Monte Carlo renormalization-group calculations of critical behavior in the simple-cubic Ising model

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The Monte Carlo renormalization group is applied to the three-dimensional Ising model on simple cubic lattices with 8^3, 16^3, 32^3, and 64^3 sites. The comparison of block-spin correlation functions from the largest lattices yields the nearest-neighbor critical coupling $K_1^c = 0.221\,654(6)$. After allowing for (i) interpolation to this best estimate for K_1^c, (ii) an apparent finite-size effect in the renormalization-group transformation due to the measurement of correlation functions of too few (seven) operators, and (iii) the extrapolation for the effect of a slow transient towards the fixed point, the values $\nu = 0.629(4)$ and $\eta = 0.031(5)$ are obtained for the thermal and magnetic exponents. The correction-to-scaling exponent ω is estimated to be around 1; to obtain an accuracy competitive with other methods requires measurements with more than seven operators. We briefly review the problem of redundant operators and indicate the future prospects for this kind of calculation.

I. INTRODUCTION

The Monte Carlo (MC) approach, simulating directly a physical problem of interest, can be implemented to produce excellent results for finite systems. Near a continuous phase transition, or critical point, however, where the correlation length ξ diverges in an ideal infinite system, the behavior is dominated by finite-size effects whenever the ideal ξ would be greater than the linear dimension of the system. Therefore, in the finite systems which we simulate by MC methods the various singularities of interest at a critical point are always rounded off. This prevents us, in this direct approach, from taking much useful data very close to the critical point, and leaves us with the problem of extrapolating from results at various finite sample sizes to the infinite system.

A number of approaches can be adopted to tackle this problem; the one which we apply here is the MC renormalization group (MCRG).[1] This has been applied successfully to a number of problems, mainly in two dimensions. In this paper we report results for the critical behavior in the three-dimensional (3D) Ising model. This model is of interest in this context for several reasons. The Ising model is the prototype spin system whose random variables take the value ± 1 on each site of a regular (in our case, simple cubic) lattice. It is the simplest representation of the universality class which includes uniaxial magnets, fluids, binary alloys, etc. Although an exact solution is not known, long series expansions can be developed which yield extremely accurate values for the critical coupling K^c, or temperature T_c, and for critical exponents. When the effects of corrections to the leading singular behavior are included in the analysis, the results from series expansions[2] seem to be in good agreement with independent field-theory calculations[3] and with experiment.[4] These results set a very demanding benchmark against which to test the MCRG in this model. Of particular significance in this connection is the existence of a "slow transient" correction to the leading scaling behavior in this model,[5] which must be identified and isolated from the leading critical behavior; this aspect provides a severe challenge to the MCRG method.

The MCRG method has been recently reviewed (see, e.g., Swendsen[1]). Our starting point is the Hamiltonian with a nearest-neighbor coupling K_1,

$$\mathscr{H} = K_1 S_1, \quad S_1 = \sum_{\langle ij \rangle} \sigma_i \sigma_j \ , \tag{1}$$

where $\sigma_i = \pm 1$ is the spin variable on site i and the sum is over nearest-neighbor pairs $\langle ij \rangle$ on the simple cubic lattice. Correlation functions involving any operator $B(\sigma)$ are defined in the usual way by the trace over the equilibrium distribution

$$\langle B \rangle = \mathrm{Tr}_{\sigma}[B(\sigma)\exp\mathscr{H}(\sigma)] / \mathrm{Tr}_{\sigma}[\exp\mathscr{H}(\sigma)] \ . \tag{2}$$

For any given configuration $\{\sigma\}$ $(=\{\sigma^{(0)}\})$ of these spins generated by a MC method, we define a sequence of

block-spin configurations $\{\sigma^{(n)}\}$ on lattices whose spacing is scaled by successive factors, in our case of 2, 2^2, etc. (corresponding to $n=1$, 2, etc.). For the calculations reported here we have adopted the majority rule: The block spin $\sigma^{(1)}$ takes the values ± 1 according to the sign of the total spin of the 2^3 $\sigma^{(0)}$'s which are being blocked; if this total spin is 0, a value of ± 1 is assigned to $\sigma^{(1)}$ by using a pseudorandom logical variable. Thus, from an ensemble of configurations of the original spins $\{\sigma^{(0)}\}$ on a lattice of N sites, we generate, by n successive applications of this rule to blocks of 2^3 spins, an ensemble of configurations of the block spins $\{\sigma^{(n)}\}$ for each $n=1$, 2, etc. on lattices of $N/2^3$, $N/2^6$, etc. sites. Estimates for any correlation function of the $\{\sigma^{(n)}\}$ ($n=0$, 1, 2, . . .) can be made from this ensemble.

If the ensemble of original configurations of $\{\sigma^{(0)}\}$ follows the equilibrium distribution of (1), the block-spin configurations of $\{\sigma^{(n)}\}$ for a given blocking level n will be distributed according to a renormalized Hamiltonian

$$\mathcal{H}^{(n)}=\sum_{\alpha} K_{\alpha}^{(n)} S_{\alpha}^{(n)} , \tag{3}$$

where the sum is over nearest-neighbor, second-neighbor, etc. interactions (labeled by α) for the block spins $\{\sigma^{(n)}\}$. The renormalization-group (RG) transformation implicitly specifies $K_{\alpha}^{(n+1)}$ as functions of $K_{\beta}^{(n)}$, with fixed points of this transformation determining the critical surface, critical exponents, etc. by the standard theory.[5] Characteristic RG trajectories are shown schematically in Fig. 1. In the approach we follow here, only K_1 ($\equiv K_1^{(0)}$) is required explicitly; the critical value K_1^c and critical exponents are determined as follows.

To determine K_1^c, we perform independent MC simulations at some fixed K_1 value on lattices of size N and $N/2^{3m}$, $m=1,2,\ldots$. The coupling K_1 is estimated to have its critical value when

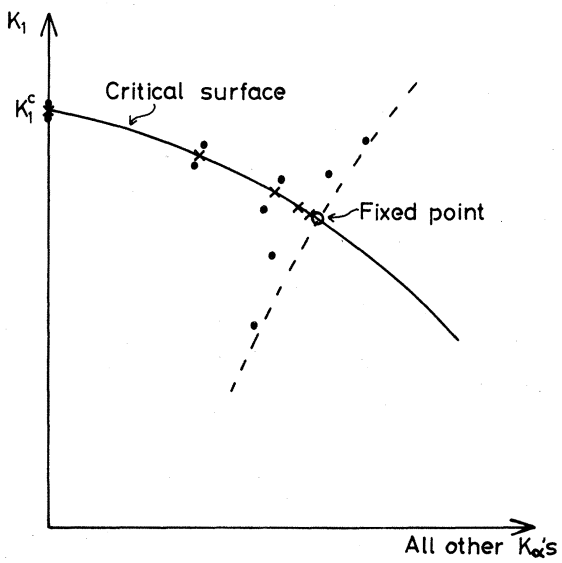

FIG. 1. Schematic diagram for RG flows in the many-dimensional space of coupling constants, indicating the transient into the fixed point starting from the critical value K_1^c, and the instability of the fixed point to perturbations out of the critical surface.

