

## Numerical computation of finite size scaling functions: An alternative approach to finite size scaling

Jae-Kwon Kim, Adauto J. F. de Souza,<sup>\*</sup> and D. P. Landau  
*Center for Simulational Physics, The University of Georgia, Athens, Georgia 30602*

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Using single cluster flip Monte Carlo simulations we accurately determine new finite size scaling functions which are expressed only in terms of the variable  $x = \xi_L/L$ , where  $\xi_L$  is the correlation length in a finite system of size  $L$ . Data for the  $d=2$  and  $d=3$  Ising models, taken at different temperatures and for different size lattices, show excellent data collapse over the entire range of scaling variable for susceptibility and correlation length. From these finite size scaling functions we can estimate critical temperatures and exponents with rather high accuracy even though data are not obtained extremely close to the critical point. The bulk values of the renormalized four-point coupling constant are accurately measured and show strong evidence for hyperscaling. [S1063-651X(96)02708-0]

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### I. INTRODUCTION

True critical phenomena can possibly take place only in the limit in which the size of the system becomes infinite (i.e., the thermodynamic limit). The singular behavior of a system near a critical point is characterized by the bulk values of various physical quantities; it is technically impossible, however, to directly obtain information about infinite lattices from Monte Carlo simulation. Practically, however, it is not necessary to make the size of the lattice infinite in order to estimate a thermodynamic value through a Monte Carlo simulation of finite lattices: The concept of finite size scaling (FSS) [1], introduced to extrapolate the information available from the finite system to the infinite volume limit, has been remarkably successful. The most frequent application of FSS [2] has been primarily concerned with extracting some universal quantities such as the critical exponent  $\nu$  or some ratios of the critical exponents, without knowledge of the bulk values in the scaling regime. The standard finite size scaling variable is  $x = tL^{1/\nu}$  with the reduced temperature  $t \equiv |K_c - K|/K_c$ , where  $K$  is the inverse coupling  $K = J/kT$  and  $K_c$  is the inverse critical coupling. Of course, use of this variable presupposes knowledge of the correct critical coupling and the uncertainty in  $K_c$  introduces a source of error into the analysis. Another formulation proposed by Fisher used  $\tilde{t} = |K_c^L - K|/K_c^L$ , but since this requires knowledge of multiple finite lattice "critical couplings" it has seldom been used. Some nonuniversal critical parameters like  $K_c$  can also be calculated by different FSS techniques, e.g., the fourth order cumulant ratio method [3] or the microcanonical Monte Carlo (MC) method [4].

Nonetheless, determining bulk values (i.e., in the thermodynamic limit) is an important task of MC simulations, because physical quantities can then be directly compared with experiment. Also, the variation of a suitable thermodynamic

quantity with temperature near criticality characterizes its critical behavior, even if it is not describable by a power law. A criterion telling whether a quantity measured on a finite lattice at a temperature  $T$  is distinguishable from the thermodynamic value (value in the thermodynamic limit) is the ratio of the linear size of the lattice ( $L$ ) to the correlation length [ $\xi(T)$ ]: provided  $L/\xi(T)$  is sufficiently large, the measured quantity becomes essentially independent of  $L$ . Thus, one needs very large  $L$  at temperatures where  $\xi(T)$  becomes large. Unfortunately, in this situation critical slowing down limits the quality of the data. Recently, new techniques of FSS have been introduced [5,6], which enable one to extract correct thermodynamic values indirectly for a variety of physical quantities. The feature characteristic of these techniques is the calculation of some FSS functions defined in terms of a nonconventional FSS variable.

In this paper, we numerically calculate certain FSS functions which are different from the "usual" ones and extract estimates for the values of critical parameters for the two- and three-dimensional Ising models. In the next section we provide the theoretical background, and in the following section we calculate bulk values of the correlation length ( $\xi$ ), magnetic susceptibility ( $\chi$ ), and renormalized four-point coupling constant ( $g^{(4)}$ ). We summarize and conclude in the final section.

### II. THEORY AND SIMULATION

The fundamental assumption of FSS theory [1] is that  $A_L(t)$ , the value of some thermodynamic quantity  $A$  on a finite lattice of linear size  $L$ , can be expressed as

$$A_L(t) = L^{\rho/\nu} f_A(s(L,t)), \quad s(L,t) \equiv L/\xi(t) \quad (1)$$

for a bulk quantity  $A$  which has a power-law critical singularity  $A(t) \sim t^{-\rho}$  where  $t = |K_c - K|/K_c$ . Equation (1) is valid for values of  $L$  and  $\xi(t)$  which are large; otherwise, there should be corrections to FSS, which unless explicitly stated are ignored throughout this work.

