

Free energy in a magnetic field and the universal scaling equation of state for the three-dimensional Ising model

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We have substantially extended the high-temperature and low-magnetic-field (and the related low-temperature and high-magnetic-field) bivariate expansions of the free energy for the conventional three-dimensional Ising model and for a variety of other spin systems generally assumed to belong to the same critical universality class. In particular, we have also derived the analogous expansions for the Ising models with spin $s = 1, 3/2, \dots$ and for the lattice Euclidean scalar-field theory with quartic self-interaction, on the simple-cubic and the body-centered-cubic lattices. Our bivariate high-temperature expansions, which extend through 24th order, enable us to compute, through the same order, all higher derivatives of the free energy with respect to the field, namely, all higher susceptibilities. These data make more accurate checks possible, in critical conditions, both of the scaling and the universality properties with respect to the lattice and the interaction structure and also help to improve an approximate parametric representation of the critical equation of state for the three-dimensional Ising model universality class.

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I. INTRODUCTION

We present a brief analysis of high-temperature (HT) and low-field expansions for the free energy of the conventional three-dimensional (3D) Ising model in an external uniform magnetic field, extended from the presently available¹⁻⁴ order 17 up to order 24 in the case of the simple-cubic (sc) lattice, and from the order 13 up to 24 in the case of the body-centered-cubic (bcc) lattice. In addition to the conventional Ising model (i.e., with spin $s = 1/2$), we have considered also a few models with spin $s > 1/2$, and the lattice scalar Euclidean field theories with even polynomial self-interaction. All results for the simple Ising system in a field can be readily transcribed into the lattice-gas model language and therefore are of immediate relevance also for the theory of the liquid-gas transition.^{5,6} The HT and low-field expansions of the spin- s Ising models can be transformed^{7,8} into low-temperature (LT) and high-field expansions.

The spin- s Ising model in an external magnetic field H is described by the Hamiltonian⁹⁻¹²

$$\mathcal{H}\{s\} = -\frac{J}{s^2} \sum_{\langle ij \rangle} s_i s_j - \frac{mH}{s} \sum_i s_i, \quad (1)$$

where $s_i = -s, -s+1, \dots, s$ is the spin variable at the lattice site i , m is the magnetic moment of a spin, and J is the exchange coupling. The first sum extends over all distinct nearest-neighbor pairs of sites, and the second sum over all lattice sites. The conventional Ising model is recovered by setting $s = 1/2$.

The one-component self-interacting scalar-field theory on a lattice is described by the Hamiltonian¹³⁻¹⁵

$$\mathcal{H}\{\phi\} = -\sum_{\langle ij \rangle} \phi_i \phi_j + \sum_i (V(\phi_i) + H\phi_i). \quad (2)$$

Here $-\infty < \phi_i < +\infty$ is a continuous variable associated to the site i and $V(\phi_i)$ is an even polynomial in the variable ϕ_i . In

this study, we have only considered the specific model in which $V(\phi_i) = \phi_i^2 + g(\phi_i^2 - 1)^2$, although we can cover interactions of a more general form.

All these models are expected to belong to the 3D Ising universality class, therefore our extensive set of series-expansion data can be used to test the accuracy of the basic hypotheses of critical scaling and universality with respect to the lattice and the interaction structure, by comparing the estimates of the exponents and of universal combinations of critical amplitudes for the various models, as well as by forming approximate representations of the equation of state (ES). In this study our attitude^{15,16} is, to some extent, complementary to the current one. Usually, universality is essentially assumed from the outset: For example, in the renormalization group (RG) approach,¹⁷⁻²⁵ an appropriate scalar-field theory in continuum space is taken as the representative of the Ising universality class, as suggested by the independence of the renormalization procedure from the details of the microscopic interaction. Also in HT and Monte Carlo approaches, attention has been recently focused^{14-16,26,27} on particular continuous- or discrete-spin-lattice models that exhibit vanishing (or very small) leading nonanalytic corrections to scaling,^{28,29} in order to be able to estimate more accurately the physical quantities of interest. In this paper, we prefer to take advantage of our extended expansions to test a wide sample of models, expected to belong to the same universality class, and to show how closely, already at the present orders of expansion, each model approaches the predicted asymptotic scaling and universality properties.

The paper is organized as follows: in Sec. II we briefly characterize our expansions, sketch the method of derivation, and list the numerous tests of correctness passed by the series coefficients. In Sec. III we define the higher-order susceptibilities, whose critical parameters enter into the determination of the scaling ES and update an approximate representation of it. In Sec. IV we discuss numerical estimates of exponents, amplitudes, and universal combinations of these, which can

be computed from the bivariate series. In the last section, we summarize our results and draw some conclusions.

II. EXTENSIONS OF THE BIVARIATE SERIES EXPANSIONS

The HT series-expansion coefficients for the models under study have been derived by a fully computerized algorithm based on the vertex-renormalized linked-cluster (LC) method, which calculates the mean magnetization per spin in a nonvanishing magnetic field from the set of all topologically distinct, connected, 1-vertex-irreducible (1VI), single-rooted graphs.⁹ We have taken advantage of the bipartite structure of the sc and the bcc lattices to restrict the generation of graphs to the subset of the bipartite graphs, i.e., to the graphs containing no loops of odd length.

In the past, the LC method was employed mainly to derive expansions in the absence of magnetic field. In the presence of a field, the most extensive^{1,2} data so far available in 3D were derived indirectly by transforming^{7,8} bivariate LT and high-field expansions³⁰ into HT and low-field expansions. This computation was performed only for the $s = 1/2$ Ising model, although some LT and high-field data existed also for other values of the spin. Shorter HT expansions in a finite field had also been previously obtained,⁶ only for the $s = 1/2$ model, by a direct expansion of the free energy. It is worth noting that we are now in a position to follow the opposite route: namely, of transforming our bivariate HT data for the spin- s Ising systems into LT and high-field expansions, thus extending also the known LT results.

It is fair to remark that the finite-lattice (and the related transfer-matrix) methods of expansion^{31,32} have been shown to be more efficient³³ than the LC approach, at least for

$s = 1/2$ in $d = 2$ dimensions, even in the presence of a magnetic field, while they remain rather difficult and unwieldy in higher space dimensions. In the case of the 2D spin-1/2 Ising model, with the support of a variational approximation, these methods made a representation of the ES of unprecedented accuracy³⁴ possible. In the future, these techniques might prove to be competitive³² in the 3D case also for calculations in a nonvanishing field. We believe, however, that it has been worthwhile to test and develop also a LC approach, because it expresses the series coefficients in terms of polynomials in the moments of the single-spin measure and, therefore, unlike the finite-lattice method, is flexible enough to apply also to non-discrete-state models such as the one-component scalar-field model¹⁵ within the Ising universality class studied here and, more generally, to the $O(N)$ -symmetric spin³⁵ or lattice-field systems in any space dimension.

A. The algorithms

To give a hint of the strong points of our graphical algorithms, we mention that, using only an ordinary desktop personal quad-processor computer with a 4-GB fast memory [random access memory (RAM)], our code can complete in seconds all calculations already documented^{1,2} in the literature (see Table III). The whole renormalized calculation presented here can be completed in a central processing unit (CPU) time of a few days, most of which goes into producing the highest order of expansion. In what follows all timings are single-core times.

The LC computation has been split into three parts. First, we generated the simple, bipartite, unrooted, topologically distinct 1VI graphs. This part is memory intensive, but takes only a few hours. Table I lists the numbers of these graphs from order 4 through 24. In a second step, we computed the

TABLE I. The numbers of simple, connected, bipartite, unrooted 1VI graphs with l lines and with a given number v of odd vertices, which contribute to the HT expansion coefficient of the free energy at order K^l .

$l \setminus v$	0	2	4	6	8	10	12	14	16	Totals
4	1	0	0	0	0	0	0	0	0	1
5	0	0	0	0	0	0	0	0	0	0
6	1	1	0	0	0	0	0	0	0	2
7	0	1	0	0	0	0	0	0	0	1
8	2	1	1	0	0	0	0	0	0	4
9	0	3	1	1	0	0	0	0	0	5
10	3	6	5	0	0	0	0	0	0	14
11	0	11	7	2	0	0	0	0	0	20
12	9	20	31	4	1	0	0	0	0	65
13	0	49	53	22	0	0	0	0	0	124
14	20	101	194	54	7	0	0	0	0	376
15	0	258	432	238	20	2	0	0	0	950
16	84	520	1471	732	127	0	0	0	0	2934
17	0	1482	3725	2886	434	29	0	0	0	8556
18	300	3243	12233	9531	2403	97	5	0	0	27812
19	0	9646	33 608	36 067	9675	845	0	0	0	89841
20	1520	21 859	1 09 796	1 23 543	46 241	4023	133	0	0	3 07 115
21	0	68 697	3 18 283	4 60 225	1 91 416	26 435	594	13	0	10 65 663
22	8186	1 63 780	10 48 349	16 08 030	8 58 792	1 34 409	6672	0	0	38 28 218
23	0	533 569	31 66 399	59 70 246	35 66 324	75 76 96	40 686	744	0	14 035 664
24	52 729	13 28 836	10 594 514	21 241 772	15 475 018	37 96 365	3 17 259	4267	38	52 810 798

single-rooted multigraphs, their symmetry numbers, and their lattice embeddings. This part of the calculation requires little memory: In the case of the bcc lattice, completing the 24th order took approximately one day, while in the case of the sc lattice 2 weeks were necessary. In the latter case, most of the time was spent to determine the graph embeddings. These two parts of the calculation were implemented by C++ codes, and used the “Nauty”³⁶ library to compute the graph certificates and symmetry factors. The relevant procedures of this package were supplemented with the GNU Multiprecision Arithmetics Library³⁷ to get the exact graph symmetry numbers. The third step implements the algebraic vertex-renormalization⁹ procedure by deriving the magnetization from the single-rooted 1VI graphs and then, by integration, the free energy $\mathcal{F}(K, h) = \sum f_n(h)K^n$. Here $K = J/k_B T$, with k_B the Boltzmann constant and T the temperature, while $h = mH/k_B T$ is the reduced magnetic field. The magnetization is expressed in terms of the bare vertices $M_i^0(h)$ obtained deriving i times with respect to h the generating function $M_0^0(h) = \ln\left[\frac{\sinh(h(2s+1)/2s)}{\sinh(h/2s)}\right]$ in the case of the spin- s Ising systems, or, in the case of the scalar-field system, $M_0^0(h) = \ln\left[\int d\phi e^{-V(\phi)+h\phi}\right]$. For example, the HT expansion coefficient of the free energy at order K^2 , on the bcc lattice, is given by

$$f_2(h) = 2[M_2^0(h)]^2 + 32[M_1^0(h)]^2 M_2^0(h), \quad (3)$$

while on the sc lattice

$$f_2(h) = \frac{3}{2}[M_2^0(h)]^2 + 18[M_1^0(h)]^2 M_2^0(h). \quad (4)$$

TABLE II. The numbers of monomials in the bare vertices, with a given number v of odd vertices, which contribute to the HT expansion coefficient of the free energy on a bipartite lattice, at order K^l .

