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Computer Investigations of the Three-Dimensional Ising Model

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We have been studying the three-dimensional Ising model using some finite-size scaling ideas. The simulation is done by a fast microcanonical method. Here we present our results for the critical exponents ν and α.

KEY WORDS: Ising models; computer simulation; microcanonical ensemble; Monte Carlo simulation; finite-size scaling.

The Ising model is one of the simplest theoretical systems for the study of phase transitions. This model can be solved analytically in two dimensions[1] and exhibits the typical behavior of a ferromagnet. In particular, above a certain critical temperature the elementary magnets in a large sample are in a disordered state with no net bulk magnetization. On the other hand, below the critical temperature the magnets tend to order themselves parallel to one another, with a net overall magnetization. The more realistic three-dimensional Ising model has so far eluded analytic solution, though various parameters have been estimated by approximation techniques. Some methods, such as high-temperature series, are analytical in nature. Alternatively, one can simulate the model on a computer and effectively "measure" its properties. As bulk thermodynamic quantities are best determined on large systems, i.e., for a large number of interacting elementary magnets, clearly there is a need for large computation times and computer memory.

What are the quantities that we wish to measure? Not all details of the ferromagnetic phase transition are of equal importance. The precise value

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of the critical temperature as well as the corresponding value of the internal energy are relatively unimportant as they are specific to the details of the model and are not directly related to physical systems. They are nevertheless of some interest because they can be estimated by various methods and comparisons can be made. Moreover, their determination is an important antecedent to estimates of more important critical parameters, in particular, the critical exponents.

Quantities such as the correlation length ξ and the specific heat C of the system are expected to diverge as the temperature T approaches the critical value T_c:

$$\xi \propto |T/T_c - 1|^{-\nu}, \qquad C \propto |T/T_c - 1|^{-\alpha} \tag{1}$$

The exponents like ν, α, etc. are believed to have a universality property, i.e., they should agree for a whole class of systems, including physical ones. Testing this universality is the primary reason for the importance of measuring these parameters as accurately as possible.

Beyond universality, there are theories which predict relations among these exponents. In particular "hyperscaling"[2] predicts that ν and α satisfy the relation

$$\nu d = 2 - \alpha \tag{2}$$

where d is the number of spatial dimensions. As there is some controversy over this relation, it is of great interest to test its validity. Hyperscaling has been verified for analytically solvable models in two dimensions.

Several computer simulations of the three-dimensional Ising model have been carried out or are in progress.[3] These studies all use the conventional Monte Carlo method for generating a sample of configurations of the system. They work with the canonical ensemble, wherein the temperature is an external parameter and configuration energies are distributed according to the Boltzmann rule,

$$P(E) \propto \exp(-E/kT) \tag{3}$$

We have been following an alternative scheme[4] where the total system energy is effectively held fixed, thus sampling the microcanonical ensemble. The temperature is not an input. Rather, its value is determined through the use of a set of auxiliary variables ("demons") which exchange energy with the Ising lattice. Unlike conventional Monte Carlo, where random numbers from the computer simulate thermal fluctuations, this method sets up a deterministic dynamics which conserves the total energy. The demons interact with the spins of the system and try to invert them. If the resulting configuration is compatible with the constraints on energy, the change is

carried through. The demons then move on to act on other spins. As in conventional Monte Carlo, physical quantities are measured for different allowed configurations and subsequently averaged.

Although the simulations presented in this paper are modestly long, they are much shorter than and in no way compare with those in Ref. 3. Our purpose here is to give more substantial tests of the algorithms presented in Ref. 4. Thus we wish to verify that this method can be competitive with more conventional canonical approaches.

As discussed in Ref. 4, this technique reduces to the Metropolis *et al.*[5] algorithm in any local lattice region if the demon variables make large jumps around the lattice. For efficiency, it is particularly important that this jump size be large. In particular, if the demons only move sequentially through the lattice, it can take a large number of iterations for a local hot or cold spot to dissipate. In our program the demons hop between spins separated by several tens of sites.

