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LETTER TO THE EDITOR

A test for hyperscaling violation in the three-dimensional Ising model†

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Abstract. Monte Carlo methods are used to compute the renormalised coupling constant of the three-dimensional Ising model for different values of the correlation length. For an appropriate choice of parameters the correlation length scales like N for a lattice with N^3 sites. By increasing N from $N=3$ to $N=60$, we observed a systematic downward trend by more than twice the statistical error for a quantity which should be constant if hyperscaling is valid.

A recent high-temperature analysis of the three-dimensional Ising model by Baker and Kincaid (1981) shows a small but persistent violation in certain scaling relations among critical exponents. The major uncertainty in these calculations is the extrapolation of the correlation length series from small to large ξ^2. This is accomplished by using Padé approximant techniques to resum a truncated power series in inverse temperature into a form that exposes the singular behaviour of ξ^2 near the critical point.

An important input into this resummation was the parametrisation of the correlation length in the scaling region. Although the leading singularity is expected to diverge like a power, there are few constraints on the number and variety of weaker singularities in ξ^2. Nickel (1982) has proposed that in addition to the leading scaling term there is a cut structure in ξ^2 which produces significant corrections to the previous results of Baker and Kincaid (1981). In the analysis by Nickel all scaling violations seem to disappear to the order calculated. An additional study (McKenzie and Lookman 1982), based on an examination of the behaviour of the spatial behaviour of the series coefficients of the spin–spin correlation function, concludes that the numerical data do not support the hyperscaling relation $d\nu = 2-\alpha$ in three dimensions.

Although scaling may indeed hold for the three-dimensional Ising model, clearly another approach is needed to resolve the issue. In this article we use Monte Carlo methods to evaluate thermodynamic quantities numerically as a function of lattice size. By increasing N we can study the approach to scaling. An important feature about Monte Carlo is that thermodynamic averages are determined at least in theory without resorting to approximation schemes. The errors we encounter in practice are easier to analyse since they are statistical in nature. For the range of correlation lengths we studied, we believe that Monte Carlo provides a reliable non-perturbative guide to the physics.

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The standard spin-$\frac{1}{2}$ Ising model is defined by the partition function

$$Z = \sum_{\{S_i\}} e^{-H}, \qquad H = \beta \sum_{NN} S_i S_j + h \sum_i S_i, \tag{1}$$

where the Ising Hamiltonian consists of a sum over nearest-neighbour spin pairs with $\beta = J/kT$ and the interaction of all the spins in a constant magnetic field h. We have incorporated the temperature dependence into the Hamiltonian and J is the exchange energy. The spins are defined on lattice sites in a d-dimensional cubical crystal, where each $S(i)$ can take two values denoted by $+1$ and -1. Given a polynomial of spin variables $F(S_1, S_2, \ldots, S_j)$, its *connected* average value is obtained from

$$\langle F \rangle_c = F(\delta/\delta h_1, \delta/\delta h_2, \ldots, \delta/\delta h_3) \ln Z(\beta, h). \tag{2}$$

In terms of Z, and the Hamiltonian H, the unsubtracted average value is defined by

$$\langle F \rangle = Z^{-1} \sum_{\{S_i\}} F(S_1, S_2, \ldots, S_j) \exp(-H). \tag{3}$$

From now on both $\langle F \rangle_c$ and $\langle F \rangle$ will be evaluated at $h = 0$ unless otherwise indicated.