$l \setminus v$	0	2	4	$v > 4$	Totals
1	0	1	0	0	1
2	1	1	0	0	2
3	0	3	1	0	4
4	3	4	3	0	10
5	0	10	6	2	18
6	6	14	15	6	41
7	0	27	25	18	70
8	14	39	45	39	137
9	0	70	77	86	233
10	25	94	130	164	413
11	0	157	201	305	663
12	53	222	318	541	1134
13	0	348	481	924	1753
14	89	457	742	1529	2817
15	0	699	1091	2519	4309
16	167	941	1589	3972	6669
17	0	1379	2289	6213	9881
18	278	1796	3314	9566	14954
19	0	2577	4635	14487	21699
20	480	3370	6492	21662	32004
21	0	4711	9010	32134	45855
22	760	5965	12430	46887	66042
23	0	8257	16858	67949	93064
24	1273	10664	22895	97543	132375

Table II lists the number of monomials of the bare vertices, with a given number v of odd indices that contribute to the free-energy HT expansion coefficient at order K^l . Equivalently, this is the number of admissible vertex-degree sequences of the (far more numerous) graphs contributing to this coefficient. Notice that the monomials containing at least two bare vertices of odd order are the overwhelming majority. They all vanish in zero field, which shows that the finite-field calculation has a substantially higher complexity. The renormalization through 24th order was performed in a few hours. The third step of the calculation is based on codes written in the Python and Sage³⁸ languages.

It is also not without interest that in a preliminary step of our work, we have been able to employ the simple *unrenormalized* linked-cluster method,⁹ which uses *all* topologically distinct unrooted connected graphs (including multigraphs) to compute the bivariate expansions of the free energy through order 20. It takes only 1 day to complete this calculation. Of course, while the unrenormalized procedure is algebraically straightforward, it would make further extensions of the series impractical, using our desktop computers, for the rapid increase with order of the combinatorial complexity and, as a consequence, of the memory requirements. The computation of the 21st order does not fit in 4 GB of RAM, but would require some increase of memory. These calculations are, however, interesting by themselves, both because the unrenormalized method is still generally (and too pessimistically) dismissed as unwieldy beyond just the first few orders, and because they provide a valuable cross check, through order 20, of the results of the algebraically more complex vertex-renormalized procedure, which remains necessary to push the calculation to higher orders. Our improvements of the presently available HT series in a field are summarized in Table III, in the case of the sc and the bcc lattices. Similar extensions for the same class of models, in the case of the simple quadratic lattice and for bipartite lattices in $d > 3$ space dimensions, will be discussed elsewhere. The series-expansions coefficients will be tabulated in a separate paper.

The feasible correctness checks of our computations are inevitably partial, because the extended expansions include information much wider than that already available in the literature. The easiest nontrivial check is that our procedure yields the known bivariate expansion of the free energy for the spin-1/2 Ising model in a finite field on the 1D lattice. Of course, we have also checked that our results agree, through

TABLE III. Maximal order in K of the HT and low-field expansions of the free energy for the models in the Ising universality class considered in this note.

	Existing data (Ref. 2)	This work
	sc lattice	
Ising $s = 1/2$	17	24
Ising $s > 1/2$	0	24
ϕ^4	0	24
	bcc lattice	
Ising $S = 1/2$	13	24
Ising $s > 1/2$	0	24
ϕ^4	0	24

their common extent, with the old data cited above^{1,2} for the spin-1/2 Ising system in a magnetic field, both on the sc and the bcc lattices. Otherwise, our results can only be compared with the related data in zero field, in particular, with the HT expansions of the free energy and its second field derivative, both for the Ising model with general spin s and for the scalar-field model, on the sc and the bcc lattices, which have been tabulated^{15,16} through order K^{25} , while the fourth field derivative is already known^{15,16} through K^{23} for both lattices. Our results agree, through their common extent, also with the expansions of the sixth field derivative in zero field, tabulated³⁹ up to order K^{19} , and of the eighth field derivative, tabulated³⁹ up to order K^{17} , in the case of the spin-1/2 model on the bcc lattice. We have finally checked that our expansions reproduce the sc lattice calculations of the sixth field derivative (known up to order K^{19}), of the eighth (known up to order K^{17}), and of the tenth (known up to order K^{15}) in the case of the sc lattice scalar field with quartic self-coupling $g = 1.1$, which have been tabulated in Ref. 14.

III. ASYMPTOTIC SCALING AND THE EQUATION OF STATE

The hypothesis of asymptotic scaling⁴⁰⁻⁴⁴ for the singular part $\mathcal{F}_s(\tau, h)$ of the reduced specific free energy, valid as both h and τ approach zero, can be expressed in the form

$$\mathcal{F}_s(\tau, h) \approx |\tau|^{2-\alpha} Y_{\pm}(h/|\tau|^{\beta\delta}). \quad (5)$$

where $\tau = (1 - T_c/T)$ is the reduced temperature. The exponent α specifies the divergence of the specific heat, β describes the small τ asymptotic behavior of the spontaneous specific magnetization M on the phase boundary ($h \rightarrow 0^+, \tau < 0$),

$$M \approx B(-\tau)^{\beta}, \quad (6)$$

and B denotes the critical amplitude of M . The exponent δ characterizes the small h asymptotic behavior of the magnetization on the critical isotherm ($h \neq 0, \tau = 0$),

$$|M| \approx B_c |h|^{1/\delta}, \quad (7)$$

and B_c is the corresponding critical amplitude. For the exponents α and β , we have assumed the values $\alpha = 0.110(1)$ and $\beta = 0.3263(4)$, obtained using the scaling and hyperscaling relations, from the HT estimates¹⁵ of the susceptibility exponent $\gamma = 1.2373(2)$ and of the correlation-length exponent $\nu = 0.6301(2)$.

The functions $Y_{\pm}(w)$ are defined for $0 \leq w \leq \infty$ and have a power-law asymptotic behavior as $w \rightarrow \infty$. The $+$ and $-$ subscripts indicate that different functional forms are expected to occur for $\tau < 0$ and $\tau > 0$. The usual scaling laws follow from Eq. (5). The simplest consequence of Eq. (5), which will be tested using our HT expansions, is that the critical exponents of the successive derivatives of $\mathcal{F}_s(\tau, h)$ with respect to h at zero field are evenly spaced by the quantity $\Delta = \beta\delta$, usually called the ‘‘gap exponent.’’ More precisely, let us define the zero-field n -spin connected correlation functions at zero wave number (also called *higher susceptibilities* when $n > 2$) by the equation

$$\chi_n(K) = [\partial^n \mathcal{F}(h, K) / \partial h^n]_{h=0} = \sum_{s_2, s_3, \dots, s_n} \langle s_1 s_2 \dots s_n \rangle_c. \quad (8)$$

For odd values of n , these quantities vanish in the symmetric HT phase, while they are nontrivial for all n in the broken-symmetry LT phase. For even values of n in the symmetric phase, and for all n in the broken phase, scaling implies that, as $T \rightarrow T_c^+$ along the critical isochore ($h = 0, \tau > 0$) or, as $T \rightarrow T_c^-$ along the phase boundary, we have

$$\chi_n(\tau) \approx C_n^{\pm} |\tau|^{-\gamma_n} (1 + b_n^{\pm} |\tau|^{\theta} + \dots), \quad (9)$$

where $\gamma_n = \gamma + (n - 2)\Delta$, and b_n^{\pm} and θ are, respectively, the amplitude and the exponent that characterize the leading nonanalytic correction to asymptotic scaling. The value⁴⁵ $\theta = 0.52(2)$ has been estimated for the universality class of the 3D Ising model. Assuming also the validity of hyperscaling, we can conclude that $2\Delta = 3\nu + \gamma$.

An important bonus of our bivariate calculations is the significant extension the HT expansions of the higher susceptibilities. As mentioned above, we have added one more term to the existing¹⁶ HT expansion of $\chi_4(K)$, five terms to that³⁹ of $\chi_6(K)$, seven to that¹⁴ of $\chi_8(K)$ and nine to that of $\chi_{10}(K)$. In the case of the susceptibilities of order $2n > 10$, no data were available so far, except those for the $s = 1/2$ Ising model, which can be derived from the expansions listed in Table III. We have now extended, uniformly in the order, the HT expansions of all higher susceptibilities $\chi_{2n}(K)$ with $2n \geq 4$, for several models in the 3D Ising universality class. In this paper, we shall present only a preliminary analysis of these quantities, while a more detailed discussion of our bivariate expansions will be postponed to a forthcoming article.

The scaling form of the ES, $M = \mathcal{M}(h, T)$, relating the external reduced magnetic field h , the reduced temperature τ , and the magnetization M , when h and τ approach zero, is simply obtained by differentiating Eq. (5) for $f_s(\tau, h)$ with respect to h ,

$$M \approx -|\tau|^{\beta} Y_{\pm}^{(1)}(h/|\tau|^{\beta\delta}). \quad (10)$$

Here we have used the relation $\gamma = \beta(\delta - 1)$. By further differentiation of Eq. (10) with respect to the field, also the higher susceptibilities are recognized to have a scaling form

$$\chi_n(h, \tau) = (\partial^{n-1} M / \partial h^{n-1}) \approx -|\tau|^{-\gamma_n} Y_{\pm}^{(n)}(h/|\tau|^{\beta\delta}). \quad (11)$$

The hypothesis of universality states that, in addition to the critical exponents, the function $Y_{\pm}(w)$, [and therefore also its n th derivative $Y_{\pm}^{(n)}(w)$] is universal⁴⁶ up to multiplicative constants (*metric factors*⁴⁷) that fix the scales of h and τ in each particular model within a universality class. Accordingly, one can conclude that a variety of dimensionless combinations of critical amplitudes are universal.