$$\langle S_{\alpha}^{(n)}\rangle_L=\langle S_{\alpha}^{(n-m)}\rangle_S , \tag{4}$$

where L and S denote the large and small lattices, respectively; since the effective lattice sizes on the left- and right-hand sides of Eq. (4) are the same, unknown finite-size effects should be systematically canceled. The most sensitive determination is obtained by choosing n as large as possible to amplify any contribution from the relevant perturbation $K_1-K_1^c$ and to deamplify irrelevant perturbation from the fixed-point Hamiltonian as indicated in Fig. 1. Noting that

$$\frac{\partial\langle S_{\alpha}^{(n)}\rangle}{\partial K_1}=\langle S_{\alpha}^{(n)} S_1^{(0)}\rangle-\langle S_{\alpha}^{(n)}\rangle\langle S_1^{(0)}\rangle , \tag{5}$$

we can solve the set of linear equations

$$\langle S_{\alpha}^{(n)}\rangle_L-\langle S_{\alpha}^{(n-m)}\rangle_S=\left[\frac{\partial\langle S_{\alpha}^{(n)}\rangle_L}{\partial K_1}-\frac{\partial\langle S_{\alpha}^{(n-m)}\rangle_S}{\partial K_1}\right]\delta K_1 \tag{6}$$

to estimate the deviation from criticality, $\delta K_1 \simeq K_1-K_1^c$, using the appropriate correlation functions measured from the MC ensembles for the large and small lattices.

The stability matrix $T_{\alpha\beta}$ of the RG transformation is defined by

$$T_{\alpha\beta}=\frac{\partial K_{\alpha}^{(n+1)}}{\partial K_{\beta}^{(n)}} . \tag{7}$$

Critical exponents y_a are obtained from the eigenvalues λ_a of the stability matrix $T_{\alpha\beta}^*$ (evaluated at the fixed-point Hamiltonian) according to

$$\lambda_a=2^{y_a} . \tag{8}$$

By performing simulations at K_1^c, we obtain estimates for $T_{\alpha\beta}^*$ by solving the linear equations

$$\frac{\partial\langle S_{\gamma}^{(n+1)}\rangle}{\partial K_{\beta}^{(n)}}=\sum_{\alpha}\frac{\partial K_{\alpha}^{(n+1)}}{\partial K_{\beta}^{(n)}}\frac{\partial\langle S_{\gamma}^{(n+1)}\rangle}{\partial K_{\alpha}^{(n+1)}} , \tag{9}$$

using estimates as in Eq. (5) from the MC ensemble. In principle, the best estimate for $T_{\alpha\beta}^*$ is obtained by using Eq. (9) for the largest value of RG blocking n on the largest available lattice, to eliminate as much as possible of the transient effect towards the fixed point; a detailed discussion of various systematic effects is given in Sec. IV.

This paper is organized as follows. Section II summarizes the computational aspects of the calculation. In Secs. III and IV we give the data and the analysis thereof for the critical coupling and exponents, respectively. We conclude in Sec. V with a discussion, making particular reference to various ways of improving upon our results with presently available computing resources.

II. COMPUTATIONAL ASPECTS

We have implemented the above equations in three independent programs: (i) for a serial machine, (ii) vectorized optimally for the array processor model no. AP190-L from Floating Point Systems Inc. (FPS), and (iii) in distributed array processor- (DAP-) FORTRAN for the International Computers Limited (ICL) distributed array proces-

sor. Where the parameters are the same we obtain entirely compatible results. We have taken data on 8^3, 16^3, and 32^3, and on the DAP alone, 64^3 lattices; the data presented here are those obtained from the DAP computer. The 64×64 array size and the logical software facility on the DAP are advantageous for this particular problem;[6] compact and efficient routines can be written in DAP-FORTRAN both for the MC updating and the RG blocking.

In the updating, spin flips which do not increase the energy are always accepted, and spin flips which cost energy $\Delta\mathscr{H}$ (>0) are accepted with probability $\exp(-\Delta\mathscr{H})$. In order to ensure convergence to equilibrium one should not attempt to update simultaneously and independently spins which interact with one another in $\mathscr{H}$. A sweep of the lattice is achieved with complete efficiency by updating all the spins on even sites, taking pairs of adjacent 64×64 bit planes at a time, and then all the spins on the odd sites for the planes. For the lattices smaller than 64^3, multiple independent simulations are run simultaneously to increase statistics.

All data were taken using a tested Numerical Algorithms Group (NAG) pseudo-random-number generating routine,[7] with an additional random shuffle amongst the 4096 parallel processors in the DAP array. With this extra precaution, the machine makes approximately 2.7×10^6 update attempts per second. We further checked this random-number generator in a two-dimensional program, which revealed no discrepancies with the exact results.[7] [We have subsequently run the 3D problem at 6×10^6 update attempts per second using a shift-register generator[7] assembler routine written by K. Smith (DAP Support Unit, Queen Mary College). A special Ising-model assembler routine written by D. M. Scott (University of Edinburgh), operates at 9.5×10^6 update attempts per second and further improvements are expected.]

In the RG blocking the choice of origin at each blocking level is systematically permuted among the eight possibilities. This is important particularly at the higher blocking levels, where it substantially improves the quality of the statistics.[8] We chose to block one configuration in four, thereby reducing the speed to approximately 1.2×10^6 update attempts per second. Even with the permutation of the origin for the block spins, one might expect that this is too frequent because of the long-time correlation in large lattices at criticality. However, there is preliminary indication that the correlation functions which are used for calculating critical exponents do not suffer the same critical slowing down because of large cancellations of statistical errors. The data we present comes from 32, 16, 4, and 2×10^6 sweeps on lattices of 8^3, 16^3, 32^3, and 64^3 spins, respectively, at each of three values of the nearest-neighbor coupling K_1(0.221 61, 0.221 66, 0.221 69; on the 64^3 lattice at the last value, in fact, only 1×10^6 sweeps were done). The error bars given in parentheses in all "raw" data tables in Sec. IV are the standard deviations in the mean obtained from eight bins of successive configurations, each bin involving one-eighth of the total relevant data. Thus, for the 64^3 lattice we are presuming that independent configurations are obtained typically at least every 2.5×10^5 sweeps; on the basis of our data this is not an overestimate of the long-time correlations, and indeed in the final estimate for the critical coupling a 50% increase in error bars on data from the 64^3 simulation has been made on the basis of χ^2 confidence levels (see Sec. IV A). We note that this number of sweeps is typical of the total data at a single K_1 value taken in some previous studies on large lattices.[9]

Approximately 15 h of calculation were done to equilibrate the 64^3 lattice at $K_1=0.221\,69$. A subsequent 5 h was used to change this configuration to one at $K_1=0.221\,61$, and 5 h more was needed to equilibrate for the final value, $K_1=0.221\,66$.

