# Updated tests of scaling and universality for spin-spin correlations in the two- and threedimensional spin-S Ising models using high-temperature expansions

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We have extended, from order 12 through order 25, the high-temperature series expansions (in zero magnetic field) for the spin-spin correlations of the spin-*S* Ising models on the square, simple-cubic and body-centered-cubic lattices. On the basis of this large set of data, we confirm accurately the validity of the scaling and universality hypotheses by resuming several tests which involve the correlation function, its moments and the exponential or the second-moment correlation lengths.

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## I. INTRODUCTION AND CONCLUSIONS

Moderate-length high-temperature (HT) expansions (through order 12) and low-temperature (LT) expansions for the spin-spin correlation function (sscf)  $G(\vec{r},T;S)$  of the nearest-neighbor Ising models with general spin S were first computed<sup>1-3</sup> three decades ago on various lattices in twodimensions (2D) and in 3D. Motivations for the study of these models came not only from their direct phenomenological interest, but mainly from the conjecture<sup>4</sup> that, in a given space dimension, the exponents characterizing the critical behavior are independent both of the lattice structure and of the spin magnitude S. This conjecture was the first step towards the modern notion of universality class. In the same years also the hypothesis of critical scaling<sup>5</sup> was put forward. Many studies<sup>1-3,6-13</sup> of the mentioned HT and LT series were devoted to test the validity and the main consequences of these basic hypotheses.<sup>4–6,13–19</sup> Although the results sometimes were not as precise as was hoped, or covered only the S = 1/2 case, the scaling tests suggested that the critical sscf is a homogeneous function of appropriate variables, while the universality tests indicated that the critical indices and suitable combinations<sup>20</sup> of critical amplitudes are independent of the spin S and lattice structure. A few years later, the first substantial extension<sup>21,22</sup> of HT Ising series in 3D [through order 21 on the body-centered-cubic (bcc) lattice only] did not make higher expansion coefficients available for the sscf, but only for its two lowest even moments and therefore various tests could not be repeated and updated.

We are now resuming the HT part of those pioneering analyses in order to improve their extent and accuracy by taking advantage of our recent extension<sup>23–25</sup> from order 12 through order 25 of the HT expansions for the sscf of the Ising model with general spin *S*, in 2D on the square (sq) lattice and in 3D on the simple-cubic (sc) and the bcc lattices. From these data we have also derived series for related quantities, in particular for a variety of moments of the sscf, which are computed through order 25, and for the exponential (or "true") correlation length defined via the exponential decay of the sscf, which, however, can be extended only through order 19. For reasons of space we have not tabulated in this paper the series analyzed, but have included them into our on-line library<sup>24</sup> of HT data for the spin-S Ising model in order to make them more widely available for further study. Since this is the largest body of series data so far computed for these systems, we have already been studying other aspects of them in previous papers. In particular, in Ref. 23 we have accurately confirmed that the residual weak spin dependence observed<sup>26</sup> in lower-order studies of the susceptibility exponent  $\gamma$  and of the correlation-length exponent  $\nu$  in 3D on the bcc lattice, should not be ascribed to small violations of universality, but can be simply explained away as numerical inaccuracies due to expected non-negligible spindependent corrections to the leading scale behavior. Moreover we have tested the universality of several amplitude combinations obtaining similar results. In Ref. 25 an analogous survey of universal quantities was performed in 2D for the sq-lattice case. Shorter series (but only for the S = 1/2case) had been analyzed in Ref. 27.

From the evidence presented here we can conclude that our HT data for the sscf have by now reached an extension sufficient to make the use of modern series-extrapolation techniques possible and generally reliable. Therefore we are able to exhibit more convincingly both in 2D and in 3D many expected properties related to scaling and universality also in some cases in which the old analyses led to inconclusive or not very precise results.

The rest of the paper is organized as follows. In Sec. II we shall outline the main features of the model, introduce our notations and conventions, and very briefly recall the scaling and universality properties expected for the sscf along with the corresponding tests discussed in full detail by the above cited papers.<sup>6-12</sup> Therefore, in Sec. III we can restrict ourselves to only a few comments on the numerical results.

#### II. THE SPIN-S ISING MODELS

The spin-S Ising models with nearest-neighbor interaction are defined by the Hamiltonian

$$H\{s\} = -\frac{J}{2} \sum_{(\vec{r},\vec{r}')} s(\vec{r}) s(\vec{r}') - h \sum_{\vec{r}} s(\vec{r}), \qquad (1)$$

where *J* is the exchange coupling, and  $s(\vec{r}) = s^{z}(\vec{r})/S$  with  $s^{z}(\vec{r})$  a classical spin variable at the lattice site  $\vec{r}$ , taking the 2S+1 values  $-S, -S+1, \ldots, S-1, S$ . The sum runs over all nearest-neighbor pairs of sites. For simplicity, the nearest-neighbor lattice spacing will be set equal to 1 everywhere. We shall consider expansions in the usual HT variable  $K = J/k_BT$  where *T* is the temperature,  $k_B$  the Boltzmann constant, and *K* will be called "inverse temperature" for brevity. In the critical region we shall also refer to the standard "reduced-temperature" variable  $t(S)=1-T_c(S)/T=1-K/K_c(S)$ .

We shall study the HT expansion of the (connected) sscf defined as

$$G(\vec{r},T;S) = \langle s(\vec{0})s(\vec{r}) \rangle_c.$$
<sup>(2)</sup>

In order to estimate numerically  $G(\vec{r},T;S)$  as  $T \rightarrow T_c +$ , we have allowed for its expected<sup>6,28</sup> behavior: in the 2D case

$$G(\vec{r},T;S) \approx G(\vec{r},T_c;S) - E^+(\vec{r};S)t(S)\ln t(S) + \cdots$$
 (3)

and in the 3D case

$$G(\vec{r},T;S) \approx G(\vec{r},T_c;S) - E^+(\vec{r};S)t(S)^{1-\alpha} + \cdots$$
 (4)

Here  $E^+(\vec{r};S)$  is the critical amplitude of the leading singular correction,  $\alpha = 0.110(1)$  (Ref. 23) denotes the critical exponent of the specific heat in 3D and the dots indicate higher-order corrections.