The ES can also be written in the equivalent form^{40,41,48}

$$h(M, \tau) \approx M |M|^{\delta-1} f(\tau/|M|^{1/\beta}), \quad (12)$$

in which a single scaling function $f(x)$, universal up to metric factors, describes both the regions $\tau < 0$ and $\tau > 0$. The function $h(M, \tau)$ is known⁴⁸ to be regular analytic in a neighborhood of the critical isotherm and of the critical isochore. From general thermodynamic arguments⁴⁸ one can infer that $f(x)$ is a positive monotonically increasing regular function of its argument, in some interval $-x_0 \leq x \leq \infty$, with $x_0 > 0$. Moreover, $f(-x_0) = 0$. The local behavior of the

function $f(x)$ can be further determined, by the requirement of consistency with the scaling laws, in terms of critical amplitudes of quantities computable from our HT and LT series. By differentiating this form of the ES with respect to M , we get the asymptotic behavior $f(x) \propto x^\gamma$ for large positive x . Setting $\tau = 0$, the ES reduces to Eq. (7) and $f(0) = B_c^{-\delta}$. If $h \rightarrow 0$ at fixed $\tau < 0$, we expect to find a nonvanishing spontaneous magnetization M , therefore the ES implies that $f(x)$ must vanish. Because $f(-x_0) = 0$, we have $-\tau/M^{1/\beta} = x_0$ and, from Eq. (6), we conclude that $x_0 = B^{-1/\beta}$. We can then fix the metric factors by normalizing the field to $B_c^{-\delta}$ and the reduced temperature to $B^{-1/\beta}$. The expansion of $f(x)$ for large positive x is expressed in terms of the critical parameters characterizing the HT side of the critical point. The small x expansion, which uses the parameters of the critical isotherm, and the negative x region related to the parameters of the LT side of T_c , will be discussed in a forthcoming paper presenting our analysis of the extended LT expansions.

Summarizing the more detailed discussion of Ref. 19, we can also observe that, in the large positive x (small magnetization) region, where the magnetic field $h(M, \tau)$ has a convergent expansion in odd powers of M , the ES is more conveniently expressed in terms of the variable $z = M\tau^{-\beta}x_0^\beta$. The ES takes then the form

$$h(M, \tau) = \bar{h}|\tau|^{\beta\delta}F(z), \quad (13)$$

where \bar{h} is a constant and $F(z)$ is normalized by the equation $F'(0) = 1$. The small z expansion of $F(z)$ can be written as

$$F(z) = z + \frac{1}{6}z^3 + F_5z^5 + F_7z^7 + \dots \quad (14)$$

The coefficients F_5, F_7, \dots are defined by the equation $F_{2n-1} = r_{2n}^+ / (2n-1)!$, in terms of the ratios r_{2n}^+ that will be introduced in the next section. They have been computed within the RG approach,^{20,22} by the ϵ expansion ($\epsilon = 4 - d$) up to five loops, by the perturbative g expansion at fixed dimension $d = 3$ up to the same order, by other RG approximations,²³⁻²⁵ by HT expansions,^{14,49} and by Monte Carlo methods.^{50,51} Our estimates of the first few r_{2n}^+ by extended HT expansions are listed in Table X.

A. A parametric form of the ES

A parametric form⁵²⁻⁵⁴ has been introduced to formulate an approximate representation of the ES in the whole critical region and as an aid in the comparison with the experimental data. The parametrization is chosen to embody the analyticity properties of $h(M, \tau)$ and the scaling laws. These properties make the parametric form convenient to approximate the ES in the whole critical region by using only HT inputs, such as the small z expansion equation (14) of $F(z)$. In this approach, the scaled field and the reduced temperature are expressed as the following functions:

$$M = m_0 R^\beta \theta, \quad (15)$$

$$\tau = R(1 - \theta^2), \quad (16)$$

$$h = h_0 R^{\beta\delta} l(\theta), \quad (17)$$

of generalized radial and angular coordinates $R \geq 0$ and $-\theta_0 \leq \theta \leq \theta_0$, with $\theta_0 > 1$ the smallest positive zero of the

function $l(\theta)$. The radial coordinate R measures the distance in the h, T plane from the critical point, and the angular coordinate θ specifies a direction in this plane. Therefore, $\theta = 0$ corresponds to the critical isochore, $\theta = \pm 1$ is associated to the critical isotherm, and $\theta = \pm\theta_0$ is associated to the coexistence curve. The function $l(\theta)$, normalized by $l'(0) = 1$, is odd and regular for $|\theta| < \theta_0$, as implied by the regularity of $f(x)$ and the invertibility of the above variable transformation in this interval.

The variable z is then expressed as

$$z = \frac{\rho\theta}{(1 - \theta^2)^\beta} \quad (18)$$

and the function $F(z)$ of Eq. (14) is related to $l(\theta)$ by

$$l(\theta) = \frac{1}{\rho} [(1 - \theta^2)^{\beta+\gamma} F(z(\theta))]. \quad (19)$$

Here $\rho = m_0 x_0^\beta$ is a positive constant related to the arbitrary normalization constant m_0 appearing in Eq. (15). If $F(z)$ were exactly known, the corresponding $l(\theta)$ given by Eq. (19) should not depend on ρ . However, the polynomial truncations of $l(\theta)$ that can be formed from the first few available terms of the expansion equation (14) of $F(z)$ will have coefficients $l_{2n+1}(\rho)$ depending not only on the coefficients F_5, F_7, \dots and on the exponents β and γ , but also on ρ .

In particular,¹⁹ expanding both sides of Eq. (19), one obtains

$$l_3(\rho) = \frac{1}{6}\rho^2 - \gamma, \quad (20)$$

$$l_5(\rho) = \frac{1}{2}\gamma(\gamma - 1) + \frac{1}{6}(2\beta - \gamma)\rho^2 + F_5\rho^4, \quad (21)$$

$$l_7(\rho) = -\frac{1}{6}\gamma(\gamma - 1)(\gamma - 2) + \frac{1}{12}(2\beta - \gamma)(2\beta - \gamma + 1)\rho^2 + (4\beta - \gamma)F_5\rho^4 + F_7\rho^6, \quad (22)$$

$$l_9(\rho) = \frac{1}{24}\gamma(\gamma - 1)(\gamma - 2)(\gamma - 3) + \frac{1}{36}(2\beta - \gamma)(2\beta - \gamma + 1)(2\beta - \gamma + 2)\rho^2 + \frac{1}{2}(4\beta - \gamma)(4\beta - \gamma + 1)F_5\rho^4 + (6\beta - \gamma)F_7\rho^6 + F_9\rho^8, \quad (23)$$

etc.

The dependence on ρ of the coefficients l_{2n+1} has been exploited to improve the approximation of $l(\theta)$. A first approach consists in fixing ρ to the value ρ_m that minimizes¹⁹ the modulus of the highest-order expansion coefficient $l_{2n+1}(\rho)$ of $l(\theta)$ that can be determined reliably from the available coefficients F_{2n-1} . A second method¹⁴ is based on computing some universal combinations of critical amplitudes in terms of $l(\theta)$ and then in choosing for ρ the unique value that makes all such quantities stationary. We may follow this route and consider, for example, the dependence on ρ of the universal ratio of the susceptibility amplitudes above and beneath T_c , namely, C_2^+ / C_2^- , and of the ratios $C_4^+ B^2 / (C_2^+)^3$ and $C_2^+ B^{\delta-1} / B_c^\delta$. If we plot these quantities versus ρ^2 , we obtain Fig. 1, which indicates that the choice $\rho^2 = 2.615$ should be optimal. Then, using the central values both of the coefficients F_{2n-1} up to $n = 7$, as obtained from our Table X, and of the exponents β and γ as indicated above and fixing

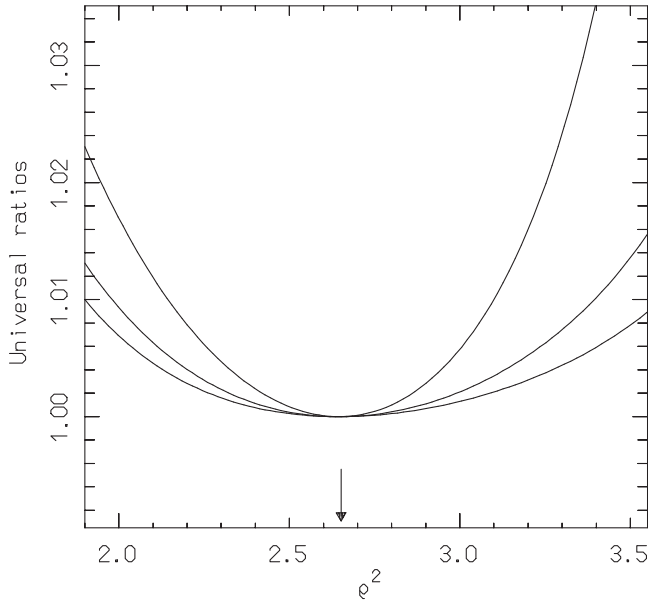


FIG. 1. A plot vs the parameter ρ^2 , of the universal combinations of critical amplitudes C_2^+/C_2^- (upper curve), $C_2^+ B^{\delta-1}/B_c^\delta$ (middle curve), and $C_4^+ B^2/(C_2^+)^3$ (lower curve) obtained from the truncated polynomial approximation of $l(\theta)$, Eq. (24). The computation is based on the coefficients F_{2n-1} with $n = 1, \dots, 7$, estimated in this work. For convenience, the curves are normalized to their minimum values.

ρ to its optimal value, the following form of $l(\theta)$ can be determined:

$$l(\theta) \approx \theta - 0.8014(50)\theta^3 + 0.00946(30)\theta^5 + 0.00141(40)\theta^7 + 0.00029(10)\theta^9 - 0.00011(5)\theta^{13}. \quad (24)$$

Here we have neglected the term in θ^{11} , whose coefficient is $O(10^{-6})$, and have indicated the last three terms only to show that their contribution in the interval of interest $|\theta| < \theta_0$ is very small. The function $l(\theta)$ vanishes at $\theta = \theta_0 \approx \pm 1.1273$.

The analogous result for this auxiliary function obtained in Ref. 20, fixing ρ by the first method and choosing the values $\beta = 0.3258(14)$ and $\gamma = 1.2396(13)$ of the critical exponents, is

$$l(\theta) \approx \theta - 0.762(3)\theta^3 + 0.0082(10)\theta^5, \quad (25)$$

which vanishes at $\theta \approx \pm 1.1537$. In this case, the coefficients F_{2n-1} were obtained by a RG five-loop perturbation expansion in $d = 3$. On the other hand, computing the F_{2n-1} by the RG ϵ expansion to fifth order and choosing $\beta = 0.3257(25)$ and $\gamma = 1.2355(50)$ leads²⁰ to

$$l(\theta) \approx \theta - 0.72(6)\theta^3 + 0.0136(20)\theta^5. \quad (26)$$

More recently, in Ref. 14, using values of the exponents very near to those used in our paper, and deriving the F_{2n-1} from a HT expansion of sc-lattice scalar-field models with self-couplings appropriately chosen to suppress the leading correction to scaling, the following expression was obtained,

$$l(\theta) \approx \theta - 0.736743\theta^3 + 0.008904\theta^5 - 0.000472\theta^7, \quad (27)$$

which vanishes at $\theta \approx \pm 1.1741$. As stressed in Refs. 19 and 20, the alternative forms, Eqs. (24)–(27), cannot be directly compared, because they are associated to different

TABLE IV. Some universal amplitude combinations obtained in this work from the parametric form Eq. (24) of the ES. For comparison, we have reported also the results obtained from the parametric form Eq. (27) of the ES in Ref. 14, based on shorter HT expansions, and from the parametric forms, Eqs. (25) and (26) in Ref. 20. The latter representations were obtained, either from the RG ϵ expansion or from the g expansion, choosing values of the exponents slightly different from those used to get the estimates listed in the first two rows.