III. CRITICAL COUPLING K_1^c

The first set of runs was made at $K_1=0.221\,69$, favored from previous series expansions (see, e.g., D. S. Gaunt, Ref. 2 and references therein), and the second at $K_1=0.221\,61$. From these runs we estimated a new critical value $K_1=0.221\,66$, and a third set of data was taken at this value. In Table I we show the estimate for the deviations $\delta K_1=K_1-K_1^c$ obtained from the various lattice sizes at various blocking levels using Eqs. (5) and (6) for the nearest-neighbor spin operator S_1 (the mean energy). Error bars in parentheses are the standard deviation in the mean from eight successive data bins as discussed in Sec. II. In the final column we show the corresponding best estimates for K_1^c by averaging the (statistically independent) results from the three different K_1 values.

In interpreting the results in Table I, we must recall that Eq. (6) estimates the deviation from criticality on the assumption that $K_1-K_1^c$ is the only difference between the effective Hamiltonians for the two systems which are being compared. This is true only after a number of RG blockings sufficiently large that the transient within the critical surface towards the fixed point is negligible compared with the statistical error (see Fig. 1). The discrepancies among the various numbers in the final column of Table I reflect the transient behavior towards the fixed point. Note that these discrepancies are not even monotonic; estimates for K_1^c can decrease and then increase as the RG blocking level is increased. In principle, the best estimates for K_1^c come from the comparisons among the largest lattices at the highest blocking levels; we record the values 0.221 652(7), 0.221 656(4), and 0.221 651(7) obtained from comparisons between 64^3, 32^3, and 16^3 lattices. While data involving the 8^3 lattice confirm underlying trends, it does not appear possible to use it to enhance the quality and consistency of data from the larger lattices, at least in a simple extrapolation with a single slow transient.

The three results quoted above are from a comparison of block correlation functions on lattices of effectively 2^3 spins. Within the MCRG formalism, one may also query the validity of blocking to this level since the effective Hamiltonian, although expected to be technically short ranged, may have significant couplings (e.g., $\langle 200\rangle$), which cannot be incorporated on a 2^3 lattice. To check this point we note the value 0.221 650(6) from comparing the 64^3 and 32^3 data each blocked to 4^3 lattice sites; in

TABLE I. Estimates for $(K_1-K_1^c)\times 10^6$ using Eqs. (5) and (6) at three K_1 values, comparing various large (L) and small (S) lattices at various RG blocking levels. For this and all subsequent tables, statistical errors on the least significant figures are shown in parentheses. The final column gives the corresponding estimates (with errors) for K_1^c from the weighted average of the three runs.

L	S	RG	$K_1=0.221\,61$ Change	0.221 66 Change	0.221 69 Change	Mean
64	32	1	−528(11)	−423(10)	−365(9)	0.222 086(5)
64	32	2	2(8)	57(7)	81(7)	0.221 606(4)
64	32	3	−32(9)	28(8)	54(8)	0.221 636(4)
64	32	4	−50(12)	16(10)	42(11)	0.221 650(6)
64	32	5	−58(13)	17(10)	38(15)	0.221 652(7)
64	16	1	−144(5)	−79(6)	−43(6)	0.221 744(3)
64	16	2	−12(4)	43(7)	70(7)	0.221 621(3)
64	16	3	−38(6)	21(8)	49(9)	0.221 644(4)
64	16	4	−52(6)	14(9)	39(12)	0.221 656(4)
64	8	1	−53(4)	6(6)	35(6)	0.221 659(2)
64	8	2	−20(5)	40(7)	66(8)	0.221 626(3)
64	8	3	−40(6)	28(8)	52(11)	0.221 643(4)
32	16	1	−556(11)	−492(6)	−447(6)	0.222 147(3)
32	16	2	45(12)	87(6)	120(7)	0.221 571(4)
32	16	3	−5(15)	36(7)	69(9)	0.221 622(5)
32	16	4	−34(21)	5(10)	44(14)	0.221 651(7)
32	8	1	−97(8)	−42(4)	−11(3)	0.221 702(2)
32	8	2	43(10)	92(4)	122(4)	0.221 568(2)
32	8	3	1(14)	51(6)	84(6)	0.221 607(4)
16	8	1	−519(7)	−435(5)	−420(11)	0.222 107(3)
16	8	2	185(8)	263(7)	282(16)	0.221 409(5)
16	8	3	103(11)	191(9)	204(21)	0.221 484(6)

practice, therefore, this appears not to be a problem given the range of the statistical errors.

On the basis of the consistency of all of these results within statistical errors we believe now that there is no compelling evidence for attempting to extrapolate them to an infinite system.[10] The weighted mean of the three values quoted together above is 0.221 654. If all three results were statistically independent, the standard deviation in this mean would be 3 in the last significant figure. They are not independent, however, since each lattice size appears twice in the three comparisons. Furthermore, one may also ask about the χ^2 confidence levels of the averaging of the three data runs to obtain the numbers we use from the fourth column in Table I; they are 0.3, 0.8, and 0.3, respectively. The small confidence levels involve the 64^3 data. If we increase the error bars on the $64^3/32^3$ and $64^3/16^3$ comparisons by 50% to obtain confidence levels of 0.6, the weighted mean is unchanged at 0.221 654 and the standard deviation would drift up to 4. In order to accommodate both the nonindependence of the three comparisons used, and to enhance confidence levels, we give as our present best estimate

$$K_1=0.221\,654(6)\ , \tag{10}$$

where the error is intended to represent one standard deviation in this mean. It must be stressed that this estimate is based on the presumption, supported by the data from the larger lattices, that no extrapolation to the infinite system is required which is significant in comparison with the statistical error bars.

The result (10) is in excellent agreement with recent series-expansion estimates which allow for the existence of corrections to scaling from the slow transient: 0.221 655(10) (Ref. 11), 0.221 66(1) (Ref. 12), and 0.221 655(5) (Ref. 13).