The correlation-function moment  $\mu_n(T;S)$  of order *n* is defined as

$$\mu_n(T;S) = \sum_{\vec{r}} |\vec{r}|^n \langle s(\vec{0})s(\vec{r}) \rangle_c \tag{5}$$

(for n < 0 the sum extends to  $\vec{r} \neq 0$ ).

The expected asymptotic behavior of  $\mu_n(T;S)$  as  $T \rightarrow T_c +$  is

$$\mu_n(T;S) \approx m_n^+(S)t(S)^{-(\gamma+n\nu)} [1 + a_n^+(S)t(S)^{\theta} + \cdots].$$
(6)

In 2D the exponent  $\theta$  of the leading singular correction is larger than unity, while in 3D a recent simultaneous study<sup>29</sup> of a set of models in the Ising universality class has suggested the very precise estimate  $\theta$ =0.517(4).

The scattering function, namely the Fourier transform of  $G(\vec{r},T;S)$ ,

$$\hat{G}(\vec{k},T;S) = \sum_{\vec{r}} \exp[-i\vec{k}\cdot\vec{r}]G(\vec{r},T;S),$$
 (7)

for  $\vec{k} = 0$  yields the zero-field reduced susceptibility

$$\hat{G}(\vec{0},T;S) = \mu_0(T;S) = \chi(T;S) = \sum_{\vec{r}} \langle s(\vec{0})s(\vec{r}) \rangle_c.$$
 (8)

The second-moment correlation length is defined in d spatial dimensions by

$$\xi_{sm}^{2}(T;S) = \frac{\mu_{2}(T;S)}{2d\chi(T;S)} = \frac{d\ln\hat{G}(\tilde{k},T;S)}{dk^{2}} \bigg|_{k=0}.$$
 (9)

For  $T > T_c$  the sscf is exponentially decreasing for large *r* and therefore following Ref. 6, beside the "second-moment" correlation length we can also define the inverse "exponential" (or "true") correlation length in the direction  $\vec{e}$  as

$$k_{\vec{e}}(T;S) = -\lim_{r \to \infty} \frac{1}{r} \ln |G(r\vec{e},T;S)|.$$
(10)

Since the singularity of  $\hat{G}(\vec{k},T;S)$  closest to the real axis in the complex *k* plane is located at  $\pm ik_{\vec{e}}(T;S)$ , the exponential correlation length can be obtained by solving recursively<sup>9</sup> the equation

$$\hat{G}(i\vec{k}_{e},T;S)^{-1}=0.$$
 (11)

Rather than working directly with  $k_e^-(T;S)$  which is not an ordinary power series in *K*, it is expedient<sup>6</sup> to form the quantity

$$\xi_{\vec{e}}^{2}(T;S) = \frac{f^{2}}{2[\cosh(fk_{\vec{e}}) - 1]}$$
(12)

which is an ordinary power series in K. In Eq. (12) f is a geometrical factor depending on the unit vector  $\vec{e}$  and on the lattice considered. In particular, if  $\vec{e}$  is directed along a lattice axis, we have f=1 for the sq and the sc lattices, while  $f = 1/\sqrt{3}$  for the bcc lattice.

So far, 3D data for this quantity were published exclusively for S = 1/2, and did not extend beyond order 15 in the sc-lattice case<sup>30</sup> or beyond order 10 in the bcc-lattice case.<sup>9</sup> In 2D the HT expansion can be computed exactly<sup>6,28</sup> for S = 1/2, but no data have been published for  $S \neq 1/2$ . In Ref. 24, we have tabulated the expansion of  $\xi_{\vec{e}}^2(T;S)$  through order 19 for  $\vec{e}$  directed along a lattice axis, in the case of the sq, sc, and bcc lattices and with  $S = 1/2, 1, 3/2, 2, 5/2, 3, \infty$ .

In order to avoid possible confusion, it should be pointed out that in Ref. 6 our  $\xi_{\vec{e}}^2$  was denoted by  $\Lambda'_2(\vec{e})$ , while the symbol  $\xi_e^-$  was used to denote  $k_e^{-1}$ . Our notation might be more suggestive since our  $\xi_{\vec{e}}^2$  compares very closely with  $\xi_{sm}^2$ . Indeed, the true and second-moment correlation lengths are almost identical in magnitude above the critical temperature. In particular on the sq lattice, when  $\vec{e}$  is directed along a lattice axis, the HT expansion coefficients of  $\xi_e^2$  and  $\xi_{sm}^2$ coincide through sixth order for S = 1/2, through fourth order for S = 1, and through second order for higher values of the spin. In 3D, in the sc-lattice case, the expansion coefficients of  $\xi_e^2$  and  $\xi_{sm}^2$  coincide through seventh order for S = 1/2, through fifth order for S=1 and through third order for higher values of S. In the case of the bcc lattice, the expansion coefficients coincide through third order for all values of the spin. Moreover, up to the maximum order of our computation, the noncoinciding coefficients differ by less than 0.1%.

The two correlation lengths  $\xi_e^-$  and  $\xi_{sm}$  are expected to share the same critical exponent  $\nu$  so that their asymptotic behavior when  $T \rightarrow T_c^+$  can be written as

$$\xi_{sm}(T;S) \approx f_{sm}^+(S)t(S)^{-\nu} [1 + a_{sm}^+(S)t(S)^{\theta} + \cdots]$$
(13)

and

$$\xi_{e}(T;S) \approx f^{+}(S)t(S)^{-\nu}[1+a^{+}(S)t(S)^{\theta}+\cdots].$$
(14)

Here the critical amplitude  $f^+(S)$  is independent of e, since the sscf becomes spherically symmetric near the critical point. The ratio

$$Q_{\xi}^{+}(S) = f^{+}(S) / f_{sm}^{+}(S)$$
(15)

is a universal combination of critical amplitudes,<sup>20</sup> i.e., it is expected to depend only on the lattice dimensionality d, but not on the spin S or the lattice structure.