Universal ratios	A^+/A^-	C_2^+/C_2^-	$\alpha A^+ C_2^+/B^2$	$C_2^+ B^{\delta-1}/B_c^\delta$
This work	0.530(3)	4.78(3)	0.0563(5)	1.66(2)
Ref. 14	0.529(6)	4.78(5)	0.0562(1)	1.665(10)
ϵ expans. (Ref. 20)	0.527(37)	4.73(16)	0.0569(35)	1.648(36)
g expans. (Ref. 20)	0.537(19)	4.79(10)	0.0574(20)	1.669(18)
MC (Ref. 27)		4.756(28)		1.723(13)
MC (Ref. 57)	0.536(2)	4.713(7)		
MC (Ref. 58)		4.75(3)		
MC (Ref. 56)	0.540(10)	4.67(3)		
MC (Ref. 55)	0.532(7)			

parametrizations (different values of ρ). One should rather compare the universal predictions obtained from them, for example, for the universal amplitude combinations, which we have reported in Tables IV and V.

In the Table IV, A^+ and A^- denote the amplitudes of the specific heat above and beneath T_c . Our estimates are compared with the corresponding ones obtained²⁰ from the polynomials $l(\theta)$ in Eqs. (25) and (26) and with those obtained¹⁴ from Eq. (27). The results from the various approaches show a good overall consistency. In Table IV, we have reported also a few recent^{27,55–57} Monte Carlo estimates, for the ratios A^+/A^- , $C_2^+ B^{\delta-1}/B_c^\delta$, and C_2^+/C_2^- . It is worth to remark that the computation of the first quantity is difficult, because the weak singularity of the specific heat forces to extend the simulation very close to the critical point. The recent estimates^{55–57} of this ratio, in the range 0.532(7)–0.540(4), based on simulations of large lattices, might now supersede older results, which were $\approx 6\%$ larger, thus improving the agreement with the ES estimates of Table IV. Also the second ratio, involving the amplitude B_c of Eq. (7) is difficult to measure by simulations, for similar reasons. The result of Ref. 27 is somewhat larger than the estimates from the ES. In the case of the third ratio,

TABLE V. More universal amplitude combinations obtained in this work from the parametric form Eq. (24) of the ES. For comparison, we have reported also the results obtained from the parametric form Eq. (27) of the ES in Ref. 14, based on shorter HT expansions, and from the parametric forms Eqs. (25) and (26) in Ref. 20. They were obtained, either from the RG ϵ expansion or from the g expansion, choosing values of the exponents slightly different from those used to get the estimates listed in the first two rows.

Universal ratios	$-C_4^+ B^2/(C_2^+)^3$	C_4^+/C_4^-	$-C_3^- B/(C_2^-)^2$
This work	7.8(1)	-9.2(3)	6.015(15)
Ref. 14	7.83(4)	-9.3(5)	6.018(20)
ϵ expans. (Ref. 20)	8.24(34)	-8.6(1.5)	6.07(19)
g expans. (Ref. 20)		-9.1(6)	6.08(6)

the recent simulations^{27,56,57} have changed the previous larger estimates to values in a range closer to the ES results. It should be noted that the simulations of Refs. 27 and 57 are performed on models on the sc lattice with reduced corrections to scaling such as the ϕ^4 model²⁷ and the Blume-Capel model.⁵⁷ On the other hand, the simulations of Refs. 55, 56, and 58 are based on the conventional sc lattice $s = 1/2$ Ising model. In these tables, we have not reported the few available experimental measures of some of these combinations, nor the estimates based on a direct evaluation of the amplitudes by LT and HT expansions. These data, tabulated in Refs. 14, 19, 20, and 47, are completely compatible with the ES results of Tables IV and V, but sometimes the comparison is not stringent, owing to the still large uncertainties. Therefore, it will be useful to improve the series determinations of the amplitudes on the critical isotherm and on the coexistence curve, exploiting our extended bivariate LT expansions of the free energy for the spin- s Ising models. A more detailed analysis of our results, along with estimates of other universal amplitude combinations, and a

wider comparison among the results in the literature is deferred to a forthcoming paper.

B. The HT zero-momentum renormalized couplings

The HT expansions of the higher susceptibilities⁴¹ will be used to evaluate their critical amplitudes C_n^+ , defined in Eq. (9), and correspondingly the critical limits of the zero-momentum n -spin dimensionless HT renormalized couplings (RCCs). These quantities enter into the approximate representations of the scaling ESs, Eqs. (10) and (12).

In the HT phase the first few $2n$ spin RCCs are defined as the critical limits as $K \rightarrow K_c^-$ of the following expressions:

$$g_4^+(K) = -\frac{V}{\xi^3(K)} \frac{\chi_4(K)}{\chi_2^2(K)}, \quad (28)$$

$$g_6^+(K) = \frac{V^2}{\xi^6(K)} \left[-\frac{\chi_6(K)}{\chi_2^3(K)} + 10 \left(\frac{\chi_4(K)}{\chi_2^2(K)} \right)^2 \right], \quad (29)$$

$$g_8^+(K) = \frac{V^3}{\xi^9(K)} \left[-\frac{\chi_8(K)}{\chi_2^4(K)} + 56 \frac{\chi_6(K)\chi_4(K)}{\chi_2^5(K)} - 280 \left(\frac{\chi_4(K)}{\chi_2^2(K)} \right)^3 \right], \quad (30)$$

$$g_{10}^+(K) = \frac{V^4}{\xi^{12}(K)} \left[-\frac{\chi_{10}(K)}{\chi_2^5(K)} + 120 \frac{\chi_8(K)\chi_4(K)}{\chi_2^6(K)} + 126 \frac{\chi_6^2(K)}{\chi_2^6(K)} - 4620 \frac{\chi_6(K)\chi_4^2(K)}{\chi_2^7(K)} + 15400 \left(\frac{\chi_4(K)}{\chi_2^2(K)} \right)^4 \right], \quad (31)$$

$$g_{12}^+(K) = \frac{V^5}{\xi^{15}(K)} \left[-\frac{\chi_{12}(K)}{\chi_2^6(K)} + 220 \frac{\chi_{10}(K)\chi_4(K)}{\chi_2^7(K)} + 792 \frac{\chi_8(K)\chi_6(K)}{\chi_2^7(K)} - 17160 \frac{\chi_8(K)\chi_4^2(K)}{\chi_2^8(K)} - 36036 \frac{\chi_6^2(K)\chi_4(K)}{\chi_2^8(K)} + 560560 \frac{\chi_6(K)\chi_4^3(K)}{\chi_2^9(K)} - 1401400 \left(\frac{\chi_4(K)}{\chi_2^2(K)} \right)^5 \right], \quad (32)$$

$$g_{14}^+(K) = \frac{V^6}{\xi^{18}(K)} \left[-\frac{\chi_{14}(K)}{\chi_2^7(K)} + 364 \frac{\chi_{12}(K)\chi_4(K)}{\chi_2^8(K)} - 50050 \frac{\chi_{10}(K)\chi_4^2(K)}{\chi_2^9(K)} + 2002 \frac{\chi_{10}(K)\chi_6(K)}{\chi_2^8(K)} + 1716 \frac{\chi_8^2(K)}{\chi_2^8(K)} + 3203200 \frac{\chi_8(K)\chi_4^3(K)}{\chi_2^{10}(K)} - 360360 \frac{\chi_8(K)\chi_6(K)\chi_4(K)}{\chi_2^9(K)} - 126126 \frac{\chi_6^3(K)}{\chi_2^9(K)} + 10090080 \frac{\chi_6^2(K)\chi_4^2(K)}{\chi_2^{10}(K)} - 95295200 \frac{\chi_6(K)\chi_4^4(K)}{\chi_2^{11}(K)} + 190590400 \left(\frac{\chi_4(K)}{\chi_2^2(K)} \right)^6 \right]. \quad (33)$$

Here $\xi(K)$ is the second moment correlation length, defined by

$$\xi^2 = \frac{\mu_2}{6\chi_2}, \quad (34)$$

with μ_2 the second moment of the correlation function expressed as

$$\mu_2 = \sum_{s_x} x^2 \langle s_0 s_x \rangle_c. \quad (35)$$

Both the HT expansions of $\chi(K)$ and $\mu_2(K)$ are tabulated,^{15,16} through order K^{25} , for the spin- s Ising models and for the lattice scalar field.

The volume V per lattice site takes the value 1 for the sc lattice and $4/3\sqrt{3}$ for the bcc lattice. The definitions of the quantities $g_{2n}^+(K)$ given here differ by a factor $(2n)!$ from those of Ref. 49.

Also the quantities,

$$I_{2n+4}^+(K) = \frac{\chi_2^n(K)\chi_{2n+4}(K)}{\chi_4^{n+1}(K)}, \quad (36)$$

with $n \geq 1$, whose critical values are the universal amplitude combinations first described⁴⁶ in the literature, and the closely related quantities

$$r_{2n}^+(K) = \frac{g_{2n}^+(K)}{g_4^+(K)^{n-1}}, \quad (37)$$

which share the computational advantage of being independent of the correlation length, will be of relevance in what follows. The finite critical limits g_n^+ , r_{2n}^+ , and I_{2n+4}^+ of the RCCs, of the ratios $r_{2n}^+(K)$ and of the quantities $I_{2n+4}^+(K)$, represent universal combinations of HT amplitudes that should be considered together with those listed in Tables IV and V. We have not included the expressions of higher-order RCCs, because, in spite of our extensions, the available series might not yet be long enough to determine safely their critical limits. One should notice that, from the point of view of numerical approximation, the g_{2n}^+ , and also the quantities derived from them such as r_{2n}^+ , are difficult to compute, unless $2n$ is small, because they result from relatively small differences between large numbers. These estimates can be reliable provided that the uncertainties of the large numbers are much smaller than their difference. For the same reason, these quantities are notoriously even more difficult to compute by stochastic methods.

IV. METHODS AND RESULTS OF THE SERIES ANALYSIS

A. Extrapolation methods

In the numerical analysis of the series expansions of physical quantities, we shall follow two procedures aimed to determine the critical parameters, namely, the values of these quantities at the critical point, whenever they are finite, or if they are singular, the locations, amplitudes, and exponents of the critical singularities on (or nearby) the convergence disk in the complex K plane.