Notice that using the critical form for  $\xi$ ,  $\xi(t) \sim t^{-\nu}$ , we can rewrite the scaling variable  $s(L,t)$  as

<sup>\*</sup>Permanent address: Departamento de Física e Matemática, Universidade Federal Rural de Pernambuco, 52171-900, Recife, Pernambuco, Brazil.

$$s(L,t)=[A(t)/L^{\rho/\nu}]^{-\nu/\rho}, \quad (2)$$

so that Eq. (1) may be rewritten as

$$A_L(t)=A(t)\mathcal{F}_A(s(L,t)), \quad (3)$$

where the relation between the scaling functions  $f_A$  and  $\mathcal{F}_A$  is given by

$$\mathcal{F}_A(s)=s^{\rho/\nu}f_A(s). \quad (4)$$

For  $A=\xi$ , Eq. (3) shows that  $\xi_L(t)/L$  is just a function of  $\xi(t)/L$  and vice versa, and this leads to the relation

$$A_L(t)=A(t)\mathcal{Q}_A(x(L,t)), \quad (5)$$

where  $x(L,t)\equiv\xi_L(t)/L$  is the ratio of the correlation length on a finite lattice to the lattice size, and  $\mathcal{Q}_A(x)$  is given by

$$\mathcal{Q}_A(x)=\mathcal{F}_A(f_\xi^{-1}(x)). \quad (6)$$

Using the same observation, it is trivial to obtain [7] another equivalent form,

$$A_{bL}(t)=A_L(t)\mathcal{G}_A(x(L,t)), \quad (7)$$

where  $b$  is a scaling factor and  $\mathcal{G}_A(x)$  is another scaling function.

It is evident that given  $f_A$  one can determine the other two scaling functions from Eqs. (4) and (6), and all the scaling functions,  $f_A$ ,  $\mathcal{F}_A$ ,  $\mathcal{Q}_A$ , and  $\mathcal{G}_A$  should be universal. It has also been argued [8] that a certain asymptotic form of  $f_A(s)$  can be expressed in terms of the critical exponent  $\delta$ ; by fitting this functional form one can extract an estimate for the critical exponent.

It is worth stressing that use of the scaling function  $\mathcal{Q}$  rather than  $\mathcal{F}$  would be more convenient in many cases, particularly because one does not need the bulk correlation length to define the former. Note that there is no explicit  $t$  dependence of the scaling variables, so that knowledge of the critical coupling is not required, and that  $x$  becomes independent of  $L$  at criticality. This  $L$  independent value of  $x$  at criticality,  $x_c$ , which characterizes a universality class for a given geometry [9], forms the upper bound of  $x$ . In other words, the scaling function  $\mathcal{Q}$  is defined only over  $0\leq x\leq x_c$ . *A priori*, the two limits of the scaling function  $\mathcal{Q}$  are known for a continuous phase transition:  $\lim_{x\rightarrow 0}\mathcal{Q}(x)\rightarrow 1$  and  $\lim_{x\rightarrow x_c}\mathcal{Q}\rightarrow 0$ , because  $A_L$  converges to its bulk value in the former case while  $A(t)$  diverges in the latter case with  $A_L(t)$  finite. In general, as we will show in this work, for  $A=\xi$ ,  $\chi$ , or  $g^{(4)}$ ,  $\mathcal{Q}_A(x)$  turns out to be a monotonically decreasing function of  $x$ .

It is important to realize that the knowledge of the scaling function  $\mathcal{Q}$  near  $x=0$  plays as relevant a role as that near  $x=x_c$  to the extraction of necessary information of the critical behavior in (deep) scaling region. It can be easily seen by noting that  $x(L,t)$  for a fixed temperature arbitrarily close to criticality can be made arbitrarily close to zero by simply choosing a value of  $L$  sufficiently large.

Equations (3) and (5) do not include any critical exponents, so that one might conjecture that their validity can be extended to non-power-law singularities. Although a general proof of this conjecture is missing, Lüscher [10] obtained an

explicit expression for the inverse correlation length (mass gap), that is consistent with Eq. (5), for the two-dimensional (2D)  $O(N)$  ( $N>2$ ) spin models, which exhibits an exponential critical singularity. Also, very extensive numerical verification [5] of Eq. (5) was given for  $\chi$  and  $\xi$  for the 2D  $O(N)$  models with  $N=2$  and 3.

