RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 33, NUMBER 11 1 JUNE 1986

Finite-size scaling and the three-dimensional Ising model

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(Received 6 January 1986)

We give results of an extensive finite-size-scaling analysis of the three-dimensional Ising model on lattices of size up to 44^3. Contrary to the results of Barber *et al.* [Phys. Rev. B **32**, 1720 (1985)], our data show a smooth approach to the thermodynamic limit for all the lattice sizes we studied. We estimate from our data that $\gamma/\nu = 1.964(3)$. We also describe a method to implement the Metropolis algorithm using only logical commands. Our program currently achieves a speed of one spin update approximately every 11 nsec (93 million updates per second) on a 2-pipe CDC CYBER 205.

The three-dimensional Ising model is the simplest model of the dynamics of ferromagnets. Near the critical point, it is also the simplest field theory which is not obviously trivial. On the other hand, it has resisted all attempts at an exact solution. The spin variables $s = 1 - 2\sigma = -1, 1$ in the model have only two possible values and can therefore be represented by a single bit in the computer. This makes it possible to write extremely fast simulation algorithms for this model using bit operations and multispin coding techniques.[1] The reason one wants fast algorithms is that near the critical point (i.e., as the correlation length $\xi \to \infty$), the computer time to generate successive independent configurations diverges (approximately as ξ^2). With improvements in numerical techniques and the increasing availability of computing power for scientific applications, the critical behavior of this model has been the subject of extensive numerical studies in recent years.[2] A powerful tool used to study the model is Monte Carlo simulation on finite lattices followed by a finite-size-scaling analysis.[3]

Recently, the utility of finite-size-scaling methods for the three-dimensional Ising model has become very unclear. This situation is due primarily to the very high-precision data[4] obtained with the special purpose machine developed at the University of California, Santa Barbara and popularly known as the "Ising Model Processor" (IMP).[5] The data obtained with the IMP show unambiguous anomalous behavior for lattices of size 32^3 and smaller and casts doubt on the validity of hyperscaling. More recently, less precise data from Parisi and Rapuano[6] on a 24^3 lattice and Hoogland, Compagner, and Blöte[7] on lattices of size 4^3, 8^3, 16^3, and 32^3 are consistent with smooth finite-size behavior.

In this paper we present extensive new data that demonstrate a smooth finite-size scaling behavior for the three-dimensional Ising model. Our present results span lattices with linear extent L in the range 8–44, and achieve an accuracy comparable to the results of Ref. 4. We have obtained our results by inventing a new implementation of the traditional Metropolis *et al.*[8] algorithm. We use our method on a two-pipe, four-megaword CDC CYBER 205 supercomputer taking complete advantage of the vector architecture of that machine to achieve a speed of 93 million spin updates per second. The previous top speed on a two-pipe CYBER 205 was 21 million updates per second using a conventional multispin coding method.[9] By comparison, the IMP achieves about 25 million updates per second as does the microcanonical method of Creutz[10] when implemented on a CDC 7600.

The major bottleneck in a parallel implementation of the Metropolis algorithm is that each decision to update the spin involves comparing the change in the action with a floating-point random number. Since it takes about 20 nsec to generate a single new random number even on our machine, it is impossible, using the usual serial method, to exceed about 50 million updates per second. In fact, as noted above,[9] one is apparently limited in practice to about 21 million updates per second. Our new algorithm is designed to avoid this bottleneck by arranging to effectively make the required floating-point comparison using only a short sequence of simple binary instructions with no floating-point operations whatsoever while updating. We now briefly describe our method as implemented on a CYBER 205.

We represent the Ising variable at site i by σ_i, with $\sigma_i = 0, 1$ corresponding to the spin being up or down, respectively. Let N be the number of lattice sites. The spin variables are labeled even or odd in a checkerboard pattern on the lattice and the even and odd site variables are stored in two separate arrays which are updated one after the other. In our algorithm, we update 64 independent lattices simultaneously. Spins occupying the same position on these 64 lattices are arranged in the 64-bit positions of a single word. At the start of the simulation, each of the 64 lattices is initialized independently to a configuration with spins randomly up or down.