A first procedure used in our series analysis is the differential approximant (DA) method,⁵⁹ a generalization of the well-known Padé approximant method⁵⁹ having a wider range of application. In this approach, the values of the quantities or the parameters of the singularities can be estimated from the solution, called a differential approximant, of an initial value problem for an appropriate ordinary linear (first- or higher-order) inhomogeneous differential equation. This equation has polynomial coefficients defined in such a way that the series-expansion coefficients of its solution equal, up to a certain order, those of the series under study. Various possible equations and therefore various DAs can be formed by this prescription. They are usually identified by the sequence of the degrees of the polynomial coefficients of the equation. The approximants are called first-order, second-order DAs, etc., according to the order of the defining equation. The convergence of the procedure, in the case of the Ising models, can be improved by first performing in the series expansions the variable transformation⁶⁰

$$z = 1 - (1 - K/K_c)^\theta, \quad (38)$$

aimed at reducing the influence of the leading corrections to scaling. Here θ is the exponent that characterizes these corrections. A sample of estimates of the parameters of the critical singularity is obtained from the computation of many high-order “quasidiagonal” DAs, namely, approximants with small differences among the degrees of the polynomial coefficients of the defining differential equation, which use all or most of the given series coefficients. A first estimate of a parameter, along with its uncertainty, results from computing

the sample average and standard deviation. The result can then be improved by discarding from the sample single estimates that appear to be obvious outliers, and recomputing the average of the reduced sample. A conventional guess of the uncertainty of the parameter estimate is finally obtained simply, and rather roughly, as a small multiple of the spread of the reduced sample around its mean value. This subjective prescription might, to some extent, allow for the difficulty to infer possible systematic errors, and to extrapolate reliably a possible residual dependence of the estimate on the maximum order of the available series.

A second approach is based on a faster converging modification of the standard analysis of ratio sequence of the series coefficients and will be denoted here as the *modified ratio approximant* (MRA)^{28,59} technique. Let us assume that the singularity of a physical quantity, which is nearest to the origin of the complex K plane, is the critical singularity, located at K_c , and characterized by the critical exponent λ and the exponent θ of the leading correction to scaling (this hypothesis is generally not satisfied for the LT series). Then Eq. (9) implies the following large r behavior of the series-expansion coefficients c_r :

$$c_r = C \frac{r^{\lambda-1}}{\Gamma(\lambda)} K_c^{-r} \left[1 + \frac{\Gamma(\lambda)}{\Gamma(\lambda-\theta)} \frac{b}{r^\theta} + O(1/r) \right]. \quad (39)$$

In this case, the MRA method evaluates K_c by estimating the large r limit of the approximant sequence

$$(K_c)_r = \left(\frac{c_{r-2}c_{r-3}}{c_r c_{r-1}} \right)^{1/4} \exp \left[\frac{s_r + s_{r-2}}{2s_r(s_r - s_{r-2})} \right] \quad (40)$$

with

$$s_r = \left[\ln \left(\frac{c_{r-2}^2}{c_r c_{r-4}} \right)^{-1} + \ln \left(\frac{c_{r-3}^2}{c_{r-1} c_{r-5}} \right)^{-1} \right] / 2. \quad (41)$$

By using the asymptotic form Eq. (39), we can obtain¹⁶ the large r asymptotic behavior of the sequence of MRA approximants of the critical inverse temperature,

$$(K_c)_r = K_c \left[1 - \frac{\Gamma(\lambda)}{2\Gamma(\lambda-\theta)} \frac{\theta^2(1-\theta)b}{r^{1+\theta}} + O(1/r^2) \right]. \quad (42)$$

The method estimates also the critical exponent λ from the sequence

$$(\lambda)_r = 1 + 2 \frac{(s_r + s_{r-2})}{(s_r - s_{r-2})^2}, \quad (43)$$

with s_r defined by Eq. (41). In this case, the large r asymptotic behavior of the sequence $(\lambda)_r$ is

$$(\lambda)_r = \lambda - \frac{\Gamma(\lambda)}{\Gamma(\lambda-\theta)} \frac{\theta(1-\theta^2)b}{r^\theta} + O(1/r). \quad (44)$$

If the available series expansions are sufficiently long (how long cannot unfortunately be decided *a priori*), the estimates of the critical points and exponents obtained from extrapolations based on Eqs. (42) and (44) can be competitive in precision with those from DAs. If, on the other hand, the series are only moderately long or the exponent $\lambda \gg 1$, then corrections of order higher than $1/r^{1+\theta}$ in Eq. (42) [or higher than $1/r^\theta$ in Eq. (44)] might still be non-negligible. The same remark applies if the $O(1/r)$ terms in Eq. (39) are not sufficiently

small. Therefore, in some cases, Eqs. (42) and (44) might be inadequate to extrapolate the behavior of the few highest-order terms of the MRA sequences.

B. Critical parameters of the higher susceptibilities

For both methods sketched above, the main difficulties of the numerical analysis of the HT expansions are related to the presence of the leading nonanalytic corrections to scaling that appear in the near-critical asymptotic forms of all physical quantities. It was, however, observed^{28,29} that the amplitudes of these corrections are nonuniversal and therefore, by studying families of models expected to belong to the same universality class, one might be able to single out special models for which these amplitudes have a very small or vanishing size. These models would then be good candidates for a high-accuracy determination of the critical parameters of interest. In the literature, various models that share this property to a good approximation have been subjected to analysis: among them, the lattice ϕ^4 model on the sc lattice with the value $g = 1.1$ of the quartic self-coupling,^{14,61} or the same model on the bcc lattice with the self-coupling¹⁵ $g = 1.85$. Also the spin- $s = 1$ and

$s = 3/2$ Ising systems on the bcc lattice¹⁶ show very small corrections to scaling. All these models will be considered here.

An accurate estimate $2\Delta = 3.1276(8)$ of the gap exponent that improves the four-decade-old⁴ estimate $2\Delta = 3.126(6)$, based on 12th-order series, had been already obtained from the known 23rd-order HT expansions of $\chi_4(K)$ for the spin- s Ising models¹⁶ and for the lattice scalar field,¹⁵ on the sc and bcc lattices. The addition of a single coefficient to the expansion of $\chi_4(K)$ does not urge resuming a full discussion of the estimates of this exponent and of the validity of hyperscaling on the HT side of the critical point, already tested with good precision in Refs. 15, 16, and 62.

To get some feeling of the reliability of the estimates that can be obtained from a study of our HT expansions of the higher susceptibilities $\chi_{2n}(K)$, it is convenient to test how accurately the critical inverse temperature K_c and the critical exponents γ_{2n} can be determined from them by using MRAs. Let us, for example, consider the above-mentioned self-interacting lattice scalar-field model of Eq. (2) on the sc lattice with quartic self-coupling $g = 1.1$. In Fig. 2, we have plotted versus $r^{1+\theta}$ the sequences of the MRA estimates $(K_c)_r$ for K_c , as obtained from the HT expansions of $\chi_{2n}(K)$ with $2n = 2, 4, \dots, 22$. The MRA sequences are normalized by the appropriate limiting value of the sequence $(K_c)_r$, estimated in Ref. 16 and reported in Table VI, to make

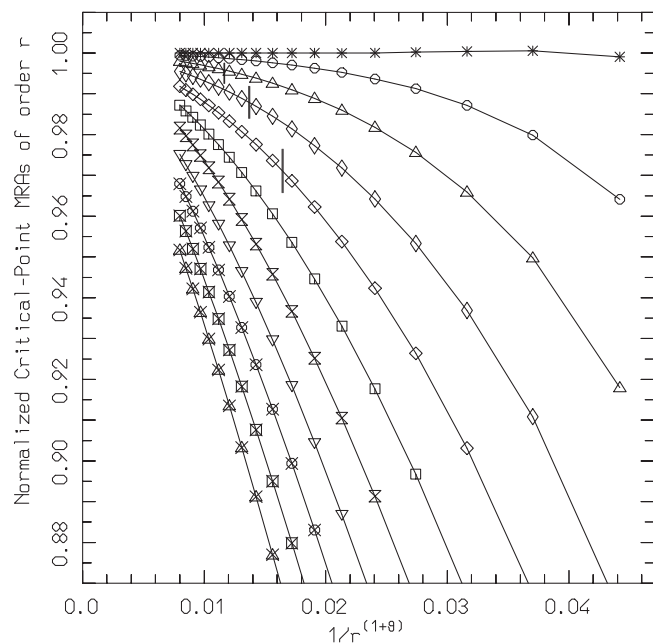


FIG. 2. The sequences of MRAs of the critical point for the scalar-field model with self-coupling $g = 1.1$ on the sc lattice, plotted vs $1/r^{1+\theta}$. Here r is the order of the approximant and θ is the exponent of the leading correction to scaling. We have normalized the MRAs to the estimated value of K_c . The MRAs are obtained from the HT expansions of $\chi_2(K)$ (stars), $\chi_4(K)$ (circles), $\chi_6(K)$ (triangles), $\chi_8(K)$ (rhombs), $\chi_{10}(K)$ (rotated squares), $\chi_{12}(K)$ (squares), $\chi_{14}(K)$ (double triangles), $\chi_{16}(K)$ (rotated triangles), $\chi_{18}(K)$ (crossed circles), $\chi_{20}(K)$ (crossed squares), and $\chi_{22}(K)$ (crossed triangles). The symbols representing the MRAs are connected by straight lines as an aid to the eye. Small vertical segments on the third, fourth, and fifth curve from above indicate the order at which our extension of the $\chi_6(K)$, $\chi_8(K)$, and $\chi_{10}(K)$ series begins to contribute to the MRAs. The six lowest curves refer to higher susceptibilities for which no data exist in the literature.

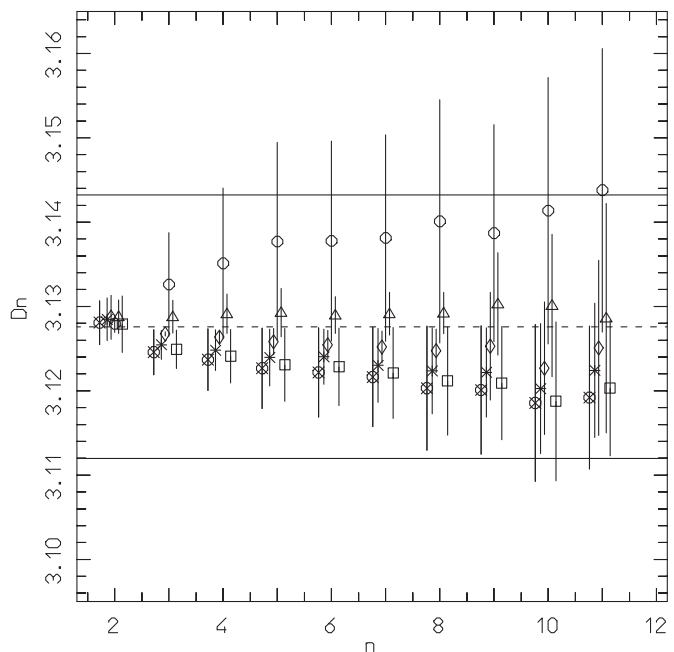


FIG. 3. As a simple consequence of the scaling hypothesis, the exponent differences $D_n = \gamma_{2n} - \gamma_{2n-2}$ should not depend on n and equal 2Δ . Here they are obtained by forming second-order DAs of the ratios $\chi_{2n}(K)/\chi_{2n-2}(K)$ for $n = 2, 3, 4, \dots, 11$, obtained from the expansions of the bcc lattice Ising model with spin $s = 1/2$ (circles), $s = 1$ (triangles), $s = 3/2$ (rhombs), $s = 2$ (stars), $s = 5/2$ (squares), and $s = 3$ (crossed circles). For each value of n , the symbols referring to the various values of the spin s have been slightly shifted apart to avoid cluttering and keep the uncertainty of each estimate visible. The dashed horizontal line represents the estimated (Ref. 16) value $2\Delta = 3.1276(8)$ of twice the gap exponent. The continuous horizontal lines indicate a relative deviation of 0.5% from the expected central value.