To extract the critical exponents we use a variation of finite size scaling.[6] We take correlations between spins at various separations and form ratios which would represent dimensionless physical observables in a field theoretical continuum limit. Using renormalization arguments previously developed for lattice gauge theory,[6] we match these observables on different length scales and on finite lattices. For example, consider an Ising system of linear size L and take the ratio of the correlation between spins separated by $L/4$ to the correlation for a separation of $L/2$, both measured at temperature T. This ratio will remove any wave function renormalization factors from the correlations. Now consider the same quantity on a new lattice of size L' and at temperature T'. In general the above ratio R will differ. However, if the temperatures are related in such a manner that the correlation lengths are in the same ratio as the sizes, then, as discussed for ratios of Wilson loops in Ref. 6, the ratios should be equal except for corrections of order the inverse corelation length. These corrections should become small near the critical point. In equations, if we adjust T' so that we have the matching

$$R(L, T) = R(L', T') \tag{4}$$

then we should have

$$L/\xi = L'/\xi' \tag{5}$$

From Eq. (1), this implies

$$(L/L')^{-1/\nu} = |(T - T_c)/(T' - T_c)| \tag{6}$$

Now consider plotting $R(L, T)$ versus $1/T$ in a small region around the

critical point. As the lattice is finite, R is analytic and we can approximate it with a linear function

$$R(L, T) = A_1 + A_2/T \tag{7}$$

$$R(L', T') = A_1' + A_2'/T' \tag{8}$$

The matching condition of Eq. (4) then takes the form

$$A_1 + A_2/T = A_1' + A_2'/T' \tag{9}$$

As T approaches T_c and the correlation length diverges, dimensionless quantities involving scales much less than the correlation length should become scale invariant. Thus we determine T_c to be the temperature at which $R(L, T)$ and $R(L', T)$ match. This occurs at

$$A_1 + A_2/T_c = A_1' + A_2'/T_c \tag{10}$$

Now Eq. (9) becomes

$$A_2(1/T_c - 1/T) = A_2'(1/T_c - 1/T') \tag{11}$$

To first order in the difference from the critical temperature, this combines with Eq. (7) to give

$$A_2/A_2' = (L/L')^{1/\nu} \tag{12}$$

or

$$1/\nu = \ln(A_2/A_2')/\ln(L/L') \tag{13}$$

Thus the ratio of the slopes yields the exponent ν.

To determine α we use a more conventional finite-size scaling analysis. We work directly with the internal energy E. For an infinite system near the critical point this behaves as

$$|E - E_c| \propto |T/T_c - 1|^{1-\alpha} \tag{14}$$

where E_c is the value of the internal energy at the critical point. With a finite-volume system, however, the internal energy is an analytic function of the temperature. Standard finite-size scaling arguments as presented in Ref. 7, or in Ref. 8 in the context of lattice gauge theory, indicate that near the critical temperature two finite systems of different size satisfy

$$[E(L, T) - E_C(L)]L^{(1-\alpha)/\nu} = [E(L', T') - E_c(L')]L'^{(1-\alpha)/\nu} \tag{15}$$

where T' is determined from Eq. (5). To use this, we do a linear fit to the energy on our finite system in the critical region

$$\begin{aligned} E(L, T) &= B_1 + B_2/T \\ E(L', T') &= B_1' + B_2'/T' \end{aligned} \tag{16}$$

With a little algebra, Eqs. (15), (16), and (6) relate the ratio of the slopes to the ratio α/ν:

$$\alpha/\nu = \ln(B_2/B_2')/\ln(L/L') \tag{17}$$

We note at this point that although one goal would be to test the hyperscaling relation of Eq. (2), the above finite-size scaling analysis is not independent of that relation. Indeed, finite-size scaling as well as hyperscaling follow from the assumption that only a single length scale is diverging at the critical point. If there were two distinguishable correlation lengths diverging at different rates, both hyperscaling and finite-size scaling could be questioned. Thus our analysis is not purely a test of Eq. (2), but should be regarded as a consistency test on both that relation and finite-size scaling.[9]

We have worked on lattices of size 16, 32, 48, and 64 sites for two of the three dimensions. The third dimension of the lattices was kept at 128 sites for technical reasons related to the details of the multispin coded program. The above scaling arguments require scaling the size in all dimensions by the same ratio. Our hope is that 128 is sufficiently larger than the other dimensions that it can be regarded as infinite, hence insensitive to scale changes.