The change in the action on flipping the sign of σ_i may be written as

$$\Delta S_i = S_{\text{final}} - S_{\text{initial}} = 4\Omega_i - 12 \ , \tag{1a}$$

where

$$\Omega_i = \sum_{\hat{\mu}} \text{XOR}(\sigma_i, \sigma_i + \hat{\mu}) \ . \tag{1b}$$

Here XOR stands for the logical exclusive OR function, and $\hat{\mu}$ runs over the directions of the six neighbor spins. The decision on whether or not to accept the spin flip is made using three bit vectors B_2, B_1, B_0 which are initialized to the values 0,0,1, respectively. Think of the integer $I \in (0, 7)$ constructed by using B_0, B_1, B_2 as the zeroth, first, and second bits in its binary representation. First, Ω_i is added to I using only logical operations. In the case where the spin-flipped state is not less probable than the original state, $\Omega > 2$. This will result in $B_2 = 1$ after the addition. In this case, the spin flip is accepted.

The decision in the case where the spin-flipped configuration is less probable is made using two additional vectors D_1 and D_0. Once again, think of the integer J whose zeroth and first bits are D_0 and D_1, respectively. Initially, the D vectors are set so that n_1, n_2, n_3 entries in the vectors have $J = 1, 2, 3$, respectively, where

$$n_1 = \tfrac{1}{2}N(e^{-4\beta} - e^{-8\beta}) \ , \tag{2a}$$

$$n_2 = \tfrac{1}{2}N(e^{-8\beta} - e^{-12\beta}) \ , \tag{2b}$$

$$n_3 = \tfrac{1}{2}Ne^{-12\beta} \ . \tag{2c}$$

The remaining positions in the D vectors are set to 0,0. J is then added to the I and the flip is accepted if the result has $B_2 = 1$. Note that this corresponds to accepting the spin flip with probabilities $e^{-4\beta}$, $e^{-8\beta}$, and $e^{-12\beta}$ for $\Omega = 2, 1, 0$, respectively. This is exactly what is required to implement the Metropolis algorithm.

Our algorithm currently runs at a speed of about 93 million spin updates per second. This great speed is because of the gain in statistics by simultaneously measuring order parameters over 64 independent lattices. There are several additional details that we have not mentioned which are necessary to successfully implement the algorithm described above. The most important detail is that the n's in Eq. (2) are integers while the right-hand side is not. This essentially means that we are operating at a β value slightly different from the one we want. Fortunately, it is possible to correct any order parameter measured via our algorithm and readjust to the correct value of β. The only place one might worry about this is near the critical point. However, this correction in β is $O(L^{-d})$ for d dimensions, and for large enough L it becomes less than the inherent inaccuracy of $O(L^{-1/\nu})$ in estimating the critical β.[3] In three dimensions, it turns out that the correction in β, near $\beta_c \sim 0.221\,65$ is smaller than the accuracy with which β_c is known. This and other issues relevent to the algorithm will be described in great detail elsewhere.[11].

Our vector length is $\frac{1}{2}N$ which, for $L > 8$, is more than sufficient to obtain very nearly the maximum possible vector speed for our computer. The algorithm is completely expressed, in the crucial parts, in terms of explicit vector machine instructions and so is ideally adapted to the available architecture. Of course, the algorithm is sufficiently general that it could be implemented on any machine. We use the definitions,

$$M = \sum s_i, \ C_u = \frac{\partial E}{\partial \beta}, \ m = \frac{\langle |M| \rangle}{N}, \ E = \frac{1}{dN}\frac{\partial \ln Z}{\partial \beta} \ ,$$

$$\chi_m = \frac{\langle M^4 \rangle - 3\langle M^2 \rangle}{N}, \ gR = \frac{\langle M^4 \rangle - 3\langle M^2 \rangle}{\langle M^2 \rangle^2} \ .$$

We have tested our algorithm (and the programs which implement it) by simulating, on finite lattices, the exactly solvable[12] two-dimensional Ising model. We find that there is excellent agreement between our Monte Carlo runs and the exact answers for the order parameters. We show in Table I a sample of these results. We have also used these results to test the sensitivity of our method to the choice of the pseudorandom number generator used during the simulation. For the two-dimensional case we note a slight preference for the feedback shift-register method using the primitive trinomial $x^{127} + x^{97} + 1$, as compared to the CYBER 205's built-in multiplicative congruential generator which uses the multiplier 4C65DA2C866D(hex) and operates modulo 2^{47}. Similar tests for the three-dimensional simulations do not give a clear indication of favor between the shift register and congruential generators. For most of the three-dimensional data reported here we used shift-

TABLE I. Comparison of our simulation algorithm results with the exact answers for the two-dimensional Ising model on a 20^2 lattice.