TABLE VI. Estimates (Refs. 15 and 16) of the critical inverse-temperatures K_c used in our study of the Ising systems with spin s and of the lattice scalar-field systems, on the sc and the bcc lattices.

	$s = 1/2$	$s = 1$	$s = 3/2$	$s = 2$	$s = 5/2$	$s = 3$	ϕ^4
K_c^{sc}	0.221 655(2)	0.312 867(2)	0.368 657(2)	0.406 352(3)	0.433 532(3)	0.454 060(3)	0.375 097(1)
K_c^{bcc}	0.157 3725(10)	0.224 656(1)	0.265 641(1)	0.293 255(2)	0.313 130(2)	0.328 119(2)	0.244 1357(5)

them easily comparable with the corresponding sequences obtained from other models in the same universality class. The choice of the plotting variable is suggested by Eq. (42). For the susceptibilities of order $2n \gtrsim 6$, the curves indicate the presence of strong corrections $O(r^{-\sigma})$, with σ between 3 and 5, and show that simply using Eq. (42), at the present orders of expansion, would be inadequate for extrapolating to $r \rightarrow \infty$ the MRA sequences. No significant quantitative difference in behavior is observed in the analogous plots for the other models examined in this study, even for those with non-negligible amplitudes of the leading corrections to scaling. On the contrary, in other cases, for example, for the Ising model with spin- $s = 1/2$ or $s = 1$ on the bcc lattice, the convergence looks even slightly faster. From these plots one may conclude that, as the order $2n$ of the susceptibility $\chi_{2n}(K)$ grows, increasingly long expansions are needed⁴⁹ in order that the MRA sequences reach the asymptotic form Eq. (42) and therefore a given precision can be achieved in the estimate of

K_c . The general features of this behavior can be tentatively explained, arguing⁴⁹ that the dominant contributions to the HT expansion of $\chi_{2n}(K)$, at a given, sufficiently large, order K^r , come from those spin correlation functions in the sum of Eq. (8), for which the average distance among the spins is $\approx r/2n$. Accordingly, it seems that the presently available expansions of the quantities $\chi_{2n}(K)$, in spite of having the same number of coefficients, might not have the same “effective length,” because they describe systems that are, in some sense, rather “small,” the more so the larger is $2n$. One might conclude that the estimates of the critical quantities, derived from the $\chi_{2n}(K)$, should probably be taken with some caution for large n , even in the case of models with very small leading corrections to scaling. However, in what follows, we shall observe that, in some cases, in spite of these difficulties, the DAs seem to yield smooth and reasonable extrapolations of these series to the critical point.

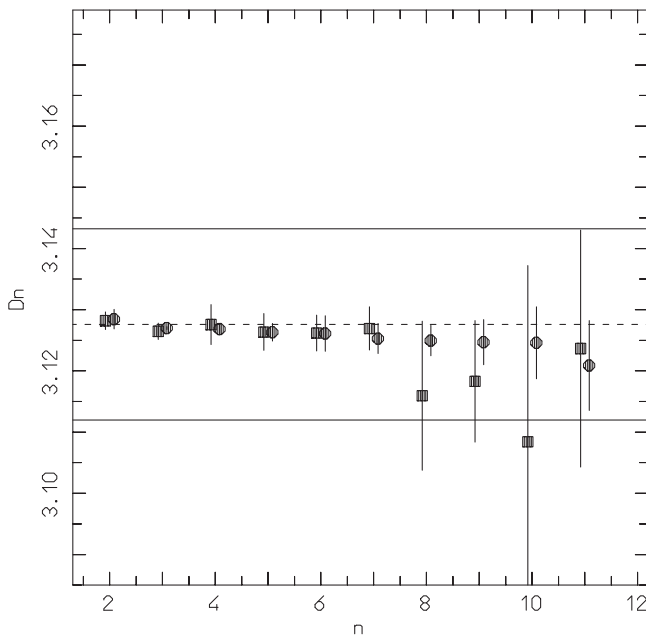


FIG. 4. Same as Fig. 3. In this case, the differences $D_n = \gamma_{2n} - \gamma_{2n-2}$ have been computed from the HT expansions of the higher susceptibilities for the lattice scalar-field theory with values of the quartic self-coupling, $g = 1.1$ on the sc lattice (black squares) and $g = 1.85$ on the bcc lattice (black circles). These values of g are chosen to minimize the leading corrections to scaling. As in Fig. 3, for each value of n , the symbols referring to the sc and the bcc estimates have been slightly shifted apart. The dashed horizontal line represents the estimated (Ref. 16) value $2\Delta = 3.1276(8)$ of twice the gap exponent. The continuous horizontal lines indicate a relative deviation of 0.5% from the central value.

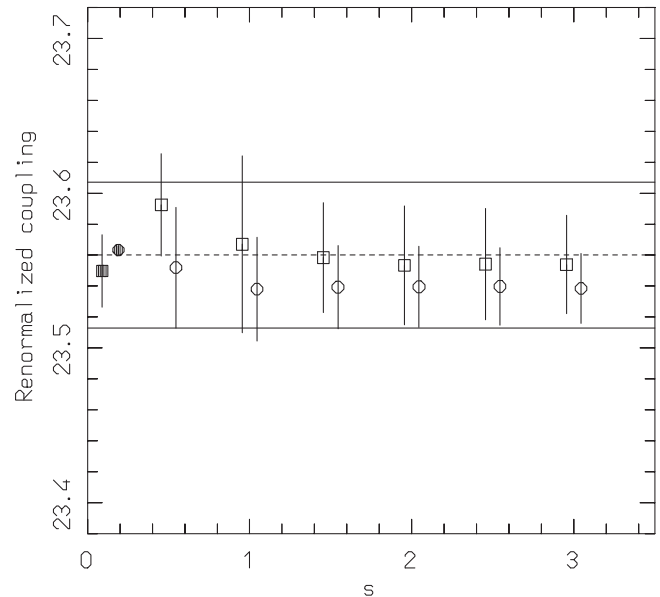


FIG. 5. The renormalized coupling constant g_4^+ for the Ising model with spin s on the bcc lattice (circles) and on the sc lattice (squares) vs the value s of the spin. The HT expansions of the Ising systems have been subjected to the variable transformation Eq. (38). For comparison, we have also computed g_4^+ for the scalar model with the value $g = 1.1$ of the quartic self-coupling on the sc lattice (black square) and with $g = 1.85$ on the bcc lattice (black circle). The latter estimates are plotted with conventional abscissas near zero. In all cases, the symbols of the sc and bcc estimates for each value of s , have been slightly shifted apart to avoid superpositions and to keep the uncertainty of each estimate visible. The dashed horizontal line represents the value $g_4^+ = 23.56(3)$ estimated in Ref. 15. The continuous horizontal lines indicate a relative deviation of 0.2% from the central value.

C. Scaling and the gap exponent

For Ising models on the bcc lattice with spin $s = 1/2, 1, \dots, 3$, we have computed the sequences of estimates of the exponent differences $D_n = \gamma_{2n} - \gamma_{2n-2}$, with $n = 2, 3, \dots, 11$. These estimates are obtained from second-order DAs of the ratios $\chi_{2n}(K)/\chi_{2n-2}(K)$, which use at least 19 series coefficients. We have imposed that the critical inverse temperatures, for the various spin systems, take the appropriate values,¹⁶ listed in Table VI. In Fig. 3, the exponent differences D_n are plotted versus n . We have observed above that, as a simple consequence of the scaling hypothesis, when the maximum order of the available HT series grows large, the D_n should all converge to the same value, equal to twice the gap exponent Δ , thus being independent of the order $2n$ of the higher susceptibilities entering into the calculation. For some particular values of the spin, e.g., $s = 1$ and $s = 3/2$, our central estimates depart by less than 0.1% from the expected result, for all values of n considered here. For other values of the spin, e.g., $s = 1/2$, a residual spread of the data remains, which, however, is quite compatible with the errors owing to the finite length of the series and to the likely presence of sizable corrections to scaling, particularly when n is large. This computation can be repeated, with similar results, but somewhat larger error bars, for the spin- s Ising system on the sc lattice. We have shown in Fig. 4 the results of the same computation for the two scalar-field systems with suppressed leading corrections to scaling studied here. In view of the above remarks concerning the effective length of the expansions of the $\chi_{2n}(K)$, our results confirm the expectation that, in general, the uncertainties of the results should grow with n . It should be noted that, both in the case of the spin- s Ising system and of the

scalar-field system, the bcc lattice expansions have a distinctly smoother and more convergent behavior than for the sc lattice, on a wider range of values of the order $2n$ of the susceptibilities, probably because the coordination number of the bcc lattice is larger. In conclusion, our results support the validity of the scaling property, while the rather accurate independence of the estimates of the gap exponent on the lattice structure and, in the case of the Ising models, on the value s of the spin, is a valuable indication of universality. Finally, it is worth to stress that the results of Figs. 3 and 4 for $n \gtrsim 4$ would be difficult to obtain by numerical approaches other than series expansions.

D. The ratios r_{2n}^+ and the critical amplitudes of the higher susceptibilities

In Ref. 4 the critical amplitudes C_{2n}^+ of the higher susceptibilities were estimated from 12th-order series, for the simple $s = 1/2$ Ising model, assuming the now outdated values $\gamma = 5/4$ and $\Delta = 25/16$ for the exponents. These series were not long enough that any estimate of the uncertainties could be tried. It is then worthwhile to update the estimates of these amplitudes by using our twice as long expansions and biasing the extrapolations by the more precise modern estimates of the exponents and the critical temperatures cited above. We can, moreover, obtain the corresponding information also for the other models under scrutiny. The critical amplitudes C_{2n}^+ with $n > 2$ can also be evaluated, with results consistent within their errors, in terms of C_2^+ , C_4^+ and of the universal critical values I_{2n+4}^+ of the quantities defined by Eq. (36). In this approach only the estimates of C_2^+ and C_4^+ need to be biased with both the critical temperatures and the exponents, while, of course,

TABLE VII. Our final estimates, by first-order DAs, of the critical amplitudes, f_ξ^+ of the second-moment correlation length, Eq. (34), and C_{2n}^+ of the susceptibilities $\chi_{2n}(K)$, Eq. (9), on the HT side of the critical point, for Ising models with various values s of the spin on the sc and the bcc lattices and for the lattice scalar field with ϕ^4 self-interaction. The quartic self-coupling has the value $g = 1.1$ for the sc lattice, while $g = 1.85$ for the bcc lattice. For convenience, following Ref. 4, we have reported the value of $C_{2n}^+/(2n)!$.