For  $T \rightarrow T_c + 0$  and in zero magnetic field, the sscf is expected to exhibit the asymptotic structure

$$G(r,T;S) \approx (1/r)^{d-2+\eta} A_l(S) D_0(C_l(S)r/\xi_{sm}(T;S)) + \cdots$$
(16)

when both *r* and  $\xi_{sm}$  are much larger than the lattice spacing (with arbitrary  $r/\xi_{sm}$ ). Equation (16) together with these assumptions on *r* and  $\xi_{sm}$  is usually referred to as the "strongscaling hypothesis" (while it is called the "weak-scaling hypothesis," if its validity is restricted to the  $r \rightarrow \infty$  limit with fixed  $r/\xi_{sm}$ ). In Eq. (16),  $\eta$  is the critical exponent describing the decay of the sscf at the critical point,  $D_0(x)$  is called the critical scaling function,  $A_l(S)$  and  $C_l(S)$  are scale factors. The dots indicate subcritical corrections proportional to a positive power of some irrelevant field. The scaling function  $D_0(x)$  is expected to be universal: its structure does not depend on the particular model under study provided that it belongs to a given universality class. On the contrary the scale factors  $A_l(S), C_l(S)$  depend on the spin and the lattice *l*. The validity of the asymptotic structure Eq. (16) was verified analytically<sup>32</sup> for the spin S = 1/2 Ising model in 2D.

For the scattering function  $\hat{G}(\vec{k},T;S)$  the analogous scaling form as  $T \rightarrow T_c +$  can be written as

$$\hat{G}(\vec{k},T;S) \approx A_l'(S)t(S)^{-\gamma} \hat{D}_0'(C_l'(S)k^2\xi_{sm}^2) + \cdots .$$
(17)

If the scale factors  $A'_{l}(S), C'_{l}(S)$  are specified adopting the normalization conditions

$$\hat{D}_{0}'(0) = 1, \quad \left(\frac{d\hat{D}_{0}'(x)}{dx}\right)_{x=0} = -1,$$
 (18)

one can write<sup>6</sup> as  $k \rightarrow 0$ 

$$\hat{G}(\vec{0},T;S)/\hat{G}(\vec{k},T;S) = 1/g_{+}(k\xi_{sm}(T;S))$$

$$= 1 + \xi_{sm}^{2}(T;S)k^{2}$$

$$-\Sigma_{4}(T,S)\xi_{sm}^{4}(T;S)k^{4}$$

$$+\Sigma_{6}(T,S)\xi_{sm}^{6}(T;S)k^{6} + O(k^{8}),$$
(19)

where the function  $g_+(k\xi_{sm}(T;S))$  is universal and thus the quantities

$$\Sigma_4(T,S) = c_4 \frac{\mu_4(T;S)\mu_0(T;S)}{\mu_2^2(T;S)} - 1, \qquad (20)$$

$$\Sigma_6(T,S) = c_6 \frac{\mu_6(T;S)\mu_0^2(T;S)}{\mu_2^3(T;S)} - 2\Sigma_4(T,S) - 1 \quad (21)$$

with  $c_4 = 1/4$  and  $c_6 = 1/36$  for d = 2, while  $c_4 = 3/10$  and  $c_6 = 3/70$  for d = 3, have finite universal values as  $T \rightarrow T_c + .$ 

All  $\Sigma_{2n}(T,S)$ , as well as the difference  $\xi_e^2 - \xi_{sm}^2$ , vanish<sup>6</sup> in the mean-field related approximations. Therefore the magnitudes of these quantities at the critical point can be taken as a measure of the deviation of a given system from Gaussian behavior, which turns out to be very small on the HT side of the critical point.

More generally, it was observed<sup>13</sup> that the scaling hypothesis, Eq. (16), implies that, at the critical point, the ratios

$$R_{m,n;r,s}(T;S) = \frac{\mu_m(T;S)\mu_n(T;S)}{\mu_r(T;S)\mu_s(T;S)}$$
(22)

with m+n=r+s are universal. These ratios are dominated by the critical singularity also for negative values of the indices m,n,r,s provided that each index exceeds  $-2+\eta$ , as follows from Eq. (6).

Finally, the determination of the amplitude  $E^+(\vec{r};S)$  of the leading singularity of the sscf [see Eqs. (3) and (4)] gives another opportunity to perform universality and scaling tests. In order that the structure of Eqs. (3) and (4) be compatible<sup>11</sup> with the strong-scaling hypothesis, Eq. (16), the amplitudes  $E^+(\vec{r};S)$  must scale as  $r^{\zeta}$  with  $\zeta = (1-\alpha)/\nu + 2 - d - \eta$ , namely

$$E^+(\vec{r};S) \approx E_0^+(S)r^\zeta \tag{23}$$

for large enough *r*, independently of the spin and the lattice structure. In 2D the value  $\zeta = 0.75$  is expected, while in 3D, adopting our recent estimate<sup>23</sup> of the values of the correlation-length exponent  $\nu = 0.6299(2)$  and of the exponent  $\eta = 0.036(1)$ , we should have  $\zeta = 0.3765(10)$ .

### **III. NUMERICAL RESULTS**

Let us first observe that, due to the leading singular corrections in Eqs. (3) and (4), whose amplitudes  $E^+(\vec{r};S)$  grow with r as indicated by Eq. (23), determining accurately  $G(\vec{r},T_c;S)$  [as well as  $E^+(\vec{r};S)$  itself] is a rather delicate matter for which it is crucial to rely on sufficiently many expansion coefficients. We should also consider that the number of nontrivial coefficients in our series decreases with increasing r, and correspondingly the precision of our estimates of  $G(\vec{r},T_c;S)$  [and  $E^+(\vec{r},S)$ ] deteriorates. In Refs.

