734985720
2665035	3680655776192			70334492560861133312
-628334	124333796033888			-633860751404958720
73849	-280645093264			276443700795959544
-3849	38043397376			-8662686665252600
72	-1849816320			34895934252920
82575360	31150080			2193913532959988000
-127169280	-17175501300347550400			-99778445927008512000
80941632	21455620135671176480			121176261659768520704000
-26663712	44087210323260808128			7022626384087459773262000
4743360	-15642657789697124480			-1925642922192003512630075
-430336	742503680786553824			-33051612061689551246119990
15360	-26406655856203916			39653789550795601009531081
	1846017281046698			-3250375947462250138101276
	-754016774052698			4260545280014969562515828
16721510740	2159864197899445			5295940710145343084417116
-3143017080	-42760245203368			-174167330989866373384864
2517065190	5645807286996			448284963652188525187408
-1095991368	-460583550768			-89486558569073685298936
278184788	19911764304			1344726493932979575632
-41029280	-321615360			-1465131837163265137344
3241016	1036800			10848722648733807680
-11013	-1152			-488294844574162636
				10250018323246000
				-510183123246000
				263363788800

Table III. (Continued)

1	SUSCEPTIBILITY	MODEL	--- KLAUDER	---	61.1066343
4	...	DIMENSION = 3	---	---	19.4664000
32	3805072568800	23401744331572782200	---	---	181066343
-4	-580902498800	-5524520276447120000	---	---	-251225220
384	4004895852900	6180402147407742170	---	---	178700029
-96	-1583181473372	-4272893082735688920	---	---	-20451944
4	3810710483304	20050892974206881976	---	---	169820854
4	-59846622508	-6610134134269369892	---	---	-106744404
6144	-2031836292	-2590171982927620782	---	---	252833548
-2532	3429888	294922349512584992	---	---	-202612798
312	-11520	-27185671494442968	---	---	-15352052
1674323193907200	1674323193907200	957852024884768	---	---	262118457
289470905339200	289470905339200	-20630074489928	---	---	-102795443
-70560	229255666263810	145074489560	---	---	-221630810
14116	-106953501915876	---	---	---	-197298182
16	33931026914752	---	---	---	341138594
695236901944	1404104661094367232000	---	---	---	-5267275760000
-47639291216	-3615224983017455408000	---	---	---	224700339
1669217152	44409108445435288517125	---	---	---	302923483
-2228400	3404498584286807033670	---	---	---	677269728
655500	179511473004043357523	---	---	---	1676114
-2218240	-678753642152995098108	---	---	---	273437903
57600	18683141292367189059	---	---	---	184579387
803631330754560	-37368871642971365654	---	---	---	125250544
135311911579600	5344025103706567667	---	---	---	667097900
89575360	-35869327317884964	---	---	---	670979000
-71747080	-7594420942343812	---	---	---	628385076
29791038	2682042914332932	---	---	---	517046938
-5546108	-632644560885028	---	---	---	970469386
477174	98803510440096	---	---	---	592439577
-16416	-8845745290304	---	---	---	104439839
1144	57992609120	---	---	---	144429800
17327707968	-17327707968	---	---	---	-152593356
-1847660	3845600	---	---	---	119207208
-48198760	-48198760	---	---	---	-65189704
187117680738152609534	187117680738152609534	---	---	---	228939406
-71596332020474385941224	-71596332020474385941224	---	---	---	342379444
4178882919923371200	4178882919923371200	---	---	---	444586030
-897083139499742200	-897083139499742200	---	---	---	444586030
50714184	22791713591436703690152	---	---	---	-445860308
-3422408	90473593269334470	---	---	---	-445860308
93120	-555841549190883672	---	---	---	445860308
-576	2275551144734074072	---	---	---	5267275760000
123941467685296056	-6401467685296056	---	---	---	334375059
-95126814720	123941467685296056	---	---	---	334375059
-161839594100752	-161839594100752	---	---	---	115516832
138228235699784	138228235699784	---	---	---	115516832
-2371682928	-2371682928	---	---	---	209173768
4386813668	4386813668	---	---	---	209173768
-450124768	-450124768	---	---	---	160768497
23353552	23353552	---	---	---	9282801
-486912	-486912	---	---	---	8928201
2304203120	2304203120	---	---	---	413658546
-2073600	-2073600	---	---	---	413658546

Table III. (Continued.)