	$s = 1/2$	$s = 1$	$s = 3/2$	$s = 2$	$s = 5/2$	$s = 3$	ϕ^4
bcc							
f_ξ^+	0.4681(3)	0.4249(1)	0.4107(2)	0.4043(1)	0.4010(1)	0.3989(2)	0.4146(1)
$C_2^+/2!$	0.5202(9)	0.3105(6)	0.2481(5)	0.2186(5)	0.2019(5)	0.1910(4)	0.2741(7)
$C_4^+/4!$	-0.1416(9)	-0.0377(1)	-0.02175(7)	-0.0161(1)	-0.0134(1)	-0.01180(8)	-0.02728(8)
$C_6^+/6!$	0.1224(9)	0.014 55(8)	0.006 05(4)	0.003 77(6)	0.002 82(4)	0.002 31(3)	0.008 62(8)
$C_8^+/8!$	-0.150(3)	-0.007 98(9)	-0.002 40(2)	-0.001 25(3)	-0.000 845(9)	-0.000 646(7)	-0.003 87(3)
$C_{10}^+/10!$	0.22(1)	0.0052(1)	0.00113(1)	0.000497(9)	0.000301(5)	0.000215(3)	0.00207(4)
$C_{12}^+/12!$	-0.35(5)	-0.0037(1)	-0.00059(2)	-0.00022(2)	-0.000119(5)	-0.000079(3)	-0.00123(4)
$C_{14}^+/14!$	0.57(9)	0.0029(2)	0.00032(3)	0.000101(8)	0.000050(3)	0.000031(2)	0.00077(5)
sc							
f_ξ^+	0.5070(5)	0.4588(4)	0.4429(4)	0.4356(4)	0.4317(5)	0.4294(5)	0.4151(1)
$C_2^+/2!$	0.5608(9)	0.338(2)	0.270(2)	0.239(1)	0.220(1)	0.208(1)	0.2384(7)
$C_4^+/4!$	-0.1608(5)	-0.0432(2)	-0.0249(2)	-0.01847(9)	-0.0153(1)	-0.0135(1)	-0.01595(3)
$C_6^+/6!$	0.146(3)	0.0175(2)	0.007 29(4)	0.004 54(3)	0.003 39(1)	0.002 77(2)	0.003 39(1)
$C_8^+/8!$	-0.187(9)	-0.0101(2)	-0.003 02(5)	-0.001 58(3)	-0.001 06(2)	-0.000 809(9)	-0.001 02(1)
$C_{10}^+/10!$	0.26(6)	0.0069(3)	0.001 48(6)	0.000 655(9)	0.000 393(9)	0.000 279(9)	0.000 367(6)
$C_{12}^+/12!$	-0.19(9)	-0.0049(9)	-0.000 79(9)	-0.000 30(3)	-0.000 162(8)	-0.000 107(6)	-0.000 146(5)
$C_{14}^+/14!$	0.026(9)	0.0016(9)	0.000 34(9)	0.000 13(4)	0.000 066(9)	0.000 041(8)	0.000 061(4)

TABLE VIII. Estimates of the amplitudes C_{2n}^+ Eq. (9), tabulated in Ref. 4 without indication of error and only in the case of the Ising model with $s = 1/2$.

	$C_2^+/2!$	$C_4^+/4!$	$C_6^+/6!$	$C_8^+/8!$	$C_{10}^+/10!$	$C_{12}^+/12!$
sc lattice	0.5299	-0.1530	0.1366	-0.1722	0.2601	-0.4526
bcc lattice	0.4952(5)	-0.1385	0.1169	-0.1397	0.2023	-0.3297

the estimates of I_{2n+4}^+ have to be biased only with the critical temperatures. Our final estimates for the amplitudes C_{2n}^+ are collected in the Table VII. The results of Ref. 4 are reproduced for comparison in Table VIII.

We have estimated the critical values of the HT expansions of the RCCs either directly, by extrapolation^{49,62} to K_c^- of the simple auxiliary function

$$w_{2n}(K) = (K/K_c)^{\frac{3n-3}{2}} g_{2n}^+(K), \quad (45)$$

designed to be regular at $K = 0$, and therefore more convenient to study by DAs, or, more conveniently, but with consistent results, from the computation of the quantities r_{2n}^+ using Eq. (37). In Fig. 5, our estimates for g_4^+ are plotted versus the value s of the spin for Ising systems on the sc and the bcc lattices and compared to our previous estimate $g_4^+ = 23.56(3)$ (dashed line) in Ref. 15. In the same figure, we have also shown the values of g_4^+ for the scalar-field model on both lattices.

Table IX lists our estimates of the quantities I_{2n+4}^+ and r_{2n}^+ , obtained from first- and second-order DAs, for a few

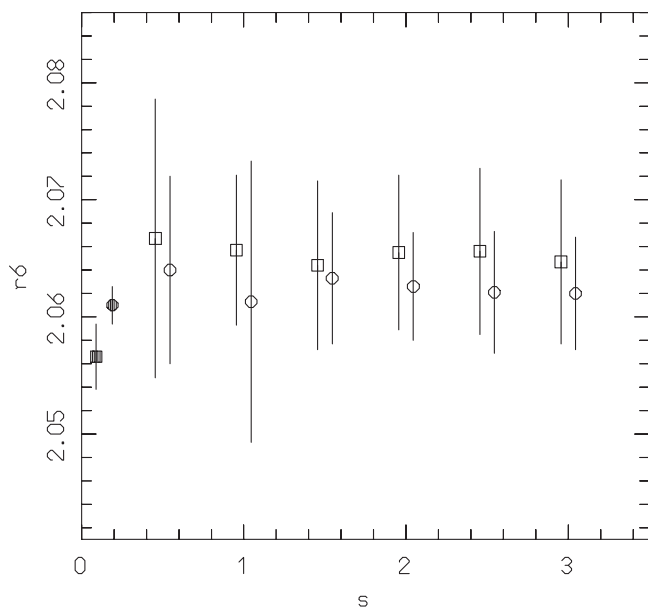


FIG. 6. The ratio r_6^+ for the Ising model with spin s on the bcc lattice (circles), for the Ising model with spin s on the sc lattice (squares) vs the spin. The expansions for the Ising systems have been subjected to the variable transformation Eq. (38). The symbols of the sc and the bcc estimates, for each value s of the spin, have been slightly shifted apart to avoid superpositions and to keep the uncertainties of each estimate visible. For comparison, we have also computed r_6^+ for the scalar model with $g = 1.1$ on the sc lattice (black square) and with $g = 1.85$ on the bcc lattice (black circle). The latter estimates are plotted with conventional abscissas near zero.

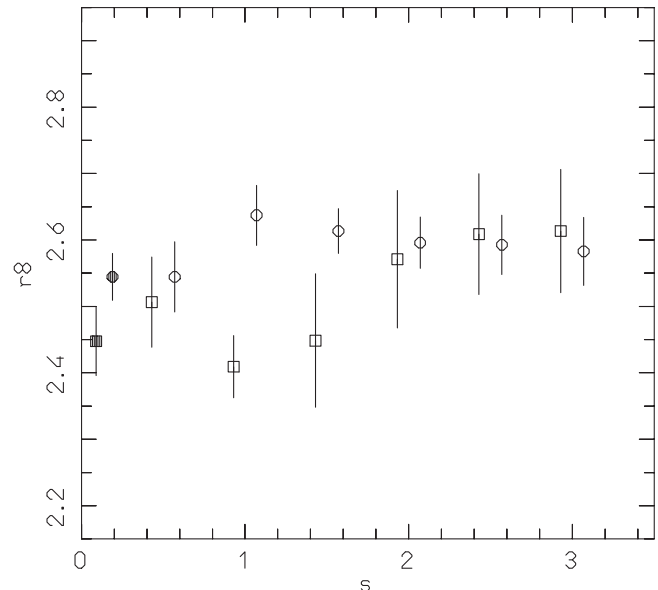


FIG. 7. Same as Fig. 6, but for r_8^+ .

spin- s Ising systems and for the lattice scalar field, on the sc and the bcc lattices. We have imposed that the critical inverse temperatures take the appropriate values reported in Table VI and that an antiferromagnetic singularity is present at $-K_c$. Only for the spin- s Ising models, we have taken advantage of the variable transformation Eq. (38) to reduce the uncertainties of the estimates and the spread among the central values for different spins. We have always taken care that the uncertainties of our results allow for the errors of the critical temperatures listed in Table VI and, whenever the variable transformation Eq. (38) is performed, also for the error of the exponent θ .

In Figs. 6–10 we have plotted versus the spin, our estimates of the quantities r_6^+ , r_8^+ , r_{10}^+ , r_{12}^+ , and r_{14}^+ for the Ising models of spin $s = 1/2, \dots, 3$ on the sc and the bcc lattices. In

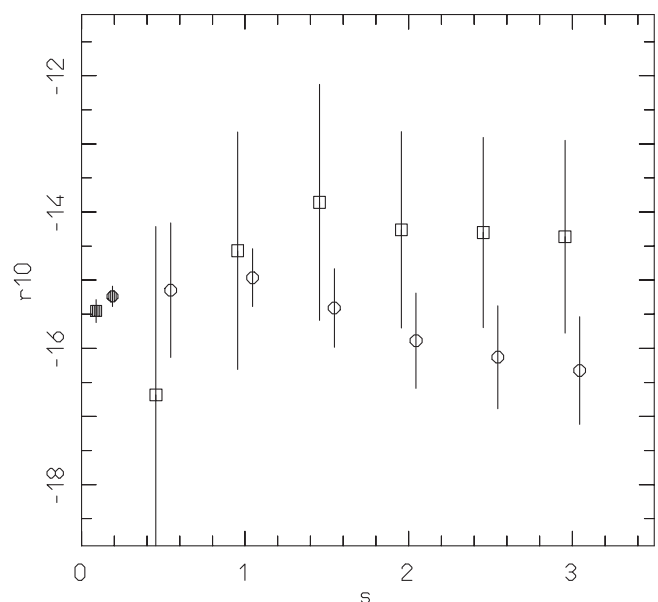


FIG. 8. Same as Fig. 6, but for r_{10}^+ .