As in Ref. 10, preliminary results from the MC Processor (MCP) at Santa Barbara have already been presented at the Les Houches workshop.[14] That study differs from the present in several features: (i) much higher statistics are obtained, including preliminary results using a 128^3 lattice, (ii) screw periodic boundary conditions result from the mapping of the lattice on to a cyclic linear data chain, and (iii) a full block-spin MCRG analysis is not carried out; instead finite-size-scaling techniques are used to estimate K_1^c. The resulting estimate $K_1^c=0.221\,650(5)$ is also in excellent agreement with the result (10). We note that the implementation of the block-spin analysis [Eqs. (5) and (6)] appears, at least for this problem, to offset considerably the advantage in statistics and lattice size generated by the MCP. In particular we note that the "crossing" estimate for K_1^c in Ref. 14 derived from the 32^3 lattice is almost an order of magnitude further from the final best estimate than is the value 0.221 651(7) obtained from com-

paring the 32^3 and 16^3 lattices in Table I.

IV. CRITICAL EXPONENTS

In this section we present the results for critical exponents obtained from the eigenvalues of the stability matrix $T_{\alpha\beta}$ as discussed in Eqs. (7)—(9). Since the fixed-point Hamiltonian is even in the spins σ, the thermal and magnetic exponents are obtained separately by considering correlation functions of operators S_γ which are even and odd, respectively, in the spins σ. The leading exponents are discussed in Secs. IV A and B and the subleading exponent in Sec. IV C.

A. Exponent ν

From the standard theory (see, e.g., Refs. 1 and 5), the even operators should have a single relevant (greater than 1) eigenvalue, with $y_1 \equiv 1/\nu$ (correlation length $\xi \propto |K_1 - K_1^c|^{-\nu}$). We allow for up to seven coupling constants by measuring the appropriate correlation functions required in Eq. (9) for the following seven operators.

(a) S_1, $\langle 100 \rangle$ neighbor coupling as in Eq. (1).
(b) S_2, $\langle 110 \rangle$ neighbor coupling [summed over the lattice as in Eq. (1)].
(c) S_3, $\langle 111 \rangle$ neighbor coupling.
(d) S_4, four-spin product, in (100) planes.
(e) S_5, four-spin product, in (110) planes.
(f) S_6, four-spin product, tetrahedral vertices in each cube.
(g) S_7, $\langle 200 \rangle$ neighbor coupling.

We can follow systematically the effect of these couplings by successively diagonalizing the 1×1, 2×2, ..., 7×7 matrix $T_{\alpha\beta}$. The results obtained for the leading thermal exponent $1/\nu$ from the run at $K_1 = 0.221\,66$ are shown in Table II with statistical errors (estimated from eight data bins as described in Sec. II) for the various lattice sizes at various blocking levels [$n = 0, \ldots, 4$ in Eq. (9)]. For the last blocking level, the $\langle 200 \rangle$ operator S_7 is discarded as it cannot be accommodated on the 2^3 blocked lattice.

Reading down the columns of Table II it is clear that there are strong transient effects as the blocking level n increases. In general, one must also expect that there will be finite-size effects in the RG transformation itself, and this appears as a variation as one reads horizontally across the table. As a benchmark one may note the value $1/\nu = 1.5922(20)$ obtained from the 64^3 data for $n = 3$ (i.e., comparing 8^3 and 4^3 block lattices); this corresponds to $\nu \simeq 0.628$ with a statistical error of less than 1 in the third significant figure. However, it is clear that the raw data does not support any "plateau" of similar values of neighboring lattice sizes and blocking levels, in contrast to the two-dimensional results (see Swendsen in Ref. 1). Therefore, it is very encouraging that the totality of

TABLE II. Estimates for $1/\nu$ from the run at $K_1 = 0.221\,66$, using Eq. (9). The sets of seven values in a column (six for the 2^3 block lattice) are the largest exponents obtained by diagonalizing 1×1, 2×2, ..., 7×7 subblocks of the stability matrix $T_{\alpha\beta}$. The successive sets in a column are for increasing blocking levels n in Eq. (9).

64^3	32^3	16^3	8^3
1.3663(7)	1.3648(5)	1.3655(3)	1.3758(3)
1.4264(7)	1.4288(7)	1.4371(2)	1.4598(3)
1.4271(6)	1.4293(8)	1.4376(3)	1.4610(3)
1.4269(6)	1.4290(8)	1.4368(3)	1.4552(2)
1.4263(6)	1.4279(7)	1.4342(4)	1.4455(3)
1.4260(7)	1.4272(8)	1.4330(4)	1.4432(3)
1.4252(7)	1.4258(8)	1.4303(4)	1.4372(4)
1.4937(9)	1.4941(7)	1.5137(4)	1.5922(3)
1.5244(7)	1.5327(8)	1.5656(6)	1.6867(3)
1.5246(8)	1.5326(9)	1.5662(6)	1.6956(3)
1.5240(8)	1.5308(9)	1.5556(6)	1.6695(3)
1.5225(8)	1.5269(9)	1.5420(8)	1.6548(3)
1.5220(8)	1.5261(9)	1.5399(8)	1.6525(3)
1.5189(9)	1.5218(9)	1.5338(8)	
1.5449(13)	1.5643(12)	1.6585(7)	
1.5768(10)	1.6099(11)	1.7460(5)	
1.5765(10)	1.6103(12)	1.7545(5)	
1.5745(9)	1.5987(12)	1.7249(7)	
1.5705(8)	1.5848(11)	1.7079(8)	
1.5699(8)	1.5825(12)	1.7051(8)	
1.5651(8)	1.5760(14)		
1.5851(31)	1.6866(30)		
1.6285(29)	1.7728(30)		
1.6285(30)	1.7810(31)		
1.6163(28)	1.7505(28)		
1.6007(25)	1.7322(27)		
1.5983(24)	1.7293(27)		
1.5922(20)			
1.6965(92)			
1.7803(87)			
1.7881(87)			
1.7565(80)			
1.7386(80)			
1.7359(79)			

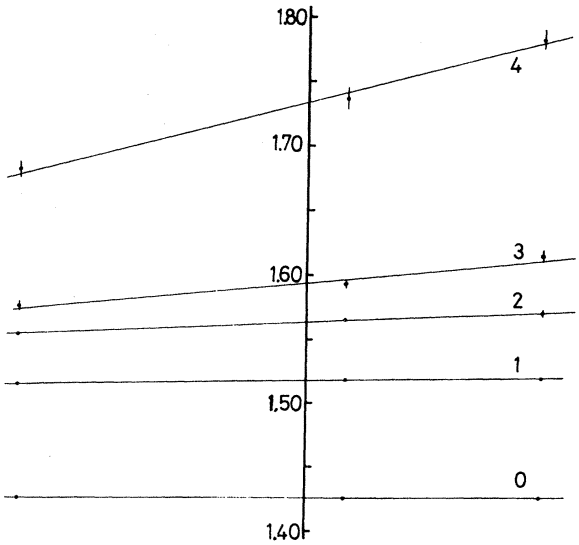

FIG. 2. Linear interpolation from the estimates of $1/\nu$ at $K_1 = 0.221\,61$, $0.221\,66$, and $0.221\,69$. The values plotted are from the 64^3 data at blocking levels $n = 0, 1, \ldots, 4$ with the maximum-size stability matrix $T_{\alpha\beta}$. The vertical line is the best estimate $K_1 = 0.221\,654$.