The magnetisation in a weak field, above the critical temperature, can be written in terms of connected cumulant averages as

$$M \equiv \left\langle \sum_i S_i \right\rangle = \sum_{n=0}^{\infty} \frac{h^{2n+1}}{(2n+1)!} \left\langle \left(\sum_i S_i \right)^{2n+2} \right\rangle_c. \tag{4}$$

Each cumulant average is extensive. The $n = 0$ term in (4) defines the zero field susceptibility

$$\chi = \left. \frac{\delta M}{\delta h} \right|_{h=0} = \left\langle \left(\sum_i S_i \right)^2 \right\rangle \tag{5}$$

which is expected to diverge as $\chi \sim (\beta_c - \beta)^{-\gamma}$ near the critical point β_c. The divergences of the high-order correlations in (4) define the gap exponents Δ_{2n}, by the relation for $n \geqslant 1$

$$\left\langle \left(\sum_i S_i \right)^{2n+2} \right\rangle_c \Big/ \left\langle \left(\sum_i S_i \right)^{2n} \right\rangle_c \sim (\beta_c - \beta)^{-2\Delta_{2n+2}}. \tag{6}$$

The correlation length ξ in units of the lattice spacing is defined as

$$\xi^2 = M_2/(2d\chi) \tag{7}$$

where M_2 is the second spin moment

$$M_2 = \sum_{i,j} (i-j)^2 \langle S_i S_j \rangle. \tag{8}$$

The correlation length is a measure of the spin–spin correlation in the lattice and is expected to diverge at the critical point as $\xi \sim (\beta_c - \beta)^{-\nu}$.

If we assume that ξ is the only relevant lengthscale for physical quantities near the critical point (Fisher 1967), then the behaviour of all the $n > 0$ terms in (4) is determined by dimensional arguments. We shall define as physical any scale-invariant function of the spin variables. One such class of functions are the ratios of cumulants given by

$$R_{n+1} \equiv \left\langle \left(\sum_i S_i \right)^{2n+2} \right\rangle_c \Big/ \left\langle \left(\sum_i S_i \right)^2 \right\rangle_c^{n+1}, \tag{9}$$

where the volume dependence of $R_{n+1} \sim V^{-n}$. Since the ratio of cumulants is dimensionless, the scaling hypothesis predicts that as ξ^2 becomes large compared with the lattice spacing

$$R_{n+1} \to k_n \xi^{nd} / V^n \tag{10}$$

where k_n is some numerical constant. Combining the known divergences of χ and ξ with equation (10), we find that the cumulants diverge as

$$\left\langle \left(\sum_i S_i \right)^{2n+2} \right\rangle_c \sim (\beta_c - \beta)^{-\gamma - n(\gamma + d\nu)}. \tag{11}$$

From (6) and (11) we finally obtain the hyperscaling relations among the critical exponents

$$2\Delta_{2n} = 2\Delta = \gamma + d\nu, \tag{12}$$

where $\Delta = \lim_{n \to \infty} \Delta_{2n}$.

Equation (12) is rigorously known as an inequality (Baker 1968, Schrader 1976, Baker and Krinsky 1977), $2\Delta_{2n} \leqslant 2\Delta \leqslant \gamma + d\nu$, since multi-spin correlations cannot extend over a larger range than the pair correlations. The simplest test of hyperscaling is based on the calculation of R_2, or equivalently, the renormalised coupling constant defined by

$$g_R = \frac{V}{\xi^d} \left\langle \left(\sum_i S_i \right)^4 \right\rangle_c \Big/ \chi^2 \tag{13}$$

where for unit lattice spacing $V = N^d$. If the exact renormalisation group equations are correct then (12) must be satisfied and the constants k_n are universal (depending only on the dimension d and the internal symmetry of the Hamiltonian) (Fisher 1967, Kadanoff 1971, 1976).