In order to define a correlation length, we consider the Fourier transform of the (connected) two-point correlation function,

$$G(\mathbf{k})\equiv\sum_{\mathbf{x}}\exp(i\mathbf{k}\cdot\mathbf{x})\langle S_0\cdot S_{\mathbf{x}}\rangle_c, \quad (8)$$

where  $S_{\mathbf{x}}$  denotes the spin variable at site  $\mathbf{x}$ . When  $\mathbf{x}$  is sufficiently large,  $\langle S_0\cdot S_{\mathbf{x}}\rangle_c\sim e^{-|\mathbf{x}|/\xi_L}$  holds [11], so we will have

$$G(\mathbf{k})^{-1}=G(\mathbf{0})^{-1}[1+k^2\xi_L^2+O(k^4)]. \quad (9)$$

By choosing  $\mathbf{k}=(2\pi/L,0)$ , we obtain

$$\xi_L=\frac{1}{2\sin(\pi/L)}\sqrt{G(\mathbf{0})/G(\mathbf{k})-1}, \quad (10)$$

for values of  $L$  that are large enough that terms  $\sim k^4$  can be safely ignored.

The renormalized coupling constant  $g_L^{(4)}$  may be defined as [12]

$$g_L^{(4)}=3(L/\xi_L)^D U_L, \quad (11)$$

where  $D$  is the lattice dimensionality and the fourth order cumulant is given by  $U_L\equiv 1-\langle S^4\rangle/3\langle S^2\rangle^2$ , with  $S$  being the order parameter. The bulk  $g^{(4)}$  has a well defined scaling behavior [7],

$$g^{(4)}(t)\sim t^{D\nu-2\Delta+\gamma}. \quad (12)$$

$g^{(4)}$  describes the non-Gaussian character of the the model, i.e., only for a Gaussian model does  $g^{(4)}(t)$  vanish as  $t\rightarrow 0$  in the absence of certain multiplicative corrections to scaling, implying the violation of the hyperscaling relation  $D\nu-2\Delta+\gamma>0$ . For a system where the hyperscaling relation is satisfied (without certain multiplicative corrections to scaling, as in the four-dimensional Ising model), its bulk value in the scaling regime remains a constant that characterizes its universality class.

Employing the single cluster Monte Carlo algorithm [13], we simulated the 2D and 3D Ising models, on the square and simple cubic lattices, respectively, with fully periodic boundary conditions imposed. For each lattice at a given temperature, we generated up to 30 bins of data each of which is composed of 10 000 measurements. In order to reduce the correlation between data points, only configurations 3–7 Monte Carlo steps apart were considered. Our quoted errors, which are purely statistical in nature, are the standard deviation of the binned values. Aware of the bad performance of some random number generators in the context of the single cluster algorithm [14], we have double-checked our results by comparing data generated by two different implementations of the algorithm, each one using a different kind of random number generator. Most of the data were obtained with a linear congruential random number generator of the

TABLE I.  $A_L$  as a function of  $L$  at  $K=0.425$ .  $\xi_\infty(K=0.425)=15.7582\dots$  from Eq. (17). Note that our  $\xi_L$  converges to its bulk value for  $L \geq 80$ , within the small statistical errors, and that the value of  $x$  monotonically decreases with  $L$ .

$L$	$\xi_L$	$x$	$\chi_L$
16	9.83(3)	0.614(2)	102.4(2)
18	10.56(4)	0.587(2)	119.8(3)
20	11.18(5)	0.559(2)	137.0(6)
22	11.74(4)	0.534(2)	153.5(5)
25	12.44(5)	0.498(2)	177.1(7)
27	12.85(5)	0.476(2)	191.9(7)
30	13.37(6)	0.446(2)	212.7(6)
32	13.69(7)	0.428(2)	224.7(9)
34	13.92(6)	0.409(2)	235.2(9)
36	14.19(6)	0.394(2)	246.6(8)
40	14.54(6)	0.363(2)	264.9(6)
50	15.19(8)	0.304(2)	296.0(1.0)
60	15.40(6)	0.257(1)	312.5(1.0)
70	15.62(7)	0.223(1)	321.3(1.4)
80	15.71(8)	0.196(1)	326.6(1.3)
100	15.75(10)	0.157(1)	329.4(1.8)
110	15.77(10)	0.143(1)	331.0(1.5)
150	15.75(14)	0.105(1)	331.4(1.6)

form  $x_{i+1} = 69\,069x_i + 1 \pmod{2^{31}}$ . The other random number generator was a multiplicative, lagged Fibonacci generator of the form  $x_{i+1} = x_i - 4423x_{i-1393}$ , which showed a good performance in a single cluster simulational test of the Ising system [15]. We observed complete agreement between the two sets of data within our statistical errors. We therefore believe that to within the error bars quoted here our data are not biased due to any correlation among the random numbers. (We also tried the well known R250 routine but the data exhibited some systematic deviation and we did not consider them in our analysis.)