TABLE III. Interpolated estimates for $1/\nu$ at $K_1=0.221\,654$, from diagonalizing the maximum size $T_{\alpha\beta}$, for various lattice sizes at various blocking levels n. The final three lower columns are the result of differencing adjacent columns of this table. Reading diagonally down yields the estimates [column (c)] for the corrections to the 64^3 data, and the accumulated corrections [column (b)]. Column (a) shows the resulting best estimates for $1/\nu$ at blocking levels $n=0, \ldots, 4$.

n	(a) "∞^3"	64^3	32^3	16^3	8^3
0	1.4251(5)	1.4251(5)	1.4268(4)	1.4299(3)	1.4371(2)
1	1.5156(12)	1.5173(6)	1.5218(4)	1.5323(4)	1.6520(2)
2	1.5576(19)	1.5633(7)	1.5748(7)	1.7025(4)	
3	1.5739(31)	1.5916(16)	1.7252(13)		
4	1.5785(93)	1.7342(40)			
	(b)	(c)	32^3-64^3	16^3-32^3	8^3-16^3
0	0.0		0.0017(6)	0.0031(5)	0.0072(3)
1	0.0017(10)	0.0017(10)	0.0035(7)	0.0105(6)	0.1197(4)
2	0.0057(18)	0.0040(15)	0.0114(9)	0.1277(8)	
3	0.0177(27)	0.0120(20)	0.1336(20)		
4	0.1557(84)	0.1380(80)			

MCRG results itself provides sufficient data to estimate and allow for the various systematic effects, as we now describe.

(i) The data in Table II does not correspond to our best estimate for K_1^c in Eq. (10); therefore, if possible, one should interpolate using the exponent estimates at the three K_1 values. In Fig. 2 we show the K_1 dependence of the estimate for $1/\nu$ from the 64^3 data at various blocking levels. Linear interpolation appears to be entirely adequate and has been used to provide a complete set of interpolations with error bars for ten K_1 values between 0.221 650 and 0.221 659. The expected analyticity in the couplings K_α of RG functions, such as the stability matrix $T_{\alpha\beta}$, underpins the use of linear interpolation (for small coupling changes); in practice, some 75% of the raw data (Table II) at $K_1=0.221\,66$ differ by one standard deviation or less from the best-fit interpolations and there are no obvious systematic discrepancies. In Table III we show the resulting interpolation at 0.221 654 for the 7×7 (6×6 for 2^3 block lattices) matrix $T_{\alpha\beta}$.

TABLE IV. Finite-size and or truncation effect, for estimates of $1/\nu$, obtained by subtracting the 64^3 data from the other columns in Table II.

32^3-64^3	16^3-64^3	8^3-64^3
−0.0015	−0.0008	0.0095
0.0024	0.0107	0.0334
0.0022	0.0106	0.0339
0.0021	0.0098	0.0283
0.0016	0.0079	0.0192
0.0013	0.0070	0.0172
0.0006	0.0051	0.0120
0.0004	0.0200	0.0985
0.0083	0.0412	0.1623
0.0080	0.0417	0.1710
0.0068	0.0316	0.1455
0.0044	0.0195	0.1323
0.0041	0.0179	0.1305
0.0029	0.0150	
0.0194	0.1137	
0.0332	0.1692	
0.0338	0.1780	
0.0242	0.1505	
0.0143	0.1374	
0.0126	0.1352	
0.0108		
0.1015		
0.1444		
0.1525		
0.1342		
0.1315		
0.1309		

(ii) Let us turn now to the estimation and elimination of finite-size effects. It is worth stressing again that here we are dealing with the short-range finite-size effects in the RG transformation itself. Table IV shows the result of subtracting the left-hand (64^3) column from successive columns *across* Table II, since we are then comparing results at the same blocking level [n in Eq. (9)] on different lattice sizes. One significant feature of Table IV is that the finite-size discrepancies *decrease* as the number of operators is increased to the maximum of seven. This systematic trend suggests strongly that the apparent finite-size effect is in large part due to the truncation of the space of operators. Of course this truncation is imposed anyway at the highest blocking level since the 2^3 block lattice cannot support, e.g., the $\langle 200 \rangle$ neighbor interaction. To estimate this finite-size and or truncation effect we show in Table III, in the last three columns below the interpolated values for $1/\nu$, the result of differencing *adjacent* columns *across* the table. Reading diagonally down these results reveals an apparently smooth and systematic trend. In column (c) of Table III we give our estimates for the "neighboring column" corrections, and in column (b) these are accumulated to provide the full corrections to the 64^3 data of blocking levels $n=1, \ldots, 4$. These numbers in column (b) must be subtracted from the 64^3 data above them; the corrected values are given in column (a) of Table III. In assessing the corrections in column (c),

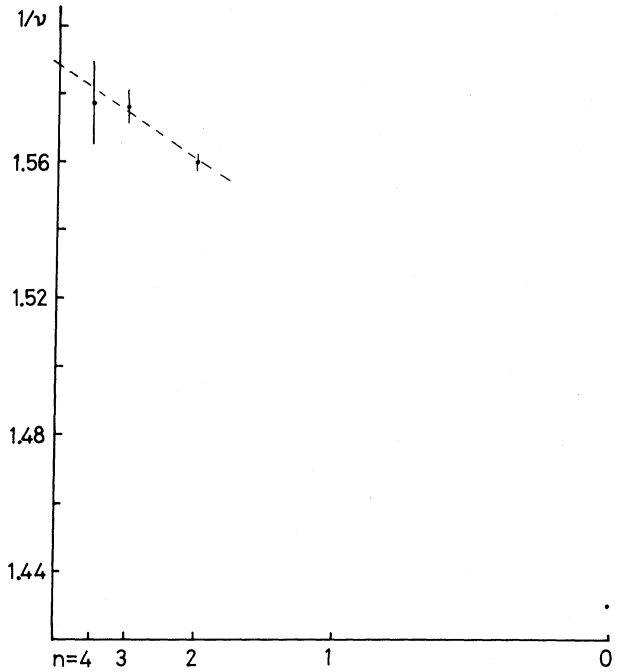

FIG. 3. Estimates for $1/\nu$ at $K_1=0.221\,654$ from Table III, column (a), plotted vs 2^{-n} for blocking levels $n=0,1,\ldots,4$. The dashed line indicates the linear fit to the data points for $n=2,3,4$.