The details of our program have been published.[10] As mentioned above, the temperatures are not inputs, as in the conventional canonical method, but averages derived from measurements of the energies, and thus they have error bars, as do the measurements of the ratios R. The internal energy is the difference between the total energy, an input, and the energy carried by the demons. The errors in this quantity are quite small, arising from the fluctuations in the small amount of energy in the demons. All these errors are incorporated into the errors in the coefficients A_1, A_2, B_1, and B_2 introduced above. These quantities are determined by least square fits to the data. The exponents $1/\nu$, α/ν, and $1/T_c$ are then determined by least square fits to the relations

$$\ln(A_2) = \text{const} + \nu^{-1} \ln(L) \tag{18}$$

$$\ln(B_2) = \text{const} + \alpha\nu^{-1} \ln(L) \tag{19}$$

$$A_1 = \text{const} - T_c^{-1} A_2 \tag{20}$$

which follow from the above analysis.

Table I. Results from the Monte Carlo Simulation for the Total Energy, Inverse Temperature, Internal Energy, and Ratio of Correlations for (a) Size = 16, (b) Size = 32, (c) Size = 48, and (d) Size = 64

Total energy	Inverse temperature	Internal energy	Ratio of correlations
		(a) $(16^2 \times 128)$	
0.67447917	0.220656 ± 0.000018	$0.67295594 \pm 0.00000013$	1.538 ± 0.002
0.67297363	0.220805 ± 0.000014	$0.67145154 \pm 0.00000010$	1.509 ± 0.002
0.67146810	0.220961 ± 0.000014	$0.66994716 \pm 0.00000010$	1.486 ± 0.002
0.66996257	0.221134 ± 0.000016	$0.66844290 \pm 0.00000012$	1.467 ± 0.002
0.66849772	0.221285 ± 0.000017	$0.66697916 \pm 0.00000012$	1.442 ± 0.002
0.66699219	0.221401 ± 0.000013	$0.66547448 \pm 0.00000009$	1.419 ± 0.002
0.66548665	0.221575 ± 0.000013	$0.66397021 \pm 0.00000009$	1.403 ± 0.001
0.66398112	0.221740 ± 0.000015	$0.66246589 \pm 0.00000011$	1.385 ± 0.002
		(b) $(32^2 \times 128)$	
0.67449951	0.221033 ± 0.000021	$0.67411941 \pm 0.00000004$	1.630 ± 0.016
0.67149861	0.221357 ± 0.000024	$0.67111911 \pm 0.00000004$	1.523 ± 0.014
0.67299398	0.221222 ± 0.000019	$0.67261422 \pm 0.00000004$	1.578 ± 0.016
0.66999308	0.221486 ± 0.000030	$0.66961381 \pm 0.00000006$	1.455 ± 0.011
0.66849772	0.221635 ± 0.000027	$0.66811872 \pm 0.00000005$	1.418 ± 0.008
0.66699219	0.221699 ± 0.000025	$0.66661331 \pm 0.00000005$	1.372 ± 0.008
0.66549683	0.221784 ± 0.000056	$0.66511810 \pm 0.00000010$	1.333 ± 0.011
0.66399129	0.221940 ± 0.000021	$0.66361285 \pm 0.00000004$	1.296 ± 0.005
		(c) $(48^2 \times 128)$	
0.67462384	0.221114 ± 0.000020	$0.67445497 \pm 0.00000002$	1.99 ± 0.14
0.67314091	0.221299 ± 0.000020	$0.67297219 \pm 0.00000002$	1.76 ± 0.05
0.67162182	0.221437 ± 0.000030	$0.67145321 \pm 0.00000002$	1.68 ± 0.05
0.67013889	0.221541 ± 0.000030	$0.66997037 \pm 0.00000002$	1.50 ± 0.06
0.66861979	0.221727 ± 0.000030	$0.66845142 \pm 0.00000002$	1.48 ± 0.04
0.66713686	0.221803 ± 0.000030	$0.66696855 \pm 0.00000002$	1.39 ± 0.02
0.66561777	0.221902 ± 0.000030	$0.66544954 \pm 0.00000002$	1.33 ± 0.04
0.66413484	0.221914 ± 0.000030	$0.66396662 \pm 0.00000002$	1.24 ± 0.01
		(d) $(64^2 \times 128)$	
0.67466227	0.221182 ± 0.000012	$0.67456731 \pm 0.00000001$	2.0 ± 0.2
0.67315674	0.221326 ± 0.000017	$0.67306185 \pm 0.00000001$	1.69 ± 0.08
0.67165120	0.221497 ± 0.000025	$0.67155639 \pm 0.00000001$	1.79 ± 0.09
0.67014567	0.221607 ± 0.000030	$0.67005091 \pm 0.00000002$	1.54 ± 0.06
0.66866048	0.221734 ± 0.000029	$0.66856578 \pm 0.00000001$	1.37 ± 0.03
0.66414388	0.221873 ± 0.000030	$0.66404924 \pm 0.00000002$	1.18 ± 0.04