TABLE I. Our estimates of the critical-point values  $G(\vec{r}, T_c; S)$  of the spin-spin correlation function for the nearest-neighbor Ising models with spin  $S = 1/2, 1, 3/2, 2, \infty$  on the sq, sc, and bcc lattices. For comparison with our results, the first column labeled [S = 1/2] shows the only available previous estimates. In the case of the sq lattice, we have cited the exact (Refs. 6 and 35) values. In the case of the nearest-neighbor correlation [r = (1,0,0)] on the sc lattice, we have reported in the first column the estimate obtained using our numerical procedure with the series  $O(K^{45})$  of Ref. 36 and have also cited a value (Ref. 37) obtained in a recent high-precision Monte Carlo simulation. In the remaining cases we have reported the estimates of Ref. 33 obtained from series  $O(K^{12})$ . We are not aware of previous calculations for S > 1/2.

Lattice	ř	[S = 1/2]	S = 1/2	S = 1	S = 3/2	S = 2	$S = \infty$
sq	(1,0)	0.707107 <sup>a</sup>	0.7071(1)	0.5806(3)	0.517(1)	0.481(1)	0.338(1)
	(1,1)	$0.636620 \dots^a$	0.6366(1)	0.5207(4)	0.463(1)	0.431(1)	0.303(1)
	(2,0)	0.594715 <sup>a</sup>	0.5947(2)	0.486(1)	0.433(1)	0.402(1)	0.282(2)
	(2,1)	0.573159 <sup>a</sup>	0.573(1)	0.467(1)	0.417(2)	0.387(2)	0.272(2)
	(2,2)	$0.540380 \ldots^{a}$	0.540(1)	0.442(1)	0.393(2)	0.365(2)	0.256(4)
sc	(1,0,0)	0.330200(5) <sup>b</sup>	0.33020(6)	0.24203(6)	0.20756(6)	0.18918(6)	0.12886(6)
	(1,0,0)	0.33017(3) <sup>c</sup>					
	(1,1,0)	$0.208(2)^{d}$	0.2086(1)	0.1529(1)	0.1311(1)	0.1194(1)	0.08141(5)
	(1,1,1)	$0.164(4)^{d}$	0.1633(1)	0.1197(1)	0.1027(1)	0.0936(1)	0.0638(1)
	(2,0,0)	$0.162(4)^{d}$	0.1608(2)	0.1178(2)	0.1010(2)	0.0921(2)	0.0627(1)
	(3,0,0)	$0.104(7)^{d}$	0.1017(3)	0.0746(2)	0.0639(2)	0.0581(2)	0.0396(1)
bcc	(1,1,1)	0.2735(7) <sup>d</sup>	0.27265(5)	0.19653(5)	0.16763(5)	0.15243(5)	0.10341(5)
	(2,0,0)	$0.200(2)^{d}$	0.19971(5)	0.14394(5)	0.12278(5)	0.11165(5)	0.07575(5)
	(2,2,0)	$0.157(2)^{d}$	0.15627(5)	0.11269(5)	0.09614(5)	0.08743(5)	0.05934(5)
	(3,1,1)	$0.129(3)^{d}$	0.12751(5)	0.09193(5)	0.07843(5)	0.07132(5)	0.04839(5)
	(2,2,2)	0.131(3) <sup>d</sup>	0.12914(5)	0.09315(5)	0.07945(5)	0.07224(5)	0.04903(5)

<sup>a</sup>Reference 6.

<sup>b</sup>Reference 36.

<sup>c</sup>Reference 37.

<sup>d</sup>Reference 33.

7, 12, and 33, due to the small number of coefficients available at that time, a generalized Neville extrapolation of the partial sums had to be used for determining  $G(\vec{r},T;S)$  and  $E^+(\vec{r};S)$  in the vicinity of  $T_c$ . Taking advantage of our new series, we can now improve substantially the numerical resummation of the HT series by resorting to first- or secondorder inhomogeneous differential approximants<sup>34</sup> (DA's) biased with  $K_c(S)$ . (Here and in what follows we have adopted the values of the critical temperatures tabulated in Refs. 23 and 25.) It does not come as a surprise that our procedures are slightly less efficient in 2D than in 3D, probably due to the presence of logarithms in the leading correction terms to the critical asymptotic behavior, Eq. (3), and also that in 3D the bcc-lattice series always yield the most accurate results. If we restrict to 1.0 < r < 6.0 the relative uncertainty of our estimates of the critical sscf should generally remain well below 1%. In 2D this can be guessed by comparing the estimates of  $G(\vec{r}, T_c; S)$  obtained from our series  $O(K^{25})$ with the known exact results in the sq-lattice case<sup>6,35</sup> for S = 1/2 and safely assuming that the precision does not deteriorate too fastly when higher values of S are considered. In 3D no exact results are available, but the HT series for the nearest-neighbor correlation function was recently extended<sup>36</sup> through order 45 in the sc-lattice case for S= 1/2. Therefore, in this case, we are able to compare our estimate at order 25 with the result obtained by applying the same numerical procedures to the series extended through order 45. (It would be very interesting if the improved finitelattice technique devised for this remarkable calculation could be generalized as effectively beyond first-neighbor correlations and to general S.) We should also mention that a completely consistent alternative estimate of the critical sclattice nearest-neighbor sscf has been obtained<sup>37</sup> in a recent high-precision Monte Carlo study. For other values of  $\vec{r}$  in the sc-lattice case and in the bcc-lattice case our results can only be compared with calculations<sup>33</sup> using the old series  $O(K^{12})$ . Table I lists our estimates of  $G(\vec{r}, T_c; S)$  with their apparent uncertainties for a small sample of values of  $\vec{r}$  and S. Previous estimates of the critical sscf from shorter series, which are available only for S = 1/2, are shown for comparison in the first column, labeled [S=1/2], of this table. In Figs. 1, 2, and 3 we have plotted our estimates of  $\ln[G(\vec{r},T_c;S)]$  vs  $\ln(r)$  for  $1 \le r \le 5$  with S = 1/2, 1, 3/2, 2 in the cases of the sq, sc, and bcc lattices, respectively. We have also shown by continuous lines the results of one-parameter fits to the leading asymptotic behaviors  $\ln[G(\vec{r},T_c;S)] \approx c(S)$  $-(d-2+\eta)\ln(r)$  expected for large r. We have taken only c(S) as a free parameter and fixed  $\eta = 0.25$  in 2D and  $\eta$ = 0.036 in 3D.