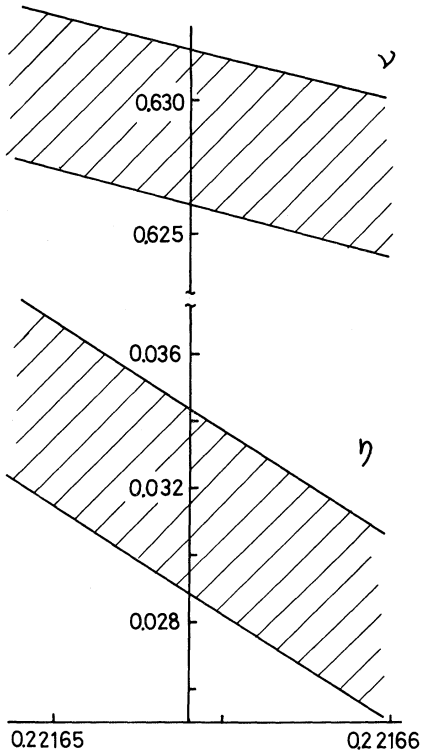

FIG. 4. Estimates for ν and η as functions of K_1^c. The vertical line is the best estimate $K_1=0.221\,654$.

we believe that we have assigned sufficiently generous errors to allow for the subjectivity which is necessarily involved. The same pattern of corrections also holds for the "raw" $1/\nu$ estimates at the three K_1 values (see Table II) and we have applied the same finite-size and truncation corrections in column (b) of Table III to all the interpolated $1/\nu$ tables. This correction procedure could probably be embellished with further refinements, but for our data we would not expect these to be significant in comparison with subsequent error estimates.

(iii) In Fig. 3 we plot the resulting corrected estimates for $1/\nu$ at the interpolated value $K_1=0.221\,654$ [from column (a), Table III] as a function of $1/2^n$, where $n=0,\ldots,4$ is the RG blocking level in Eq. (6). Since these numbers have been corrected for apparent finite-size effects, we can consider them as estimates for the exponent obtained in the first five blockings of an ideal infinite system; therefore, it remains to extrapolate these results to $n\to\infty$, where $\mathscr{H}$ will have converged to the fixed point $\mathscr{H}^*$. The choice of the extrapolation procedure should be governed by the subleading exponent ω, which ultimately controls the approach to $\mathscr{H}^*$. As we will discuss in detail in Sec. IV C, the subleading exponent is effectively $\omega\simeq 1$ on the basis of our limited data. Since the data in Fig. 3 should behave as $C_1+C_2 2^{-\omega n}$ for n sufficiently large, if $\omega=1$ then the data points should extrapolate linearly. It is clear from Fig. 3 that the effective ω is of order 1 for our values of n. On the other hand, field theory and series expansions suggest $\omega\simeq 0.8$. Therefore, we are left with the choice between using statistically accurate data points for small n with large uncontrolled systematic effects, or concentrating on the data points of larger n where the statistical errors are significant but systematic effects will be much less significant. What we have done in practice is to take the last three data points ($n=2,3,4$) and extrapolate linearly (in $1/2^n$); this yields the estimate $1/\nu=1.5892(58)$. A fit to $(C_1+C_2 2^{-\omega n})$ for any ω in the range 0.8—1.2 changes this value by less than a standard deviation; allowing an approriate increase in error bars yields $\nu=0.629(3)$ for $K_1^c=0.221\,654$.

(iv) In order to test the sensitivity to the value of K_1^c we have repeated this analysis for the range of K_1 values between 0.221 650 and 0.221 659. The results are shown in Fig. 4. Taking into account the uncertainty in K_1^c [Eq. (10)] we quote as our best estimate

$$\nu=0.629(4)\,. \tag{11}$$

The net effect therefore of all the corrections discussed in this section is to leave the value of ν, which one might guess naively from Table II, substantially unaltered, but with error estimates increased by a factor of order 5.

The result (11) is in excellent agreement with the recent estimates of 0.628—0.633 from series expansions on the simple cubic lattice,[13] 0.631(3) (Ref. 15) and 0.629(2) (Ref. 16) from the body-centered-cubic lattice, 0.630(2) from field-theory calculations,[17] and 0.635(5) from finite-size—scaling calculations.[18] The preliminary result from the Monte Carlo processor (Ref. 14) is $\nu=0.629(20)$.

B. Exponent η

The leading exponent y_H for a series of six operators (single spin, three spin, seven spin, and nine spin) is shown in Table V, in the same format as Table II. The values appear much more stable with regard to n dependence and

TABLE V. Estimates for y_H [Eq. (12)] from the run at $K_1=0.221\,66$, in similar format to Table II.

64^3	32^3	16^3	8^3
2.457 15(3)	2.457 60(3)	2.459 63(4)	2.466 49(6)
2.457 82(3)	2.457 89(3)	2.458 32(4)	2.459 09(5)
2.457 65(10)	2.457 48(3)	2.457 89(7)	2.458 53(7)
2.458 23(12)	2.458 05(4)	2.458 31(7)	2.458 21(7)
2.458 22(12)	2.458 05(4)	2.458 31(7)	2.458 22(7)
2.458 22(12)	2.458 05(4)	2.458 31(7)	2.458 22(7)
2.463 57(8)	2.466 49(16)	2.477 21(12)	2.506 78(14)
2.461 26(6)	2.461 71(15)	2.462 91(14)	2.470 63(19)
2.461 01(7)	2.461 22(14)	2.461 88(13)	2.468 98(19)
2.461 02(7)	2.461 14(14)	2.461 17(13)	
2.461 02(7)	2.461 13(14)	2.461 16(13)	
2.461 02(7)	2.461 13(14)	2.461 17(13)	
2.478 69(33)	2.490 54(32)	2.525 42(39)	
2.473 71(25)	2.474 76(32)	2.484 37(52)	
2.473 35(25)	2.473 71(34)	2.482 36(54)	
2.473 17(25)	2.472 89(33)		
2.473 15(25)	2.472 89(33)		
2.473 15(25)	2.472 89(33)		
2.497 52(110)	2.533 45(92)		
2.481 64(92)	2.489 72(67)		
2.480 60(97)	2.487 35(66)		
2.479 77(99)			
2.479 75(100)			
2.479 74(100)			
2.539 15(463)			
2.496 97(531)			
2.494 99(547)			

finite-size and truncation effects than do those for $1/\nu$ in Table II; this is just as well as it is the deviation of y_H from 2.5 which determines the standard critical exponent η [$G^{(2)}(q,\ T=T_c)\sim |q|^{-(2-\eta)}$] according to