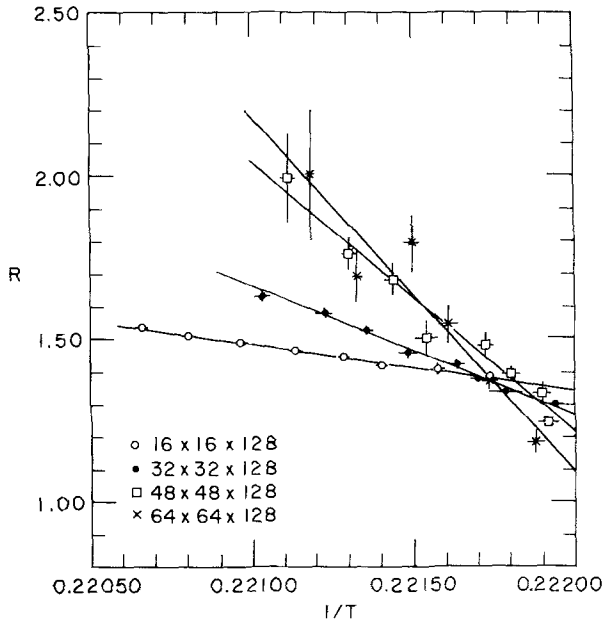

Fig. 1. Ratio of correlations quarterway and halfway across the lattice versus reciprocal temperature.

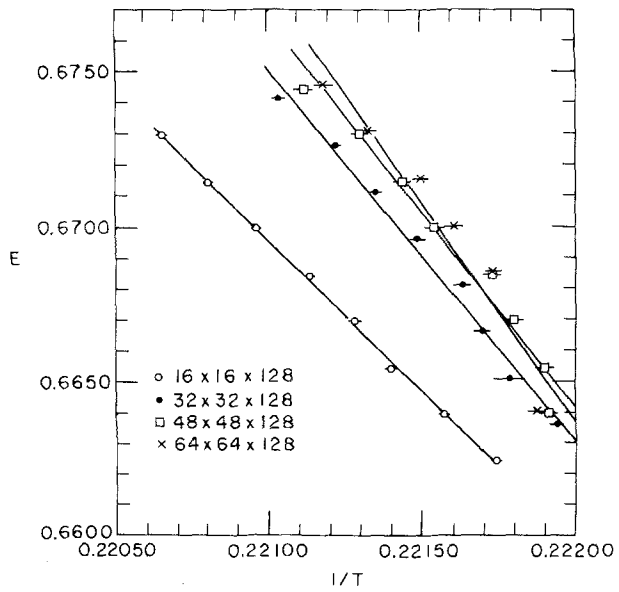

Fig. 2. Internal energy per link versus reciprocal temperature.

We measured R and T for 8 values of total energy on each of the 3 smaller lattices (sizes 16, 32, and 48), while in the case of the lattice of size 64, time constraints permitted the study of only 6 values. The number of iterations for each energy value was chosen in such a way that the errors in T were roughly the same in all cases. This meant reducing the number in inverse proportion to the number of spins. However the errors in R started increasing with lattice size (because the separations $L/4$ and $L/2$ increased) so that we had to use longer runs on our largest lattice. We did 16×10^4 iterations for $L = 16$, 4×10^4 for $L = 32$, 2×10^4 for $L = 48$ and 3×10^4 for $L = 64$. The data in each case were divided into bunches for the calculation of statistical errors. Our bunch sizes were 4000, 1000, 500, and 250 in the four cases.