### III. RESULTS

#### A. 2D Ising model

We now investigate the finite size behavior for a variety of multiplicatively renormalizable physical quantities [10] defined on a finite lattice of linear size  $L$ , in particular, the susceptibility  $\chi$  and correlation length  $\xi$ . First, we choose a certain  $K$  and perform measurements of  $A_L(K)$  for various values of  $L$ . In Table I we present our data for  $K=0.425$ , with  $L$  varying from 16 to 150. The reason for starting from  $L=16$  is that near this  $L$  the systematic error in our definition of  $\xi_L$ , Eq. (10), is about  $\sim 10^{-2}$  which is comparable to our typical statistical errors. From these data in Table I one sees that  $\xi$  is indistinguishable from its bulk value for  $L \geq 80$ , to within very small statistical error. In terms of the scaling variables, this means that  $s \geq 5.076$  or  $x \leq 0.196$ . As we stressed earlier, this condition holds (in terms of the scaling variables) regardless of the temperature as long as it remains in the scaling regime. (This is indeed the fundamental statement of FSS.) We note that for  $\chi$  the thermodynamic condi-

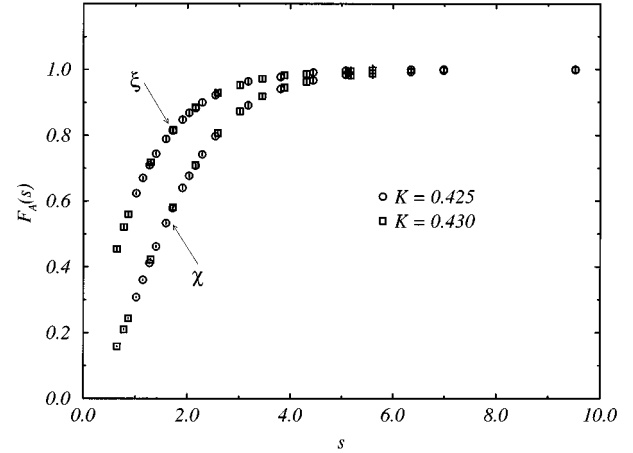


FIG. 1.  $\mathcal{F}_A(s)$  for the 2D Ising model. Each ‘‘curve’’ demonstrates the data collapse for two different values of  $K$ . Note that the lower curve converges to  $\mathcal{F}_A(s)=1$ , i.e., thermodynamic limit, more slowly than the upper curve.

tion holds for a slightly larger value of  $s$  (smaller  $x$ ) than that for  $\xi$ , namely,  $s \geq 6.346$ . Figure 1 shows the data collapse for  $\mathcal{F}_A(s)$ .

From the data in Table I, we can easily determine  $\mathcal{F}_A(s)$  and  $\mathcal{Q}_A(x)$ . In order to satisfy the asymptotic conditions, for the former one may try a polynomial function of either  $1/s$  or  $e^{-s}$ , while for the latter a polynomial of  $x$  or  $e^{-1/x}$  may be tried. That is,

$$\mathcal{F}_A(s) = 1 + b_1/s + b_2/s^2 + \dots, \quad (13)$$

$$\mathcal{Q}_A(x) = 1 + b_1x + b_2x^2 + \dots, \quad (14)$$

or

$$\mathcal{F}_A(s) = 1 + c_1e^{-s} + c_2e^{-2s} + \dots, \quad (15)$$

$$\mathcal{Q}_A(x) = 1 + c_1e^{-1/x} + c_2e^{-2/x} + \dots. \quad (16)$$

In general, it turns out that for the same number of fitting parameters the polynomial of the exponentials fits better than that of the simple scaling variables. This is especially true for the magnetic susceptibility and the four-point renormalized coupling constant. For instance, by considering terms up to the fourth order of the polynomial,  $\chi^2/N_{DF}$  (degree of freedom) = 3.3 and 0.3, respectively, for the  $\mathcal{Q}_\chi(x)$ , assuming the simple polynomial and that of the exponential. Considering up to the  $e^{-4/x}$  term, we obtain  $c_1 = -2.402, c_2 = -16.338, c_3 = 80.688$ , and  $c_4 = -134.6$  for  $\mathcal{Q}_\chi$  with  $\chi^2/N_{DF} = 0.31$ , while they are  $-0.768, -8.490, 31.032$ , and  $-89.203$ , respectively, for  $\mathcal{Q}_\xi$  with  $\chi^2/N_{DF} = 0.20$ .