$$y_H=(d+2-\eta)/2 \quad (d=3)\ . \tag{12}$$

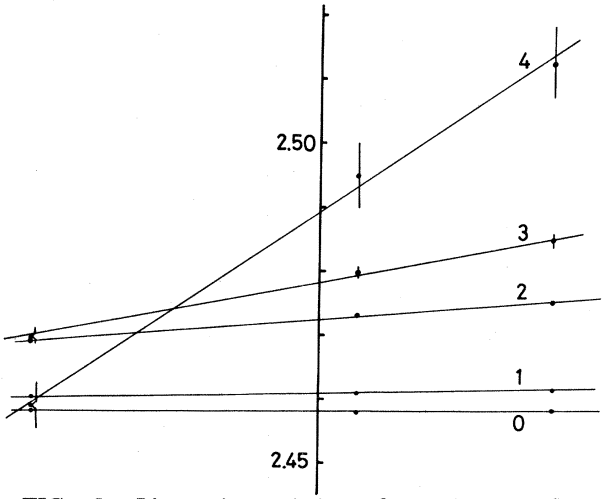

FIG. 5. Linear interpolations for estimates of y_H at $K_1=0.221\,61$, $0.221\,66$, and $0.221\,69$. The values plotted are from the 64^3 data at blocking levels $n=0,1,\ldots,4$ with the maximum-size stability matrix $T_{\alpha\beta}$. The vertical line is the best estimate $K_1^c=0.221\,654$.

We have applied the same three correction steps as for $1/\nu$. (i) The quality of the linear interpolation for y_H for K_1 between 0.221 650—0.221 659 is indicated in Fig. 5 for the 6×6 $T_{\alpha\beta}$ (3×3 for a 2^3 blocked lattice) obtained from the 64^3 data; the corresponding interpolations at 0.221 654 are shown in Table VI. (ii) We estimate finite-size and truncation corrections to η as described in Sec. IV A: $(-4\pm4)\times10^{-5}$ $(n=1)$, $(5\pm10)\times10^{-5}$ $(n=2)$, $(-17\pm15)\times10^{-5}$ $(n=3)$, and $(750\pm200)\times10^{-5}$ $(n=4)$; these values are subtracted from the last entries in the 64^3 data at 0.221 654. (iii) The "infinite-system" estimates for η obtained in this way are shown in the first column of Table VI and plotted in Fig. 4. Extrapolating to $1/2^n\to0$, and allowing again for systematic uncertainties in the extrapolation, we obtain $\eta=0.031(4)$ for $K_1^c=0.221\,654$. Finally, the dependence on K_1 of this estimate of η is shown in Fig. 4. Allowing for the uncertainty in K_1^c we quote as a final result

$$\eta=0.031(5)\ . \tag{13}$$

This result is again in excellent agreement with recent estimates, e.g., 0.031(4) from field-theory calculations.[17]

TABLE VI. Interpolation for y_H at $K_1=0.221\,654$. Column (a) contains the estimates for η after finite-size and truncation corrections.

n	(a): "∞^3"	64^3	32^3	16^3	8^3
0	0.0837(2)	2.458 14(7)	2.458 10(3)	2.458 26(5)	2.458 04(3)
1	0.0782(1)	2.460 85(4)	2.460 86(5)	2.460 70(8)	2.468 76(9)
2	0.0550(3)	2.472 53(10)	2.472 24(16)	2.481 77(39)	
3	0.0432(12)	2.478 23(57)	2.486 35(59)		
4	0.0369(70)	2.489 04(286)			

C. Exponent ω

The second-largest eigenvalue of $T_{\alpha\beta}$ in the space of even operators gives the correction-to-scaling exponent ω according to $\lambda_2=2^{-\omega}$. In Table VII we show the raw data for ω in the usual format; the successive diagonalization of submatrices of $T_{\alpha\beta}$ has a maximum of six entries, since one eigenvalue is already abstracted in the leading exponent $1/\nu$. In addition to the features also present in Tables II and IV, we note the very strong dependence of ω on the truncation (a factor of 2). It is clear that the $\langle 200\rangle$ neighbor interaction is extremely important; this suggests that longer-range interactions play a more important role in determing the correction-to-scaling exponent ω, and that our approximation of including only seven even operators might preclude any reliable estimate for ω. Nevertheless, we have followed the same procedure as described in detail in Sec. IV A; the result obtained is

$$\omega=1.0\pm0.1\ . \tag{14}$$

This value is to be compared with 0.78(13) (Ref. 13) and 0.83(8) (Ref. 19) from series expansions on the body-centered-cubic lattice (for a review and further references, see Nickel, Ref. 2), and 0.79(3) from field-theory calculations.[17] The discrepancy with (14) (which is only two standard deviations) surely derives from the truncation approximation; if the $\langle 200\rangle$ neighbor is responsible for a reduction of roughly 0.4 in ω, all the other correlation functions which are omitted may very well account for a further reduction of 0.2.

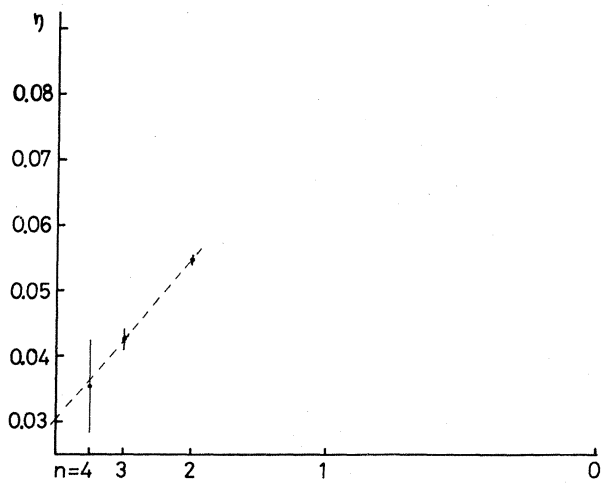

FIG. 6. Estimates for η at $K_1=0.221\,654$ from Table VI, column (a), plotted vs 2^{-n}, for blocking levels $n=0,1,..,4$. The dashed line indicates the linear fit to the data points for $n=2,3,4$.