The data are presented in Table I [(a), (b), (c), (d) for the four lattice sizes]. For each lattice size, R and E were plotted against $1/T$ and the points fitted by straight lines as indicated above. The points as well as the four lines for R are shown in Fig. 1. The fit is almost perfect for our smallest lattice but with increasing L the points get more and more scattered about the best-fit lines. This is only natural as the errors in R increase very rapidly. Figure 2 shows the points and the linear fits for E. Once again, the fits get worse with increasing size. From size 32 onwards, the points clearly show a bending near the critical region. Perhaps a quadratic fit would have been appropriate—the errors in E are neglibible and those in T are not large enough to warrant the observed deviations from linearity.

The parameters involved in the best fits are shown, complete with errors, in Table II. The variation of $\log A_2$ and $\log B_2$ with $\log L$ is shown in the lower and upper parts, respectively, of Fig. 3. The linear fit was reasonably good in both cases; the slopes, together with errors, are given in Table III. These are our "measured" values for $1/\nu$ and α/ν. For completeness we have also included our value for $1/T_c$. The errors quoted here are purely statistical. We caution the reader that in addition there may be

Table II. Coefficients of the Linear Least Squares Fit for Lattice Sizes 16, 32, 48, and 64

Lattice size	A_1	A_2	B_1	B_2
16	32.57 ± 0.7	-140.66 ± 3	2.82 ± 0.02	-9.73 ± 0.1
32	87.5 ± 4	-388.3 ± 17	3.33 ± 0.07	-12.02 ± 0.3
48	187.1 ± 17	-837.6 ± 60	3.40 ± 0.1	-12.30 ± 0.5
64	243.7 ± 30	-1093 ± 130	3.78 ± 0.1	-14.01 ± 0.6

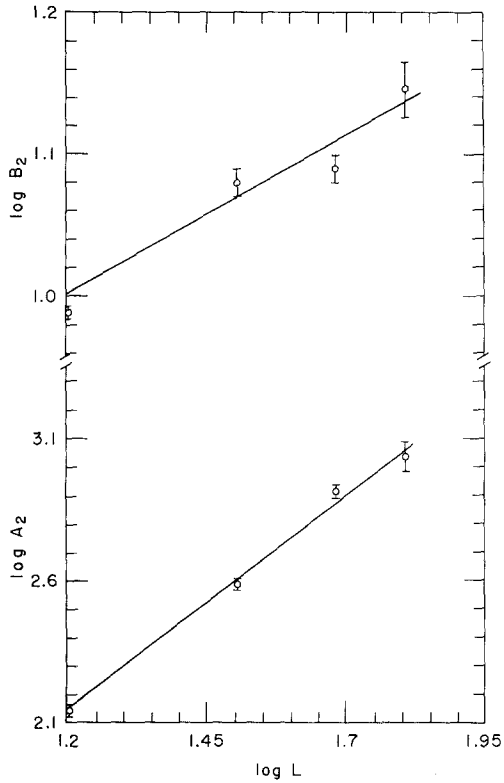

Fig. 3. Variation of (logarithms of) slopes of previous graphs with (logarithm of) lattice size.

systematic errors due to finite size and the fact that the 128 dimension of the lattices was not scaled.[11] The small errors on the critical temperature come primarily from the smallest two lattices. Longer runs on the larger lattices would be desirable to check for systematic effects. With this in mind, our results may be compared with values obtained earlier from series

Table III. Estimates for the Critical Parameters; Old Values Taken from Ref. 12

$1/\nu$		α/ν		$1/T_c$	
Our value	Series value[12]	Our value	Series & hyperscaling	Our value	Previous value
1.52 ± 0.07	1.58 ± 0.01	0.24 ± 0.03	0.17 ± 0.02	0.22169 ± 0.00002	0.221655

expansions (12) and hyperscaling. The deviations are not quite within the quoted errors. But the need for greater accuracy is obvious.

Because of uncertainties regarding the advisability of keeping our data for the lattice of size 64, we recalculated the critical exponents ignoring the last point in each of the two graphs in Fig. 3. While the value of α/ν did not change significantly, $1/\nu$ went up to 1.61 ± 0.05.

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