	---	KLAUDER	MODEL	---	---	---	---
	SECOND	MOMENT	...	DIMENSION	=	3	
4							10388127246405665292288000
							-251185587260672899650516000
							2321634170459521102095581300
							-214616132559706167533445750
							-120697257858988318838930464
64	376244	209920	2019020	2800			3110509879437017139753337567488
0	1923393	6454400	404800				-985035912867271739753337567488
	5686365	325250	215574	2600			25238046084120388813840118854788
1152	-20817225	110736	9972265	3604894451552			-51644889860672361050423788288
-96	977575	633632	464702219	11415116872			-1080080446270699424327707176
	642713	345456	605213	3648263175900			-775675929486781529591028480
24576	-2003961	4408	5266845	278432932			-31307219206008873443260
-4908	2248704	0	1135493	37676016			237714779757003295294880
296	0		-192103	2027648			-174479757003295294880
			975200	2560			23877246674534400
64400	184165	113297	9200				7919419876667161306988544000
17694720	-2355847	40361	7600				-2075663801738968512991920000
-928	1017446	79146	482				26223636831328011473147408400
	1288102	299128	410982	65993005091313925			21061429762804331986891809360
-802940	195718	3686	10131	67020432554337994			1195888269916883070820985376
1399536	-195718	3686	10131	67020432554337994			76189132567020432554337994
-101968	-222318280	57600	-2959791	136280907425180			416689134168771243875332032
2816	964357	969054	7200				821258504639964412098875356
	1408698	82315000800					-125353469483103311630551168
578027520	950309	407328	2240				1456587699499705006330304
-349614720	-383109	4492540	7616				-12503289347664002791552
86612670	106590	731515	6560				7550478706086170955776
-10431984	209945	7220	3240				-297004932891486984192
-16416	160127	40779904					66312515018193192064
	765959	595328	1437800	17296063204556800			-640396369571292360
	124500320						13939319310368000
21139292160	-16139612160						6353134612170767188858732000
5245010876	-885707680						-17937050020568110472822504000
80251776	324517959	0825600					245067554819749907403131530050
-3611680	3211517	68232260					-1398739575369504796783870
61480	100231	12247635544					13307788129369066020122427230
0	100231	12247635544					-8224147097293852105718286688
	180512	888376	571584				24616839265838829862800
856141332480	324517959	0825600					1456672909093006685160266912
-796140122400	22788885	576936					-2603417227595663494620532384
-72854664112	9315678	129504					363793504089481409295611432
9536197432	19454502	4992					-3894164757270643414825840
28686912	-146092	0320					30896565784971962717088600
-4646912	2073600						-1726645706913287241856
2304							117669261819584200
							-2366627577600
							52676205776000





Table IV. (Continued)

8	SECOND MOMENT	GAUSSIAN	---	DIMENSION = 3
0	10737418240	61572651155456	38280596882649216	23058630092136939520
128	-12828918784	-1263280353853344	-1623762629313344	-803729856176452168
0	4219305984	58277248565248	708283407618502688	70620953091831433136
1536	33037705956	607994056833408	-1594097766736384000	-177865955049704740416
-128	-44421873664	-1167385959944640	-6219651614334622208	-8814800500750437642240
0	21786657128	1386981645765120	36485659365670871040	5813536988491225217024
16384	-1472002574	-1009739379814400	-5052579841408494824	27790374375374157524992
-3072	-430965964224	-13720282608967680	-57011374311180828744	-144483261915882825449420
1024	35548856320	295121991222116352	15773862997658189824	144924005676474694919049216
0	94489280512	18908772265593920	2699819570506210893824	-15145001094474494919049216
163840	-132231674880	-1506168669871587328	-326983086070186917520	-8006145315263936958000000
-52608	48519077888	1581764669173923840	-526738686070186917520	159414982669128511927274496
4096	409286519904	58758397893296	76257331376175586279424	159414982669128511927274496
-16768	-10386727072	-58758397893296	-171841133720035119616	68782696494570788549344
2018	43856264192	653296750661024	4389547595613281782784	-17865975945552440967168
1578804	-385956264192	-13330490114252800	-8112152023469865041272	6484252439407791571599336
738304	18202695749536	42970980822953728	23532301453006059110400	39645006570098580687360
98304	-2983185088512	-225257915098120192	-4839464958080377272181504	-182799073424666410495344640
-36048	805251237888	-3136809149896960	905790754795956968443904	58182142387108425043894272
167424	824633720832	58758397893296	-127006734792686734298112	-2375396826566593825816848
163840	-1328136167424	-5699625760382640128	195246199670304267789504	4713895281095996281912861696
1968004	483268310944	53525843107782656	60184376684933439488	271810999308917909120614400
-960004	-8005282359660	5572615794673337888	-2260318663198176367869952	-1916129398433059688015638036480
1794008	8005282359660	-5572615794673337888	3397327514683195966089216	37609776349735234844951455040
11500128	-18051359963616	60184376684933439488	-2551119547240578662091488	6639676257607058483828490240
-9191424	72889338462208	-20074469638448588992	27381885734412615656	-4733419039486411274722960471120
-6109952	-7491825785888	15576564342962785280	-8866355952096944	745491857185675004630365396480
7294976	338641259185024	4503599627370496	7157973705940485216	-331689409192030825327198456480
2787072	531596922093568	-1131985514030352	-802304188237092030800	39184616002734433934000438919168
134217228	107159846912000	6870180046616361984	5128304188237092030800	
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