Physical crystals have a large but finite number of spins and for a finite system our order parameters can never become singular. It is clear since $0 \leqslant \langle S_i S_j \rangle \leqslant 1$ that for a finite-size system the correlation length can never become larger than the size of our box, that is, $\xi < N$. Nevertheless, we can examine the approach to the infinite-volume limit by increasing N with the correlation length parametrised as

$$\xi = cN, \tag{14}$$

where c is a dimensionless constant satisfying $c < 1$. In a field theory $c = 1/m_R L$, where m_R is a renormalised mass and L is the *fixed*, physical length of the system. As we increase the size of our crystal, keeping c fixed, we can solve (7) for the value $\bar{\beta}$ which satisfies (14). In the limit $N \to \infty$ we are obviously driven to the critical point of the Ising model so $\bar{\beta} \to \beta_c$. Near the critical point, $|\beta_c - \bar{\beta}| \ll 1$, g_R should behave as

$$g_R(\bar{\beta}) \sim (\beta_c - \bar{\beta})^{\gamma + d\nu - 2\Delta}, \tag{15}$$

while

$$\xi(\bar{\beta}) \sim (\beta_c - \bar{\beta})^{-\nu}. \tag{16}$$

Using (14) and (16) to write $(\beta_c - \bar{\beta})$ as $N^{-1/\nu}$, we obtain a scaling formula for the coupling as a function of the lattice size

$$g_R \sim N^{-\omega^*} \tag{17}$$

where $\omega^* = (\gamma + d\nu - 2\Delta)/\nu$. The critical exponent ω^* is often referred to as the

anomalous dimension and satisfies the inequality $\omega^* \geqslant 0$ (Schrader 1976, Baker and Krinsky 1977). If hyperscaling holds, then ω^* must be identically zero and g_R approaches a universal constant as $N \to \infty$, otherwise g_R vanishes in the infinite-volume limit.

The actual value of c in (14) is arbitrary, since in theory we can choose N large enough so that $|\beta_c - \bar{\beta}| \ll 1$ is satisfied. The larger the value of c the faster the convergence to the scaling region. This effect can be important when limitations in size are considered. To minimise finite-size effects, however, we would like to make c as small as possible. Our choice for c will be a compromise between these two requirements. In practice, c is fitted by comparing g_R versus ξ^2 for *strong* coupling perturbation theory with our numerical simulations. The convergence of a strong coupling expansion with a finite number of terms is expected to be best when N is small.

We evaluate the cumulant averages and the second spin moment by a Monte Carlo procedure. The outline of the method we use is standard. Starting with some conveniently chosen initial configuration of spin variables $S(i)$, we sweep through the lattice, updating each $S(i)$ according to a certain random algorithm. The result of each complete sweep is counted as a single new configuration. For a correctly chosen updating algorithm, the ensemble of configurations generated in this way gives a finite sequence of occurrences of random lattice spin variables distributed according to the probability $Z^{-1}\exp(-H)$. The ensemble average of F then approaches $\langle F \rangle$ in equation (3) as the size of the ensemble approaches infinity.

We used the heat bath method of Creutz (1979a, b) as our Monte Carlo algorithm to update the spin variables in the lattice. To obtain an updated spin variable at site i, we compute the local Boltzmann distribution:

$$P_i = \begin{cases} P_+(S_i) = e^{A_i}/(e^{A_i} + e^{-A_i}) \\ P_-(S_i) = 1 - P_+(S_i) \end{cases} \tag{18}$$

where P_+ is the probability that $S(i)$ is up, P_- is the probability that $S(i)$ is down, and the variable A is computed by adding all the nearest-neighbour spins around site i

$$A_i = \beta \sum_{\mu=1}^{d} (S(i+e_\mu) + S(i-e_\mu)). \tag{19}$$

Choosing a random number r uniformly distributed on the unit interval, we set $S(i) = +1$ if $r \leqslant P_+$, otherwise $S(i) = -1$. By sweeping once through the *entire* lattice updating every spin in this way, we generate *one* new spin configuration for our ensemble.