*A priori*, the estimates are accurate only for  $x \leq \xi_{L_0}/L_0 \equiv x_0$ , with  $L_0$  denoting the smallest value of  $L$  for  $K=0.425$ ; for the estimate of the coefficients for  $x > x_0$ , one needs similar data for  $A_L$  at a larger  $K$ , which might modify the values of the coefficients. Nevertheless, with the information of the finite size scaling function  $\mathcal{Q}_A$ , it is now possible to extract accurate bulk data from the Monte Carlo data on a modestly *small* lattice provided a data point (at another

TABLE II. The extraction of the  $\xi$  and  $\chi$  for the 2D Ising model based on the computation of the  $Q_A(x)$ . The ‘‘ave.’’ for each  $K$  denotes the average over the extracted bulk values from the different values of  $L(x)$ .

$K$	$L$	$\xi_L$	$x$	$\chi_L$	$\xi$	$\chi$
0.430	20	13.00(7)	0.650	158.5(4)	23.16(17)	650.4(16.2)
	30	16.67(7)	0.556	274.5(4)	23.33(11)	653.2(5.4)
	40	18.97(8)	0.474	377.3(6)	23.20(9)	647.5(4.2)
	50	20.57(8)	0.411	461.1(8)	23.31(8)	650.2(3.8)
	60	21.57(8)	0.359	524.5(1.5)	23.30(7)	651.0(5.5)
	80	22.57(10)	0.282	597.0(2.2)	23.23(8)	649.7(6.3)
	100	22.89(11)	0.229	625.3(2.3)	23.15(9)	646.6(5.9)
	120	23.12(17)	0.193	638.2(5.0)	23.23(13)	647.2(12.4)
ave.					23.21(11)	649.5(2.2)
exact					23.22	
0.434	80	32.94(7)	0.412	1047.5(2.5)	37.34(7)	1478.6(11.9)
	160	36.77(9)	0.230	1426.5(9.0)	37.19(14)	1476.0(23.1)
ave.					37.27(11)	1477.3(1.8)
exact					37.21	
0.436	50	31.58(9)	0.632	761.7(1.4)	53.10(20)	2745.0(43.7)
	60	35.35(11)	0.589	977.4(2.1)	53.18(19)	2743.8(39.8)
	70	38.54(12)	0.551	1186(3)	53.41(18)	2759.0(37.7)
	80	41.23(13)	0.515	1389(3)	53.65(17)	2779.4(31.8)
	90	43.08(7)	0.479	1563(2)	53.01(8)	2724.8(17.5)
	100	45.04(13)	0.450	1746(2)	53.37(14)	2751.1(24.7)
	120	47.96(14)	0.400	2033(5)	53.69(13)	2776.8(22.4)
	160	50.55(20)	0.316	2384(7)	52.96(17)	2724.1(22.9)
ave.					53.30(28)	2750.6(20.8)
exact					53.16	
0.438	80	51.88(13)	0.649	1777(4)	91.97(31)	7209.7(142.4)
	160	76.31(34)	0.477	4259(13)	93.66(39)	7378.2(93.0)
ave.					92.82(1.20)	7294.0(119.1)
exact					92.86	

temperature) satisfies  $x < x_0$ . Our results for  $K=0.430, 0.434, 0.436$ , and  $0.438$  are summarized in Table II.

We notice that the bulk values thus extracted for a given  $K$  do not change with respect to  $L$ , indeed verifying this form of FSS for the model (see Fig. 2 also). We also note that the values of the bulk  $\xi$  thus extracted are in excellent agreement with the corresponding exact values given by the formula

$$1/\xi(K) = \ln(\coth K) - 2K, \tag{17}$$

within typically less than 0.5% of the statistical errors. As a test of our  $\chi$ , we fitted the data over the range from  $K=0.425$  to  $0.438$  to

$$\chi \sim t^{-\gamma}. \tag{18}$$

The best  $\chi^2$  fit gives  $K_c=0.440\ 70(5)$  and  $\gamma=1.755(9)$  ( $\gamma=1.752$  by fixing  $K_c$  to the exact critical point), being

extremely close to the exact values. Since all of our data used for the analysis were for  $t > 0.006$ , the quality of the result is surprisingly good.

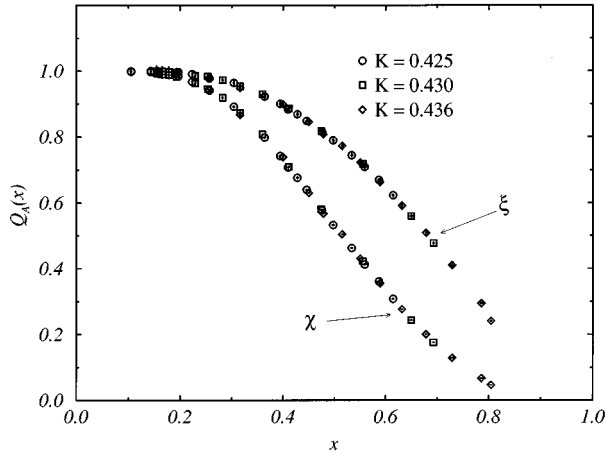
### B. The 3D Ising model

We begin with our Monte Carlo measurement at  $K=0.220$ , the results of which are summarized in Table III. We observe that the thermodynamic condition for  $\xi$  is almost satisfied for  $L/\xi_L \approx 60/10.89 \approx 5.5$ . Nevertheless, we also note that  $\chi$  and  $g^{(4)}$  increase, albeit very slowly, beyond this value. This is another indication that certain quantities converge to the thermodynamic value more slowly than the correlation length.