Both in 2D and in 3D, we have estimated also  $E^+(\vec{r};S)$  from the amplitude of the singularity of the second temperature



FIG. 1. Estimates of  $G(\vec{r}, T_c; S)$  on the sq lattice. The meaning of the symbols is as follows. Triangles, S = 1/2; squares, S = 1; rhombs, S = 3/2; circles, S = 2. The spin S points are shifted vertically by the quantity 1/2 - S in order to make the figure more legible. The continuous lines represent fits to the leading asymptotic behaviors  $\ln G(\vec{r}, T_c; S) \approx c(S) - \eta \ln(r)$  expected for large r. We have taken c(S) as a fit parameter and fixed  $\eta = 0.25$ .

derivative of  $G(\vec{r},T;S)$ , again using inhomogeneous firstand second-order DA's biased with  $K_c(S)$  and  $\alpha$ . Our estimates of  $E^+(\vec{r};S)$  for a small sample of values of  $\vec{r}$  and S are shown in Table II. They are compared with the exactly known values<sup>6</sup> for S = 1/2, in the case of the sq lattice, or with a few old estimates<sup>11</sup> from shorter series, in the case of



FIG. 2. Estimates of  $G(\vec{r}, T_c; S)$  on the sc lattice. The meaning of the symbols is the same as in Fig. 1. The spin *S* points are shifted vertically by the quantity 1/2-S in order to make the figure more legible. The continuous lines represent fits to the leading asymptotic behaviors  $\ln G(\vec{r}, T_c; S) \approx c(S) - (1 + \eta) \ln(r)$  expected for large *r*. We have taken c(S) as a fit parameter and fixed  $\eta = 0.036$ .



FIG. 3. Estimates of  $G(\vec{r}, T_c; S)$  on the bcc lattice. The meaning of the symbols is the same as in Fig. 1. The spin *S* points are shifted vertically by the quantity 1/2-S in order to make the figure more legible. The continuous lines represent fits to the leading asymptotic behaviors  $\ln G(\vec{r}, T_c; S) \approx c(S) - (1+\eta)\ln(r)$  expected for large *r*. We have taken c(S) as a fit parameter and fixed  $\eta = 0.036$ .

the sc and bcc lattices. A comparison with the exact results in 2D and with our estimate using the mentioned high-order calculation in the sc lattice<sup>36</sup> for S = 1/2 still suggests that, for all values of *S*, the relative accuracy of our estimates should not be generally worse than 1%.

In Figs. 4, 5, and 6 for S = 1/2, 1, 3/2, 2 we have plotted  $\ln[E^+(\vec{r},S)]$  vs  $\ln(r)$  in the case of the sq, sc, and bcc lattices, respectively. For r > 4.5 in the case of the sc lattice and r >6.0 in the case of the bcc lattice, we have not reported any estimates of  $E^+(\vec{r};S)$ , because the available nontrivial HT coefficients of the sscf are not sufficiently many to allow estimates at the level of precision above mentioned. In these figures we have also represented by continuous lines the results of one-parameter fits to the leading asymptotic behaviors  $\ln[E^+(\vec{r};S)] \approx b(S) + \zeta \ln(r)$  expected for large r. We have taken for  $\zeta$  the expected values  $\zeta = 0.75$  in the 2D case and  $\zeta = 0.3765$  in the 3D cases, while the free parameters b(S)have been determined using in the fits only the data with r $\gtrsim$ 1.8. Indeed, our data show visible deviations from asymptotic scaling for sufficiently small r, particularly so in the case of the sc lattice, but the asymptotic consistency with the strong-scaling hypothesis Eq. (23), is good. The behavior of  $E^+(\vec{r}; 1/2)$  as a function of r was first studied in Ref. 7 using series  $O(K^{12})$  for the face-centered-cubic lattice. In that analysis both  $\zeta$  and b(1/2) were determined by a twoparameter fit of the numerical results to the leading asymptotic behavior under the very simple assumption that the corrections to scaling are negligible even for "not very large" r. (As we have indicated above, our data show that such a strong assumption is untenable.) The authors of Ref. 7 concluded that  $\zeta = 0.47(6)$ , an estimate in sharp disagreement with the value  $\zeta = 0.33(1)$  expected from the exponent

TABLE II. Amplitudes  $E^+(r;S)$  of the leading singular correction of the sscf near the critical point for the nearest-neighbor Ising models with spin  $S = 1/2, 1, 3/2, 2, \infty$  on the sq, sc, and bcc lattices. For comparison with our results, the first column of the table labeled [S = 1/2] shows the available estimates from other sources. In the case of the sq lattice, the exact values are taken from Ref. 6. In the case of the nearestneighbor correlation on the sc lattice [r = (1,0,0)], we have reported in the first column our estimate obtained from the series  $O(K^{45})$  of Ref. 36. In the remaining cases, whenever available, we have quoted the estimates of Ref. 11 obtained from series  $O(K^{12})$ . We are not aware of other published calculations for S > 1/2.