After updating all the $S(i)$, the Fourier transform of the new spin field is constructed at zero momentum

$$\tilde{S}(0) = \sum_i S(i). \tag{20}$$

Taking ensemble averages of $(\tilde{S}(0))^n$ for various n, we obtain values for the cumulants in (4). The previous definition for the correlation length, however, must be modified for a finite-size lattice with periodic boundary conditions. We use the definition of ξ^2 of Cooper *et al* (1982),

$$\xi_F^2 = [\langle \tilde{S}(0)^2 \rangle / \langle \tilde{S}(k)^2 \rangle - 1]\hat{k}^{-2} \tag{21}$$

where $\tilde{S}(k)$ is the Fourier transform of the spin field at momentum $\hat{k} = (2\pi/N, 0, 0)$. Equation (21) is exact for a Gaussian model in any dimension and an Ising model in

one dimension provided $\hat{k}^2$ is replaced by $4\sin^2(\frac{1}{2}k)$. For $N \gg \xi$, (21) reduces to the infinite-volume definition of the correlation length.

It is important to stress that for a finite-volume system, (8) and (21) are in general not the same. Nevertheless, (21) is invariant under the rescalings $\{S_i\} \to \{S_i'\} = Z^{1/2}\{S_i\}$, and so ξ_F defines another physical length. In fact, ξ_F must scale, by dimensional arguments, like

$$\xi_F = \xi F(k\xi). \tag{22}$$

Now if we make ξ satisfy (14), then $\xi_F = F(2\pi C)\xi \sim N$ where $N^{-1/\nu} \sim (\beta_c - \bar{\beta})$. Thus replacing ξ by ξ_F in equation (13) does *not* change how g_R scales with N, even though the coupling and correlation length may be distorted by finite-size effects! From now on we will drop the subscript on ξ_F unless the context is unclear. A Monte Carlo evaluation of g_R is now straightforward.

The amount of computer time required to generate a new spin configuration is proportional to the update time, $\Delta\tau_s$, for a single spin. Minimising $\Delta\tau_s$ becomes an important cost consideration if we wish to perform computer simulations on large lattices. For this reason it was extremely useful to reparametrise each spin variable as $S(i) = 2X(i) - 1$, where the corresponding X's are either 1 or 0. Since each $X(i)$ requires only one binary digit to record the value of a spin, it is possible to record the values of many spins in the same computer word. If this packing of information is done according to the multi-spin coding prescription of Jacobs and Rebbi (1981), then beyond reducing memory requirements it also allows arithmetic operations involving many spins to be performed at once. For example, the index

$$J_i = \sum_{\mu=1}^{d} (X(i+e_\mu) + X(i-e_\mu)) + 1 \tag{23}$$

which runs from 1 to $2d+1$ can be computed for several different sites at once. If we construct an array of probabilities given by

$$P_+(J) = 1/\{1 + \exp[4\beta(J-d-1)]\} \tag{24}$$

the correct probability factor for site i is just $P_+(J_i)$. Since an array call to a small array is much faster than calculating P_+ every time we update a spin, we can use a table look-up method with multi-spin coding to parallel process the updating of spins on the lattice. Due to the simplicity of this updating procedure, we were able to optimise this portion of our program by writing it in assembly language. As a result of all these steps $\Delta\tau_s$ was estimated to be 0.4 microseconds on a CDC 7600 computer. We used of the order of 100 hours of 7600 time to measure accurately g_R for different values of ξ.

We now present our numerical results for the three-dimensional Ising model. Working first on small lattices of $N = 3$ and 4, we measured g_R for different values of c. By comparing these results with high-temperature and strong coupling predictions for the same range of ξ, we found that finite-size effects were made small (less than 5 to 10 per cent) for $c < 0.3$. Also in previous work (Cooper *et al* 1982) in two dimensions, a value of $(\xi/N)^2 = \frac{1}{36}$ was found to be satisfactory, but $(\xi/N)^2 = \frac{2}{45}$ showed slight finite-size effects. Similarly in previous work (Freedman *et al* 1982) in three dimensions, good results which compared well with the Callan–Symanzik predictions of g_R and Wegner's correction-to-scaling index, ω, were obtained with $(\xi/N)^3 \simeq 0.021$, which corresponds to $c \simeq 0.28$. It appears that the ratio of the correlated volume to