Assuming that  $A_L(K=0.220)$  reaches its bulk value for  $L=70$ , we obtain

$$c_1 \approx -0.418, \quad c_2 \approx -18.83, \quad c_3 \approx 99.38, \quad c_4 \approx -436.4, \tag{19}$$

$$c_1 \approx -0.607, \quad c_2 \approx -56.31, \quad c_3 \approx 416.75, \quad c_4 \approx -1399.9, \tag{20}$$

FIG. 2.  $\mathcal{Q}_A(x)$  for the 2D Ising model.

$$c_1 \approx -7.238, \quad c_2 \approx 21.42, \quad c_3 \approx -16.09, \quad c_4 \approx 3.67, \quad (21)$$

respectively, for  $\mathcal{Q}_\xi(x)$ ,  $\mathcal{Q}_\chi(x)$ , and  $\mathcal{Q}_{g^{(4)}}(x)$ , over the range  $0 \leq x \leq x_0 \approx 0.491$ .

Based on the knowledge of  $\mathcal{Q}_A(x)$ , we calculate the bulk values of the correlation length, magnetic susceptibility, and four-point renormalized coupling constant for various  $K$  up to  $K=0.2212$ . The largest value of  $L$  we simulated for the calculation is just 64. Obviously, the computation of the bulk value at a  $K$  larger than 0.2212 requires a larger value of  $L$  in order to keep the value of  $x$  smaller than  $x_0$ . One way to avoid the need for a larger  $L$  is to repeat the measurement of  $A_L$  at a slightly larger value of  $K$ , e.g.,  $K=0.2212$ ; this will extend the range of  $x$  over which  $\mathcal{Q}_A$  is accurately computed. In the region where  $\mathcal{Q}_A(x) \approx 0$ , however, one needs extremely precise measurements to reduce the errors in the estimates of the bulk values [16].

A summary of our results is shown in Table IV. We see that the four-point renormalized coupling constant remains unchanged, i.e.,  $g^{(4)} \approx 24.5$ , for  $K \geq 0.2206$ . Its slow variation for  $K < 0.2206$  may be due to the presence of corrections to scaling. Hence the hyperscaling relation is indeed satisfied, confirming the previous verification (within rather larger statistical errors though) based on the traditional Monte Carlo measurement [12,17]. We would like to stress, however, that it was not possible to measure  $g^{(4)}$  beyond  $K=0.2206$  in Ref. [12], even using  $L$  as large as  $L=90$ . The

TABLE III.  $A_L(K)$  at  $K=0.220$  for the 3D Ising model.

$L$	$\xi_L$	$x$	$\chi_L$	$g_L^{(4)}$
16	7.85(2)	0.491(1)	228.8(7)	9.52(5)
20	8.85(2)	0.443(1)	298.1(7)	11.43(5)
24	9.56(2)	0.398(1)	351.8(1.1)	13.44(7)
30	10.20(3)	0.340(1)	407.1(1.1)	16.5(1)
36	10.56(2)	0.293(1)	439.5(1.2)	19.2(2)
40	10.68(3)	0.267(1)	455.2(1.5)	21.4(3)
50	10.85(3)	0.217(1)	467.9(1.3)	23.5(5)
60	10.89(3)	0.182(1)	472.3(0.8)	24.2(5)
70	10.91(3)	0.156(1)	473.0(1.1)	24.7(5)

bulk  $\chi$  and  $\xi$  thus extracted are compared with those traditionally obtained, again yielding remarkable agreement (see Table IV). Figure 3 exhibits excellent data collapse for the finite size scaling function  $\mathcal{Q}_A(x)$  for  $A=\chi, \xi$ , and  $g^{(4)}$ .