Lattice	$\vec{r}$	[S = 1/2]	S = 1/2	S = 1	S = 3/2	S = 2	$S = \infty$
sq	(1,0)	0.561100 <sup>a</sup>	0.562(1)	0.621(1)	0.623(1)	0.613(1)	0.484(1)
	(1,1)	0.793515 <sup>a</sup>	0.794(1)	0.819(1)	0.812(1)	0.794(1)	0.616(1)
	(2,0)	1.0103348 <sup>a</sup>	1.01(1)	1.02(1)	1.01(1)	0.987(2)	0.759(2)
	(2,1)	1.120022 <sup>a</sup>	1.11(1)	1.13(1)	1.11(1)	1.08(1)	0.826(2)
sc	(1,0,0)	$2.252(5)^{b}$	2.27(2)	2.16(2)	2.03(2)	1.93(2)	1.42(2)
	(1,1,0)	$2.38(2)^{c}$	3.01(2)	2.72(2)	2.52(2)	2.38(2)	1.72(2)
	(1,1,1)	$2.86(4)^{c}$	3.40(2)	3.03(2)	2.78(2)	2.62(2)	1.90(2)
	(2,0,0)	$3.16(6)^{c}$	3.53(2)	3.14(2)	2.88(2)	2.71(2)	1.95(2)
	(3,0,0)		4.36(2)	3.79(2)	3.45(2)	3.24(2)	2.33(2)
bcc	(1,1,1)	2.010 <sup>c</sup>	2.325(5)	2.167(5)	2.022(5)	1.917(5)	1.401(5)
	(2,0,0)		2.707(6)	2.442(6)	2.256(6)	2.129(6)	1.545(6)
	(2,2,0)		3.126(6)	2.767(6)	2.535(6)	2.384(6)	1.720(6)
	(3,1,1)		3.41(1)	2.98(1)	2.72(1)	2.55(1)	1.83(1)
	(2,2,2)		3.44(1)	3.01(1)	2.74(1)	2.57(1)	1.84(1)

<sup>a</sup>Reference 6. <sup>b</sup>Reference 36.

<sup>c</sup>Reference 11.

values  $\nu = 0.638(2)$  and  $\eta = 0.041(6)$  generally accepted at that time. A few years later, for S = 1/2, the somewhat lower estimate  $\zeta = 0.39(4)$  was obtained<sup>11</sup> from an analysis of LT expansions in powers of  $u = \exp(-2K)$  up to order  $u^{11}$  and



FIG. 4. Estimates of  $E^+(\vec{r};S)$  on the sq lattice. The meaning of the symbols is the same as in Fig. 1. The spin *S* points are shifted vertically by the quantity 1/2-S in order to make the figure more legible. The continuous lines represent fits to the leading asymptotic behaviors  $\ln E^+(\vec{r};S) \approx b(S) + \zeta \ln(r)$  expected for large *r*. We have taken b(S) as a fit parameter and fixed  $\zeta = 0.75$ .

 $u^{13}$ , on the sc and the bcc lattices, respectively. In this latter study, however, a third fit parameter had been introduced in order to allow for small corrections to the asymptotic scaling behavior of  $E^+(\vec{r};S)$ . Also this estimate of  $\zeta$  did not agree



FIG. 5. Estimates of  $E^+(\vec{r};S)$  on the sc lattice. The meaning of the symbols is the same as in Fig. 1. The spin *S* points are shifted vertically by the quantity 1/2-S in order to make the figure more legible. The continuous lines represent fits to the leading asymptotic behaviors  $\ln E^+(\vec{r};S) \approx b(S) + \zeta \ln(r)$  expected for large *r*. We have taken b(S) as a fit parameter and fixed  $\zeta = 0.3765$ .



FIG. 6. Estimates of  $E^+(\vec{r};S)$  on the bcc lattice. The meaning of the symbols is the same as in Fig. 1. The spin *S* points are shifted vertically by the quantity 1/2-S in order to make the figure more legible. The continuous lines represent fits to the leading asymptotic behaviors  $\ln E^+(\vec{r};S) \approx b(S) + \zeta \ln(r)$  expected for large *r*. We have taken b(S) as a fit parameter and fixed  $\zeta = 0.3765$ .

with the value expected at that time, but is quite compatible with the presently preferred value.

Before any strong confidence in the results of such twoor three-parameter fits can be justified, we believe, however, that the HT series should be further extended in order to enlarge significantly the range of values of r for which  $E^+(\vec{r};S)$  can be determined with sufficient accuracy.

Having tabulated a wide sample of estimates of  $G(\vec{r}, T_c; S)$  and  $E^+(\vec{r}; S)$  with some improvement both in the extent and the accuracy, with respect to the very few estimates available in the literature, we are now in the position to exhibit more directly the scaling property by examining the near-critical sscf in the *r* space. For  $T \rightarrow T_c + 0$ , as suggested by Eq. (16), by a proper choice of the scale factors  $A_l(S)$  and  $C_l(S)$ , we should be able to plot the quantities

$$r^{d-2+\eta}G(\vec{r},T;S) \approx A_l(S)D_0(C_l(S)r/\xi_{sm}(T;S))$$
 (24)

vs  $r/\xi_{sm}$  in such a way that the curves, associated to various values of *S* and to different lattices, collapse on each other. In Fig. 7, we have plotted  $\ln[r^{d-2+\eta}G(\vec{r},T;S)]$  vs  $r/\xi_{sm}(T;S)$  in the case of the sq lattice taking  $\vec{r} = (2,0)$  and S = 1/2, 1, 3/2, 2. Our data points refer to the range of temperatures for which  $1.5 \leq \xi_{sm} \leq 200$ . Figure 8 shows the analogous plot for  $\ln[r^{d-2+\eta}G(\vec{r},T;S)]$  vs  $r/\xi_{sm}$  in the case of the sc and bcc lattices. Here we have taken  $\vec{r} = (4,0,0)$  and S = 1/2, 1, 3/2, 2 and have plotted data in the range of temperatures for which  $2.7 \leq \xi_{sm} \leq 400$ . Completely consistent results are obtained also for other choices of  $\vec{r}$ . As already observed, within these limitations, the present length of the



FIG. 7. The logarithm of the scaling function  $r^{d-2+\eta}G(\vec{r},T;S)$  vs  $x=r/\xi_{sm}(T;S)$  in the case of the sq lattice. The data represent the ssfc's with  $\vec{r}=(2,0)$  and S=1/2,1,3/2,2 in the range of temperatures for which  $1.5 \le \xi(T;S) \le 200$ . The meaning of the symbols is the same as in Fig. 1.

HT series appears sufficient to obtain reliable estimates and our results are consistent with the strong-scaling hypothesis to a good approximation.