β	E_{meas}	E_{exact}	C_v(meas)	C_v(exact)
0.432	0.685 09(9)	0.685 01	4.461(6)	4.458
0.436	0.702 78(7)	0.702 68	4.359(7)	4.364
0.440	0.719 73(9)	0.719 79	4.186(7)	4.180
0.444	0.736 05(9)	0.736 08	3.957(7)	3.954
0.448	0.751 53(8)	0.751 37	3.687(7)	3.685

TABLE II. Our current data sample. The columns referring to the results of Refs. 4, 6, and 7 show the data for $\chi_m L^{-1.96}$ from these papers. The quantities in parentheses are error estimates.

Lattice size	Number of meas.	m	E	C_v	$-g_R$	$\chi_m L^{-1.96}$	Ref. 4	Ref. 6	Ref. 7
8	$2.56\ 10^6$	0.374 34(07)	0.369 00(3)	9.444(05)	1.4454(05)	1.4912(05)	1.4919(08)	1.4942(40)	1.4909(19)
12	$6.4\ 10^5$	0.304 90(20)	0.352 10(5)	11.059(19)	1.4276(12)	1.5142(14)	1.5240(13)		
14							1.5306(13)		
16	$6.4\ 10^5$	0.263 51(14)	0.344 84(4)	12.200(21)	1.4217(11)	1.5281(13)	1.5328(08)		1.5271(13)
20	$6.4\ 10^5$	0.234 99(14)	0.340 87(3)	13.137(23)	1.4168(10)	1.5343(14)	1.5449(21)		
24	$1.6\ 10^6$	0.214 01(09)	0.338 42(2)	13.911(15)	1.4127(08)	1.5399(10)	1.5567(11)	1.5398(43)	
26							1.5545(21)		
28	$1.088\ 10^6$	0.197 63(11)	0.336 80(2)	14.565(19)	1.4105(10)	1.5424(13)	1.5537(33)		
32	$1.088\ 10^6$	0.184 41(12)	0.335 66(2)	15.165(20)	1.4084(11)	1.5445(16)	1.5498(27)		1.5469(67)
40	$6.4\ 10^5$	0.164 29(15)	0.334 17(2)	16.182(30)	1.4042(15)	1.5474(23)	1.5464(33)		
44	$1.2736\ 10^6$	0.156 41(11)	0.333 67(1)	16.595(20)	1.4038(12)	1.5488(16)			

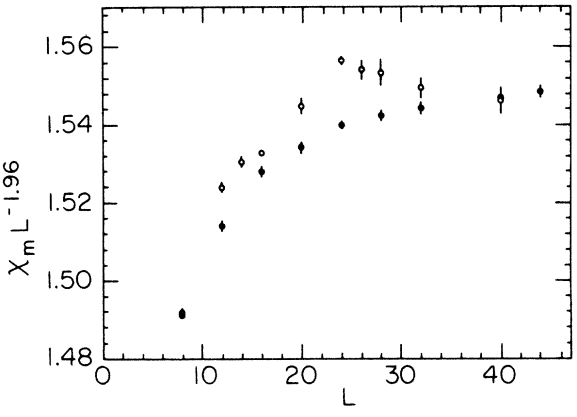

FIG. 1. Comparison of our data for $\chi_m L^{-1.96}$ (solid dots) with that of Ref. 4 (open circles).