In order to determine  $K_c$ ,  $\nu$ , and  $\gamma$  we fitted our bulk data over the range  $0.217 \leq K \leq 0.2212$  to the simple power-law singularity. We fixed the critical point in the fit, and then repeated the fit for several different fixed critical points. The results, shown in Fig. 4, indicate that the  $\chi^2$  values of the  $\xi$  and  $\chi$  data favor the range of  $K_c$  over  $0.221640 \leq K_c \leq 0.221670$ , being consistent with other recent results [18]. The empirical formulas we obtained from the best fit are as follows:

$$\xi = C_\xi (|K - K_c|/K_c)^{-\nu}, \quad C_\xi = 0.4710, \quad K_c = 0.221658, \quad \nu = 0.6418, \quad (22)$$

$$\chi = C_\chi (|K - K_c|/K_c)^{-\gamma}, \quad C_\chi = 1.0892, \quad K_c = 0.221646, \quad \gamma = 1.2388. \quad (23)$$

The value of  $\nu$  is larger by approximately 1.5% than those extracted by most other methods, while the value of  $\gamma$  agrees up to  $\sim 10^{-3}$ . The effect of including the term of the confluent correction to the scaling turns out to be minimal: the confluent correction term would usually be important when data with rather smaller bulk values of the correlation length are considered. Given the modest size lattices used and the distance from the critical points at which the actual measurements were made ( $t > 0.002$ ), we find the agreement with high resolution studies to be extremely gratifying.

#### IV. DISCUSSION AND CONCLUSION

In this paper we computed an alternative finite size scaling function, defined in terms of the scaling variable  $\xi_L/L$ , for the 2D and 3D Ising models. This type of finite size scaling function has the advantage of being defined even for small values of  $L$ , without any prior information on the critical behavior of the system. Thus, our procedure can test FSS itself by means of data collapse to the extent that  $\xi_L$  can be accurately measured; in this manner, we observed that the effect of the violation of FSS is negligibly small at least for  $L \geq 16$  for the two- and three-dimensional Ising models. We illustrated how the function can be used for the extraction of correct bulk values near criticality, and that it can be used in extracting accurate critical parameters provided the values of the correlation length are sufficiently large, i.e., approximately  $\xi \geq 5$ .

One might wonder if this technique requires an accurate bulk value of a physical quantity  $A$  at least at one point of temperature. As far as the extraction of critical parameters is concerned, however, this is not necessarily the case. To see this, imagine that we start with a fake ‘‘bulk value’’  $A'(t)$  instead of the correct one  $A(t)$ . The scaling function  $\mathcal{Q}'$  defined in terms of the fake bulk value,  $\mathcal{Q}'_A \equiv A_L(t)/A'(t) = [A(t)/A'(t)]\mathcal{Q}_A$ , simply rescales the correct scaling function by a constant; accordingly, every bulk value calculated at any other temperature using  $\mathcal{Q}'_A$  rescales the correct one with an overall factor  $A'(t)/A(t)$ . This over-

TABLE IV. The extraction of the  $\xi$  and  $\chi$  for the 3D Ising model. The uncertainties in the values of  $x$  are not considered for our error estimates. Traditional Monte Carlo measurements are in rows labeled MC.

$K$	$L$	$\xi_L$	$x$	$\chi_L$	$g_L^{(4)}$	$\xi$	$\chi$	$g^{(4)}$
0.217	16	5.30(1)	0.331	114.6(2)	17.7(1)	5.62(1)	130.8(2)	25.5(1)
	20	5.49(1)	0.275	124.5(4)	21.2(2)	5.63(1)	130.7(4)	25.4(1)
	28	5.60(1)	0.200	130.1(1)	24.6(2)	5.62(1)	131.0(3)	25.8(2)
ave.						5.62(1)	130.9(4)	25.6(3)
0.219	20	7.33(2)	0.366	212.4(7)	15.3(2)	8.04(2)	262.2(9)	24.9(6)
	30	7.88(3)	0.263	251.5(1.5)	21.8(5)	8.03(4)	260.9(1.6)	25.7(6)
	ave.					8.03(4)	261.6(2.1)	25.3(1.1)
MC	50					8.1	263	26
0.2203	30	11.16(8)	0.372	481.4(5.3)	14.8(1)	12.31(9)	602.7(6.6)	24.6(2)
	40	12.00(3)	0.300	561.4(2.6)	19.3(2)	12.44(3)	608.2(3.1)	25.1(4)
	ave.					12.38(15)	605.5(8.8)	24.9(7)
0.2206	24	11.20(5)	0.467	467.4(2.8)	10.3(2)	14.55(6)	834.2(5.0)	24.5(2)
	30	12.49(10)	0.416	589.2(2.7)	12.5(2)	14.66(12)	844.4(3.9)	24.6(2)
	36	13.28(5)	0.369	673.8(3.6)	14.9(3)	14.60(5)	836.8(4.5)	24.5(3)
	40	13.70(4)	0.343	718.0(3.4)	16.3(2)	14.66(4)	838.4(5.0)	24.4(3)
	50	14.28(5)	0.286	789.7(4.0)	19.4(3)	14.68(5)	839.7(5.3)	24.2(4)
	60	14.38(3)	0.240	809.9(1.6)	22.4(3)	14.53(5)	827.6(2.6)	25.1(4)
ave.						14.61(6)	837.0(5.7)	24.6(3)
MC	75					14.5	828	24
0.2210	40	16.75(3)	0.419	1045.0(3.1)	12.3(1)	19.73(5)	1511.5(5.5)	24.5(2)
	50	18.15(4)	0.363	1245.7(4.1)	15.1(2)	19.82(8)	1524.3(7.1)	24.4(4)
	ave.					19.77(12)	1518.(15.)	24.5(3)
0.2212	56	21.98(7)	0.393	1796.0(10.5)	13.6(1)	24.89(10)	2382(14)	24.5(2)
	64	22.89(7)	0.358	1971.6(10.4)	15.5(2)	24.86(10)	2382(13)	24.4(4)
	ave.					24.88(12)	2382(14)	24.5(3)