V. DISCUSSION

In this paper we have described the result for (3D) Ising critical behavior which can be obtained using the MCRG method with fairly high statistics on lattices with up to 64^3 states. An important aspect of the work shows how the totality of all data obtained near the best estimate for the critical point can be used to improve the statistical quality and to eliminate systematic effects in the final result. By measuring the block-spin correlations as in Eqs. (5) and (6), a run at a single K_1 value can be used to estimate K_1^c; thus all of our three runs can be used to obtain a statistically improved estimate for K_1^c. The reliability of the final result can be assessed by looking at the common trends in all blocking levels on the various lattice sizes. The expected analytic dependence of the RG transformation on the coupling K_1 underpins the linear interpolation of critical exponents from the three runs, which is essential for analysis of results at the best estimate for K_1, and can improve their statistical quality by using the three sets of data. The full MCRG tables for exponents are essential to estimate and eliminate the finite-size and truncation effects on exponents. The data on the subleading exponent ω provides one with the information on how to extrapolate from finite to infinite blocking levels to reach the fixed point. We believe that this is the first time that such systematic steps have been taken to extract data from the MCRG method. The internal consistencies of the calculations strongly support the validity of this approach. For example we have repeated the entire analysis with a different ordering for the even operators, the $\langle 200\rangle$ neighbor being promoted to the fourth order. This implies that at the 2^3 block lattice, the truncation effect is even more severe since now only three operators are used for $1/\nu$, and only two for ω. The resulting finite-size and truncation corrections are larger (30% for $1/\nu$, 100% for ω), but when they are taken into account, essentially the same final estimates for the exponents emerge, with slightly larger error bars. Finally, one can explicitly incorporate into the final results the uncertainties due to, e.g., the method of extrapolation or dependence on K_1.

An interesting aspect which should be raised here is that of redundant operators.[20] In addition to the classification of perturbations from a fixed point as relevant or irrelevant (eigenvalues greater than or less than 1, respectively), eigenoperators should also be classified as physical

TABLE VII. Estimates for ω at $K_1=0.221\,66$, in similar format to Table II.

64^3	32^3	16^3	8^3
2.009(15)	1.963(17)	1.990(8)	1.981(7)
1.427(16)	1.433(18)	1.428(6)	1.446(4)
1.432(16)	1.440(18)	1.437(7)	1.470(4)
1.447(17)	1.460(19)	1.456(7)	1.486(6)
1.457(24)	1.482(19)	1.473(10)	1.570(11)
1.069(13)	1.097(7)	1.097(5)	1.256(12)
1.970(16)	2.003(17)	2.006(7)	2.205(7)
1.447(18)	1.450(21)	1.482(10)	1.726(7)
1.441(16)	1.458(25)	1.516(12)	1.743(8)
1.428(33)	1.495(39)	1.503(4)	1.600(9)
1.441(46)	1.546(38)	1.450(4)	1.478(4)
1.061(17)	1.068(4)	1.261(10)	
1.960(32)	2.008(19)	2.186(11)	
1.406(28)	1.480(20)	1.723(8)	
1.420(31)	1.533(23)	1.740(11)	
1.571(42)	1.443(8)	1.470(8)	
1.510(36)	1.391(12)	1.357(5)	
1.054(32)	1.192(6)		
1.976(23)	2.193(22)		
1.437(46)	1.733(15)		
1.484(48)	1.749(16)		
1.392(19)	1.440(9)		
1.340(17)	1.328(9)		
1.165(16)			
2.178(28)			
1.684(28)			
1.710(35)			
1.415(26)			
1.314(22)			

or redundant.[20] The redundancy arises because the totality of all possible interactions is physically overcomplete; Hamiltonians which correspond to different points in the space of all couplings may differ in reality only by a redefinition of the basic degree of freedom, without physical content. This is perhaps most transparent in continuum field models: A redefinition of the field $\phi\rightarrow f(\phi)$ induces $\mathscr{H}(\phi)\rightarrow\tilde{\mathscr{H}}(\phi)=\mathscr{H}[f(\phi)]$ but is of no physical significance. The change in the Hamiltonian due to an infinitesimal field transformation $f(\phi)=\phi+\delta(\phi)$ is $\delta\mathscr{H}=\int\delta(\phi)\,\delta\mathscr{H}/\delta\phi$. Thus redundant perturbations of the fixed-point Hamiltonian are characterized by any function of $\phi\times$ ("equation-of-motion factor," $\delta\mathscr{H}/\delta\phi$, for the fixed-point Hamiltonian). The simplest such perturbation corresponds to $\delta(\phi)=$const. Furthermore, in field theory it is possible to formulate the RG (see Amit, Ref. 5) so that

$$\frac{\delta\mathscr{H}}{\delta\phi}(\mathscr{H}^*)=-\nabla^2\phi+g^*\phi^3\ .$$

Since $\int\nabla^2\phi$ yields 0, in the field-theory formulation $\int\phi^3$ is a redundant perturbation. Of course in the lattice calculations described here, a completely different renormalization scheme is involved but the suggestion is clear: The second largest eigenvalue in the space of odd operators is very likely to be a redundant operator. A direct confirmation of this result would be given by exposing the expected dependence of the corresponding exponent upon the precise formulation of the renormalization transformation. We have not done this. However, it is interesting to note that the actual value 0.36(4), obtained by following the same procedure as described above for other exponents, is sufficiently different from the exponent of the $\int\phi^3d^3x$ operator as calculated in field theory [$\frac{1}{2}d-1+\frac{1}{2}\eta\simeq0.515$ ($d=3$), see Chap. 10 of Amit Ref. 5] that the identification in terms of a redundant perturbation seems plausible. It is clear that further work is needed to substantiate this speculation.

Finally, let us turn to the question of future prospects for this kind of calculation. It seems perfectly feasible, provided further extrapolation problems do not emerge, to increase the accuracy of the calculation reported here by approaching an order of magnitude using computing resources presently available for this task, or in the immediate future. First, one can readily perform calculations on a 128^3 lattice. We have now increased our effective running rate on the DAP by close to a factor of 8, although of course many more sweeps would be required for high statistics with the longer-time correlations on the larger lattice. This is certainly a feasible calculation for the MPP at the National Aeronautics and Space Administration. The "demon" algorithm[21] may also provide an order-of-magnitude increase in speed. Special purpose processors which are unable to perform the RG blocking would require access to other rather powerful machines. Second, one can run with an improved energy function including second-neighbor, four-spin, etc. interactions to start as close to the fixed point as possible, and hence to eliminate substantial transient effects; this could easily be worth two extra blocking levels. Third, it is essential to measure many more correlation functions to minimize the strong truncation effect apparent in our data; the uncertainty due to these effects could be very considerably reduced. Fourth, one might also explore the optimization of the calculation by the choice of other rules for forming the block spins;[22] one may thereby eliminate transient effects in redundant operators. We note in closing that a complete calculation would look at two further effects not discussed in this paper—the variation of K_1^c estimates obtained from using other than the nearest-neighbor operator S_1 in Eqs. (5) and (6), and the "double-blocking" check that the truncation approximation made is adequate (see Swendsen, Ref. 1).

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