The very small mismatch of the curves in the extreme regions  $r/\xi_{sm} \ll 1$  or  $r/\xi_{sm} \gg 1$  which can still be observed is related (i) to the fact that the scaling property has an asymptotic character, while in practice the size of *r* still cannot exceed a few lattice spacings if we want to use a decent



FIG. 8. The logarithm of the scaling function  $r^{d-2+\eta}G(\vec{r},T;S)$  vs  $x=r/\xi_{sm}(T;S)$  in the case of the sc and the bcc lattices. For both lattices the data represent the ssfc's with  $\vec{r}=(4,0,0)$  and S = 1/2,1,3/2,2 in the range of temperatures for which  $2.7 \le \xi(T;S) \le 400$ . The meaning of the symbols is the same as in Fig. 1 for the sc-lattice case. For the bcc-lattice data we have used full symbols of the same shape.

TABLE III. Estimates of  $\Sigma_4(T_c; S)$  [see Eq. (20)] and  $\Sigma_6(T_c; S)$  [see Eq. (21)] in the case of the sq, sc, and bcc lattices for various values of S. For comparison, we have also reported a few previous estimates listed in Refs. 31 and 30, indicating the method of calculation and the expected uncertainty, when available. Only for convenience, we have listed in the S=1/2 column also the results of the renormalization group and the optimized continuous-spin calculations which, of course, do not refer to spin S=1/2.

Quantity	Lattice	S = 1/2	S = 1	S = 3/2	S = 2	$S = \infty$
$\overline{\Sigma_4(T_c;S) \times 10^4}$	sq	7.8(3)	7.9(3)	7.9(3)	7.6(3)	7.5(3)
$\Sigma_4(T_c;S) \times 10^4 \text{ (Exact)}^{a}$	sq	7.936796				
$\Sigma_6(T_c;S) \times 10^5$	sq	1.1(1)	1.1(1)	1.0(1)	1.1(1)	1.0(1)
$\Sigma_6(T_c;S) \times 10^5 (\text{Exact})^a$	sq	1.095991				
$\Sigma_4(T_c;S) \times 10^4$	sc	3.76(8)	3.9(2)	3.77(8)	3.75(8)	3.7(2)
$\Sigma_4(T_c;S) \times 10^4$	bcc	3.75(5)	3.74(5)	3.76(5)	3.76(5)	3.77(5)
$\Sigma_6(T_c;S) \times 10^5$	sc	1.0(2)	.9(2)	0.9(2)	0.8(2)	0.7(2)
$\Sigma_6(T_c;S) \times 10^5$	bcc	0.9(1)	0.86(5)	0.85(5)	0.85(5)	.85(5)
$\Sigma_4 \times 10^4$ [HT] <sup>b</sup>	sc	3.0(2)				
$\Sigma_4 \times 10^4 \text{ [HT]}^{\text{c}}$	sc	5.5(15)				
$\Sigma_4 \times 10^4 \text{ [HT]}^{\text{c}}$	bcc	7.1(15)				
$\Sigma_6 \times 10^5$ [HT] <sup>b</sup>	sc	0.5(2)				
$\Sigma_6 \times 10^5$ [HT] <sup>c</sup>	sc	0.5(2)				
$\Sigma_6 \times 10^5$ [HT] <sup>c</sup>	bcc	0.9(3)				
$\Sigma_4 \times 10^4$ (opt.cont.spin) <sup>b</sup>	sc	3.90(6)				
$\Sigma_6 \times 10^5 \text{ (opt.cont.spin)}^{b}$	sc	.88(1)				
$\Sigma_4 \times 10^4 \ (\epsilon$ -expans.) <sup>b</sup>		3.3(2)				
$\Sigma_6 \times 10^5 \ (\epsilon$ -expans.) <sup>b</sup>		0.7				
$\Sigma_4 \times 10^4$ (g-expans.) <sup>b</sup>		4.0(5)				
$\Sigma_6 \times 10^5 \text{ (g-expans.)}^{\text{b}}$		1.3(3)				

<sup>a</sup>Reference 30.

<sup>b</sup>Reference 31.

<sup>c</sup>Reference 6.

number of expansion coefficients in the estimate of  $G(\vec{r},T;S)$ , (ii) to the residual influence of the subcritical corrections.

We can further test the universality properties of the sscf in the k space, namely the critical scattering function, by simply showing that  $\Sigma_4(T_c;S)$  and  $\Sigma_6(T_c;S)$  are independent of S and of the lattice structure. Also these quantities are calculated by first- and second-order DA's biased with  $K_{c}(S)$ . Since higher-order moments of the sscf (in which the less accurately known correlations between distant spins are weighted much more than those between near spins) enter into the definitions, Eqs. (20) and (21), the convergence of the extrapolations is not expected to be very fast, particularly so in the cases of the sq and sc lattices. We should also consider that  $\Sigma_4(T_c;S)$  is the very small difference between unity and the critical value of some multiple of a ratio of moments of the sscf, so that a very high accuracy in the estimate of the latter is needed to achieve even a relatively modest precision for  $\Sigma_4(T_c;S)$ . The same remark applies also in the case of  $\Sigma_6(T_c;S)$ . In Table III we have collected our estimates of  $\Sigma_4(T_c;S)$  and  $\Sigma_6(T_c;S)$  in the case of the sc, sq, and bcc lattices for  $S = 1/2, 1, 3/2, 2, \infty$ . We have also reported a few previous estimates<sup>30,31</sup> from the existing literature.