all factor is unimportant for the extraction of the critical behavior. One can thus repeat our analysis arbitrarily close to a critical point, where the effect of corrections to scaling can be arbitrarily small. We anticipate that such an analysis will

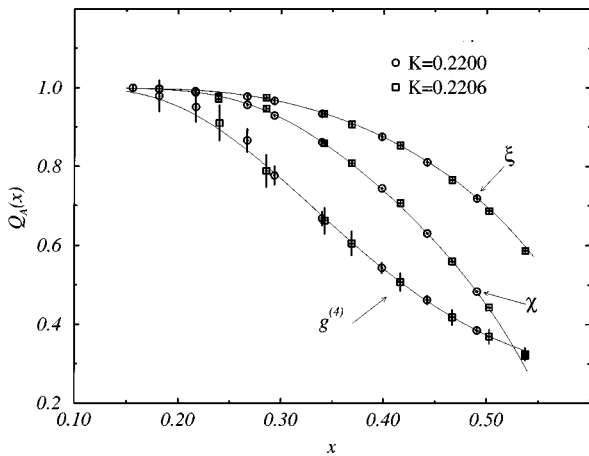


FIG. 3.  $Q_A(x)$  for the 3D Ising model. The solid lines are from the best fits.

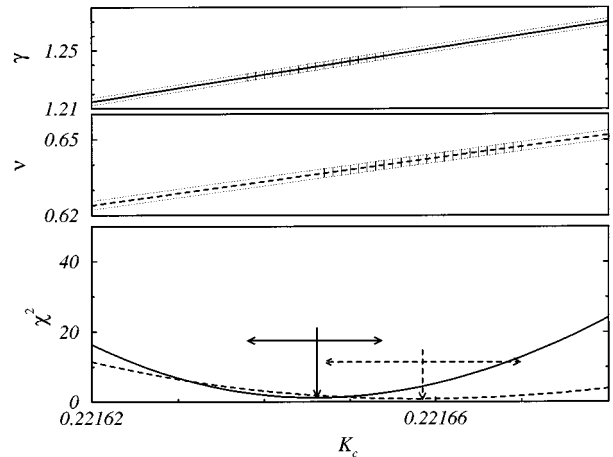


FIG. 4. The resulting estimates for the critical exponents  $\gamma$  and  $\nu$  for different choices of the critical coupling  $K_c$ . The corresponding errors are given by the light dotted lines. Solid (dashed) curves correspond to  $\chi$  ( $\xi$ ) data. The shadings show acceptable values for the critical parameters. On the bottom:  $\chi^2$  plotted against  $K_c$ ; vertical arrows locate our best estimates for  $K_c$ , whereas the horizontal ones indicate the error bars.

yield extremely accurate estimates of the critical parameters, and our study of the 3D Ising model along this line is under way. (This observation is also important for some calculations of lattice gauge theory. For example, in full lattice QCD, the computation of the ratio of the mass of various lattice hadrons is of primary concern, and for this purpose the overall factor is simply unimportant.)

We would like to stress again that the technique we have illustrated is extremely general; it holds regardless of the functional form of the critical singularity, and irrespective of the quantity as long as it is multiplicatively renormalizable. We demonstrated this point taking the example of the four-point renormalized coupling constant, whose bulk value is notoriously difficult to measure through traditional Monte

Carlo simulation [17,19]. Although our current estimate of the critical parameters cannot compete with the highest resolution Monte Carlo studies, our estimates are really surprisingly good considering how far from the critical point the data are taken. Thus, although the determination of a finite lattice correlation function is needed, this method offers a simple alternative to standard finite size scaling methods.

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