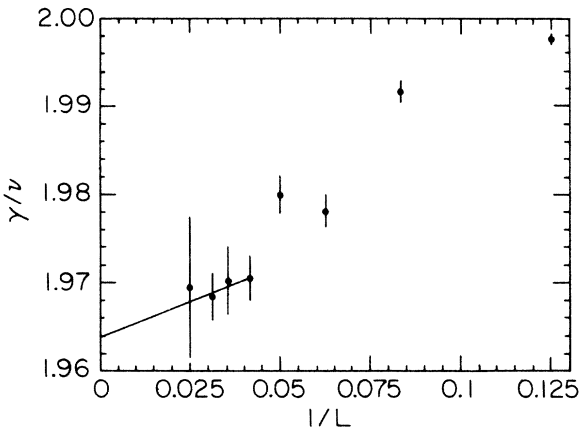

FIG. 2. Estimates of γ/ν from the data for successive lattice sizes plotted vs $1/L$. The solid line is a straight line χ^2 fit for $L = 24$ and greater.

register sequences based on primitive trinomials of the form $x^p + x^q + 1$ with the sets $(p,q) = (521, 158)$, (1279,418), (2281,715), and (4423,1393).[13] Insofar as we do not find any dependence on the random number generator, we disagree with the conclusion of Ref. 6 that the data of Ref. 4 suffer from an inadequate random number generator.

It should perhaps be recalled that the IMP data are also reported to have passed the test of comparison to exact two-dimensional results, so that evidently these tests, in view of the comparison of our three-dimensional results, are not sufficient to guarantee correct results in general. Our two- and three-dimensional results also agree (within error bars) with conventional direct Metropolis simulations of lower accuracy.

Finally, we present our current results for the three-dimensional Ising model and compare them with the previously available data. We concentrated this initial study at the value $\beta = 0.221\,650$ used by Barber, Pearson, Toussaint, and Richardson.[4] Starting from a random configuration, the lattices were all initially thermalized with 100 000 sweeps. Subsequently, measurements were made every 100 sweeps. Table I gives the data sample we have generated, so far, as well as the results of Ref. 4 (up to the lattice sizes we tested) and those of Refs. 6 and 7. In Fig. 1, we plot our results for $\chi_m L^{-1.96}$ along with those from Ref. 4. The error bars for our data were calculated by considering the variance among the means of the 64 parallel lattices. We have made extensive checks to confirm that the data from the 64 lattices are statistically independent. It is significant that our statistical errors are in fact comparable to the errors quoted in Ref. 4 even though we made, in most cases, fewer total lattice sweeps.

Figure 1 and Table II clearly show that our data are in statistically significant disagreement with the data from the IMP and are consistent with the substantially less precise results from Refs. 6 and 7. The conclusion from our data is that there are no violations of finite-size scaling[14] in the three-dimensional Ising model and that this model approaches its thermodynamic limit smoothly for all lattice sizes.

In the scaling region, one can estimate γ/ν from data for successive lattice sizes using the form $\chi_m \sim AL^{\gamma/\nu}$. In Fig. 2 we plot these estimates against $1/L$. The solid line is a straight line χ^2 fit to the last four points ($L \geq 24$). We estimate from Fig. 2 that $\gamma/\nu = 1.964(3)$. The data in Fig. 2 are clearly not accurate enough for an estimate of the nonleading exponent.

The simulation required about 40 h of CYBER 205 CPU time. In the future, we intend to improve our implementation on the CYBER 205 even further (possibly by a factor of about 10) by using only bit vectors, by changing our boundary conditions from periodic to helical (this eliminates the gather and scatter operations), and by switching to the microcanonical ensemble.[15] We also expect to significantly extend our data sample in the immediate future and should be able to present a detailed finite-size-scaling analysis of the three-dimensional Ising model soon.

Finally, we wish to point out that by a series of obvious extensions, our simulation method can be applied to any model with a sufficiently simple, discrete symmetry space, such as the n-state Potts model or the $Z(n)$ model for reasonable values of n.

One of us (D.D.) wishes to thank D. P. Landau and R. H. Swendsen for helpful conversations in the early stages of this work. The research of G.B. and R.S. and partly that of D.D. was supported by the Department of Energy under Cooperative Agreement No. DE-FC05-85ER25000. The research of D.D. was also supported by the Department of Energy under Grant No. DE-AS05-76ER3509.

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