In the case of the sq lattice our data suggest the final estimates  $\Sigma_4(T_c;S) = 7.8(3) \times 10^{-4}$  and  $\Sigma_6(T_c;S) = 1.1(1)$ 

 $\times 10^{-5}$ , independently of S and in reasonable agreement with the high-precision determinations<sup>30</sup> of  $\Sigma_4(T_c; 1/2)$  $=7.936796... \times 10^{-4}$  and of  $\Sigma_6(T_c; 1/2) = 1.095991...$  $\times 10^{-5}$  obtained by numerical integration of the analytically known<sup>38</sup> sscf of the S = 1/2 model in 2D. In 3D our results for the bcc lattice show a definitely smaller uncertainty than for the sc lattice. They suggest the final estimates  $\Sigma_4(T_c;S) = 3.8(1) \times 10^{-4}$  and  $\Sigma_6(T_c;S) = 0.9(1) \times 10^{-5}$  independently of the spin S and lattice structure. Our results are therefore consistent with the corresponding estimates in the literature, in particular with the values  $\Sigma_4(T_c)$  $=3.90(6)\times10^{-4}$  and  $\Sigma_6(T_c)=0.88(1)\times10^{-5}$  obtained<sup>30,31</sup> optimizing the parameters of a continuous-spin model, under the assumption of universality. Let us also mention that renormalization-group calculations<sup>31</sup> in the  $\epsilon$ -expansion scheme to third order yielded the estimates  $\Sigma_4 = 3.3(2)$  $\times 10^{-4}$  and  $\Sigma_6 = 0.7 \times 10^{-5}$ , while, in the coupling-constant expansion scheme to fourth order, the corresponding results were  $\Sigma_4 = 4.0(5) \times 10^{-4}$  and  $\Sigma_6 = 1.3(3) \times 10^{-5}$ .

The results of our analysis of the universal ratios  $R_{m,n;r,s}(T_c;S)$  are reported in Table IV. They also show independence of the spin and of the lattice structure within a good precision. Our series-extrapolation procedure based on first- and second-order DA's uses only our estimates of  $K_c(S)$  and does not need to be biased also with  $\gamma$  and  $\nu$  as it

$R_{m,n;r,s}$	Lattice	S = 1/2	S = 1	S = 3/2	S = 2	$S = \infty$
$R_{0,1;1/2,1/2}$	sq	1.1641(1)	1.1642(1)	1.1642(1)	1.1642(1)	1.1641(1)
$R_{0,1;1/4,3/4}$	sq	1.1211(1)	1.1211(1)	1.1211(1)	1.1211(1)	1.1210(1)
$R_{-3/4,1/4;-1/4,-1/4}$	sq	1.299(1)	1.300(1)	1.301(1)	1.300(1)	1.301(1)
$R_{-1,-1/2;-3/4,-3/4}$	sq	1.121(5)	1.124(4)	1.124(4)	1.125(4)	1.126(4)
$R_{0,1;1/2,1/2}$	sc	1.1320(1)	1.1320(2)	1.1319(1)	1.1319(2)	1.1319(2)
$R_{0,1;1/2,1/2}$	bcc	1.1320(1)	1.1319(1)	1.1319(1)	1.1319(1)	1.1319(1)
$R_{0,1;1/4,3/4}$	sc	1.0977(2)	1.0977(2)	1.0976(2)	1.0976(2)	1.0976(2)
$R_{0,1;1/4,3/4}$	bcc	1.0977(1)	1.0976(1)	1.0976(1)	1.0976(1)	1.0976(1)
$R_{1/2,1/2;1/4,3/4}$	sc	0.9697(2)	0.9697(2)	0.9698(2)	0.9697(2)	0.9697(2)
$R_{1/2,1/2;1/4,3/4}$	bcc	0.9697(1)	0.9697(1)	0.9697(1)	0.9697(1)	0.9698(1)
$R_{-1,-1/2;-3/4,-3/4}$	SC	1.084(1)	1.084(1)	1.084(1)	1.084(1)	1.083(1)
$R_{-1,-1/2;-3/4,-3/4}$	bcc	1.083(1)	1.083(1)	1.083(1)	1.083(1)	1.083(1)

TABLE IV. Estimates of the moment ratios  $R_{m,n;r,s}(T_c;S)$  [see Eq. (22)] in the case of the sq, sc, and bcc lattices for various values of S.

was necessary in the generalized Neville procedure<sup>7,12</sup> employed with the short series of Ref. 13. Considering that the values  $\gamma = 1.25$  and  $\nu = 0.625$  (or  $\nu = 0.638$ ) of the exponents accepted at the time of that study are somewhat different from the currently preferred ones and that the extrapolations are very sensitive to those values, a comparison with the numerical results of Ref. 13 has little meaning.

Finally, we have tested both in 2D and in 3D the spin independence of the ratio  $Q_{\xi}^{+}(S)$  defined by Eq. (15). In 3D also the lattice independence of  $Q_{\xi}^{+}(S)$  can be tested.

In 2D, on the sq lattice, the nontrivial expansion coefficients of the ratio  $\xi_e^2(T;S)/\xi_{sm}^2(T;S)$  are not sufficiently many and their behavior is not smooth enough to yield very accurate results. Therefore our best estimate of  $Q_{\xi}^+(S)$  [by first-order DA's biased with  $K_c(S)$ ] cannot be more precise than  $Q_{\xi}^+(S) = 1.0004(2)$ , independently of *S*. Our rough estimate is, however, consistent with the more accurate determination  $Q_{\xi}^+(1/2) = 1.000402...$  obtained in the S = 1/2 case in which, as already indicated above, very long series are available<sup>21</sup> for  $\xi_{sm}^2(T;1/2)$ , while  $\xi_e^2(T;1/2)$  is exactly known.<sup>6,28</sup>

In 3D we can use both first- and second-order DA's biased with  $K_c(S)$ . The very smooth bcc-lattice series yield the most accurate results. Our final estimate is  $Q_{\mathcal{E}}^+(S)$ =  $1.000\,200(3)$ , independently of S and of the lattice structure. So far, this ratio could be computed<sup>31</sup> only for S = 1/2from a 15 term series on the sc lattice, with the result  $Q_{\xi}^{+}(1/2) = 1.000 \ 125(50)$ . A more precise estimate<sup>31</sup>  $Q_{\xi}^{+}$ =1.000199(3) was obtained indirectly (and assuming universality), from optimized HT series for a continuous-spin model on the sc lattice. Within the renormalization-group approach,<sup>31</sup> the estimate  $Q_{\xi}^{+} = 1.000 \ 160(20)$  was obtained in the  $\epsilon$  expansion to third order, while the coupling-constant expansion technique to fourth order gave  $Q_{\xi}^{T}$ = 1.000205(30).

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