TABLE IX. Our final estimates of the universal critical values r_{2n}^+ of the quantities $r_{2n}(K)$, with $3 \leq n \leq 7$, for Ising models with various values s of the spin and for the scalar field with ϕ^4 self-interaction, on the sc and the bcc lattices. The quartic self-coupling has the value $g = 1.1$ for the sc lattice, while $g = 1.85$ for the bcc lattice. We have also reported the values of the universal amplitude ratios $I_{2n+4}^+/(2n+2)!$, with $1 \leq n \leq 5$.

bcc lattice	$s = 1/2$	$s = 1$	$s = 3/2$	$s = 2$	$s = 5/2$	$s = 3$	ϕ^4
g_4^+	23.56(4)	23.54(3)	23.54(3)	23.54(3)	23.54(2)	23.54(2)	23.56(1)
r_6^+	2.064(8)	2.061(9)	2.063(5)	2.062(5)	2.062(5)	2.062(5)	2.061(2)
r_8^+	2.54(5)	2.64(5)	2.61(4)	2.60(4)	2.59(4)	2.58(5)	2.54(4)
r_{10}^+	-15.1(9)	-15.0(5)	-15.4(6)	-15.9(7)	-16.1(8)	-16.3(8)	-15.2(2)
r_{12}^+	45(7)	40(5)	44(5)	48(6)	51(7)	53(8)	44(3)
r_{14}^+	1504(240)	1490(115)	1359(82)	1366(100)	1319(100)	1300(100)	1615(120)
$I_6^+/4!$	0.3307(3)	0.3308(5)	0.3307(2)	0.3307(2)	0.3307(2)	0.3308(2)	0.3308(1)
$I_8^+/6!$	0.2319(6)	0.2319(5)	0.2320(4)	0.2320(4)	0.2320(4)	0.2320(4)	0.2321(2)
$I_{10}^+/8!$	0.1667(2)	0.1668(3)	0.1666(2)	0.1664(3)	0.1666(4)	0.1669(5)	0.1667(2)
$I_{12}^+/10!$	0.1216(3)	0.1215(1)	0.1216(2)	0.1214(2)	0.1214(3)	0.1215(2)	0.1213(3)
$I_{14}^+/12!$	0.0894(2)	0.0892(2)	0.0894(3)	0.0894(3)	0.0893(3)	0.0893(3)	0.0897(6)
sc lattice							
g_4^+	23.59(4)	23.57(6)	23.56(2)	23.55(4)	23.55(4)	23.55(3)	23.55(3)
r_6^+	2.067(11)	2.066(8)	2.064(7)	2.065(7)	2.066(7)	2.065(7)	2.057(3)
r_8^+	2.51(7)	2.41(5)	2.45(10)	2.57(10)	2.61(9)	2.61(9)	2.45(5)
r_{10}^+	-17(2)	-14(2)	-14(2)	-14(1)	-14(1)	-14(1)	-15.4(2)
r_{12}^+	45(8)	44(8)	44(6)	52(4)	54(5)	51(6)	62(3)
r_{14}^+	1460(240)	1390(130)	1644(115)	1477(120)	1362(150)	1310(150)	1176(140)
$I_6^+/4!$	0.3306(5)	0.3306(3)	0.3307(3)	0.3306(3)	0.3306(3)	0.3306(3)	0.3310(1)
$I_8^+/6!$	0.2320(12)	0.2316(7)	0.2316(8)	0.2317(8)	0.2318(8)	0.2318(7)	0.2324(3)
$I_{10}^+/8!$	0.1678(8)	0.1670(10)	0.1665(4)	0.1665(3)	0.1665(3)	0.1665(3)	0.1665(5)
$I_{12}^+/10!$	0.1211(6)	0.1214(5)	0.1213(5)	0.1210(5)	0.1209(6)	0.1208(4)	0.1206(9)
$I_{14}^+/12!$	0.0908(12)	0.0906(12)	0.0894(10)	0.0892(10)	0.0889(12)	0.0893(8)	0.0884(7)

these figures we have reported, in correspondence with the conventional value $s = 0$ of the abscissa, also our results for the scalar model in the case of the sc lattice with quartic self-coupling $g = 1.1$ and, in the case of the bcc lattice, with self-coupling $g = 1.85$. The set of estimates shows good

universality properties and moderate relative uncertainties that slowly grow with $2n$. In the worst case, that of r_{14}^+ , the uncertainties are generally not larger than 15%.

In the first line of Table X, we have listed our final estimates of the ratios $r_6^+, r_8^+, \dots, r_{14}^+$, obtained either by simply choosing our result for the scalar-field system on the

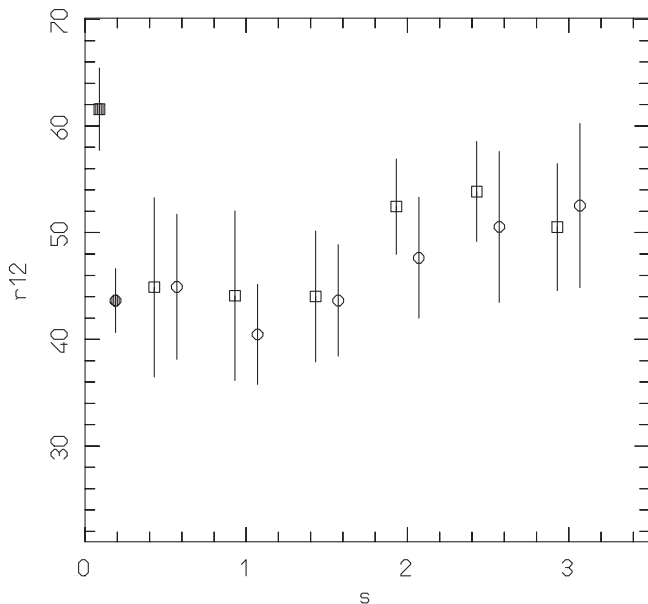


FIG. 9. Same as Fig. 6, but for r_{12}^+ .

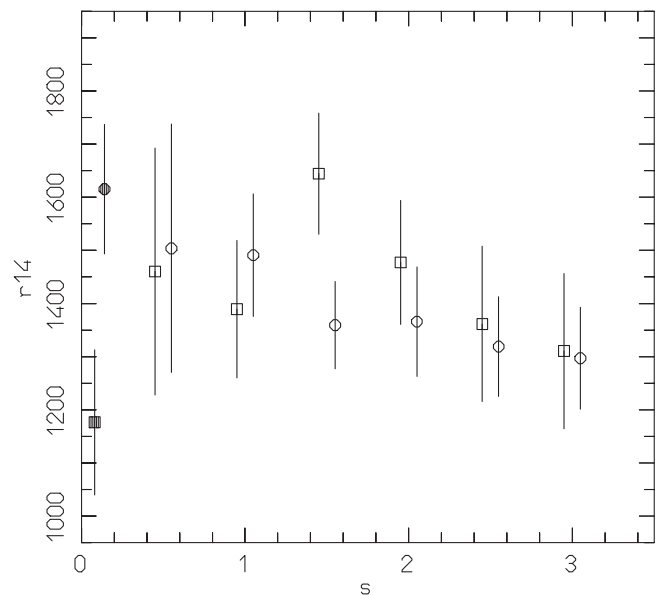


FIG. 10. Same as Fig. 6, but for r_{14}^+ .

TABLE X. Our final estimates of the quantities g_4^+ , r_6^+ , r_8^+ , r_{10}^+ , r_{12}^+ , and r_{14}^+ , obtained either from the ϕ^4 results on the bcc lattice or from a weighted average of the results on both the sc and the bcc lattices, are compared to estimates in the recent literature. These have been obtained: (i) from HT expansions (Ref. 14), shorter than those analyzed here, of the sc lattice scalar field with ϕ^4 or ϕ^6 self-interactions and appropriate self-couplings; (ii) from the expansion (Ref. 20) in powers of $\epsilon = d - 4$, within the RG approach; (iii) from the g expansion (Refs. 20 and 22) in fixed dimension $d = 3$, within the RG approach; (iv) from various approximations (Refs. 23–25) of the RG equations; v) from Monte Carlo simulations (Refs. 50 and 51).

	g_4^+	r_6^+	r_8^+	r_{10}^+	r_{12}^+	r_{14}^+
This work	23.56(1)	2.061(2)	2.54(4)	-15.2(4)	45(5)	1400(200)
HT scalar sc (Ref. 14)	23.56(2)	2.056(5)	2.3(1)	-13(4)		
ϵ exp. (Ref. 20)	23.3	2.12(12)	2.42(30)	-12(1)		
g exp. (Ref. 20)	23.64(7)	2.053(8)	2.47(25)	-25(18)		
g exp. (Ref. 22)	23.77	2.044	5.04			
Approx. RG (Ref. 23)		1.938	2.505	-12.599	10.902	
Approx. RG (Ref. 24)	20.72(1)	2.063(5)	2.47(5)	-19(1)		
Approx. RG (Ref. 25)	28.9	1.92	2.17			
MC Ising sc (Ref. 50)	23.3(5)	2.72(31)				
MC Ising sc (Ref. 51)	24.5(2)	3.24(24)				

bcc lattice, as in the case of the lowest-order ratios, or from a weighted average of the estimates on the sc and bcc lattices for the same system, as in the case of the largest-order ratios. Our values are compared with the estimates already obtained in the recent literature by various methods, including the analysis of significantly shorter HT expansions.

V. CONCLUSIONS

For a wide class of models in the 3D Ising universality class, we have described properties of the higher susceptibilities on the HT side of the critical point, which are relevant for the construction of approximate representations of the critical ES. We have based on high-temperature and low-field bivariate expansions that we have significantly extended or computed “ex novo.” The models under scrutiny include the conventional Ising system with spin $s = 1/2$, the Ising model with spin $s > 1/2$ and the lattice scalar field, defined on the 3D sc and bcc lattices. In this paper our HT data have been used to improve the accuracy and confirm the overall consistency of the current description of these models in critical conditions, by testing simple predictions of the scaling hypothesis as well as the validity of the universality property of the gap exponent and of appropriate combinations of critical amplitudes. Some of

these tests are presently feasible only within a series approach. Our main result is a set of more accurate estimates of the first three already known r_{2n}^+ parameters and a computation of two additional ratios, which enable us to formulate an update of the parametric form of the ES.

At the order of expansion reached in our study, we still observe a small residual spread of the estimates of the gap exponent and of the ratios r_{2n}^+ , around the predictions of asymptotic scaling and universality. This fact is readily explained by the obvious limitations of our numerical analysis: namely, the still relatively moderate span of our expansions, in spite of their significant extension, the notoriously slower convergence of the expansions in the case of the sc lattice, and the incomplete allowance of the nonanalytic corrections to scaling by the current tools of series analysis.

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