the total volume is the important practical criterion for g_R. Choosing $c = 0.275$, we used (14) to eliminate N in favour of ξ. Typically five values of β were tried before ξ was reproduced to within a few per cent for each N. Table 1 shows $\bar{\beta}$ versus N for $N = 3$, 6, 12, 24 and 60. High-temperature expansions yield $\beta_c \sim 0.2217$. Knowing $\bar{\beta}$ for each N, we computed the corresponding renormalised coupling constant $g_R(\bar{\beta})$. Table 1 shows g_R versus ξ^2 from our Monte Carlo simulations. Table 2 shows the results from the high-temperature series analysis by Baker and Kincaid (1981) and the strong coupling analysis of Baker *et al* (1981) over a similar range of correlation lengths. Both Monte Carlo and high-temperature investigations show a region of small ξ in which the coupling stabilises around the value $g_R = 25$. For ξ larger than 6.5 the renormalised coupling decreases with an apparent critical exponent of $\omega^* \sim 0.2$. When at most six internal lines are included in the strong coupling expansion, g_R is predicted to be 28.4 in the limit $\xi \to \infty$ (Baker *et al* 1981, Bender *et al* 1979).

Table 1. Monte Carlo data for g_R versus lattice size N, inverse temperature β, and correlation length ξ.

N	$\bar{\beta}$	ξ^2	g_R(MC)
3	0.1720	0.68	42.36 ± 1.8†
6	0.1950	2.72	27.8 ± 1.0
12	0.2120	10.89	25.0 ± 0.9
24	0.2170	43.56	24.2 ± 0.7
40	0.2200	121.00	22.3 ± 0.7
60	0.2208	272.25	19.2 ± 0.5

† Strong coupling predicts $g_R = 44.74$ for $\xi^2 = 0.68$.

Table 2. High-temperature† and strong coupling‡ estimates for g_R versus ξ.

ξ^2	g_R(HT)	g_R(SC)
1	38.80 ● 0.05	39.75
4	29.50 ± 0.05	31.41
16	25.5 ± 0.10	29.18
32	24.0 ± 1.0	28.81
64	22.8 ± 1.2	28.62
256	20.6 ± 1.8	28.47

† From the analysis in Baker and Kincaid (1981).
‡ From the analysis in Baker *et al* (1981).

A major difficulty in studying the behaviour of $g_R(\xi^2)$ on significantly larger lattices would be the enormous size of our ensembles†. On a $6 \times 6 \times 6$ lattice we used five independent subensembles each with 30 000 spin configurations to measure g_R to ~5%. In contrast, each subensemble for a $60 \times 60 \times 60$ lattice required 300 000 spin configurations to achieve the same accuracy. The longer 'time' in the Markov chain over which we sampled spin configurations was due primarily to the critical slowing down

† A fast processor for Monte Carlo simulations of the three-dimensional Ising model is being developed at Santa Barbara which will update 30 million spins per second on a $64 \times 64 \times 64$ lattice. For details see Pearson *et al* (1981).

of the crystal as we approached the critical point. Typically 20% of each run was discarded to get into equilibrium.

In conclusion, we have tested hyperscaling in the three-dimensional Ising model by measuring the renormalised coupling constant as a function of correlation length. The major difficulty in comparing our numbers with other studies is the distortion of g_R and ξ caused by our working in a finite volume, relative to the renormalised mass. We estimate this to be $\sim 10\%$ effect. However, the finite-size scaling formula for g_R, and hence the anomalous dimension, is unaffected by our choice for c. Our Monte Carlo data show a consistent downward trend in g_R as we increased N. For lattices with $N \leqslant 60$ we observed no stabilisation of the coupling. We conclude that larger lattices are required to see hyperscaling in these numerical simulations, if it is to be seen at all. Finally, the large value for g_R predicted by strong coupling as $\xi \to \infty$ was probably due to the shortness of the series used to Padé g_R and ξ.

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