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LETTER TO THE EDITOR

Vectorised dynamic Monte Carlo renormalisation group for the Ising model

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Abstract. Applying the dynamic Monte Carlo renormalisation group to the Glauber kinetic Ising model, the dynamical critical exponent z is found by simulation of up to 8192^2 and 512^3 spins on the vector computer CDC Cyber 205, using the new 'Method of 2^d colours' for the Monte Carlo part (update speed 22 megaspins/s). The two-dimensional result $z = 2.14 \mp 0.02$ disagrees with Domany's hypothesis. For three dimensions, a systematic trend in z with increasing blocksize leads to an extrapolated value $z = 1.965 \mp 0.010$, which is consistent with a theoretically expected value 2.02.

Since the idea of combining Monte Carlo (MC) simulation and renormalisation group analysis was initiated by Ma (1976), successive work refined and applied it to the Glauber and Kawasaki kinetic Ising model (Tobochnik *et al* 1981, Swendsen 1982, Katz *et al* 1982, Yalabik and Gunton 1982, Pawley *et al* 1984). This sort of analysis allows only for the simulation of relative small systems such as 16^3; thus the resulting values for critical exponents are possibly systematically wrong because of boundary and finite-size effects.

The present work will use the new and simple dynamic Monte Carlo renormalisation group (MCRG) analysis of Jan *et al* (1983) to determine the dynamical critical exponent z. Previous results using different methods resulted in different values for z in three dimensions; $z = 2.17 \mp 0.06$ was found (Chakrabarti *et al* 1981) by MC simulations above T_c, MC renormalisation resulted in $z = 2.08$ (Yalabik and Gunton 1982), and an earlier study using the dynamic MC renormalisation group of Jan *et al* (1983) gave $z = 2.11 \mp 0.03$. By interpolation between two epsilon expansions a value of $z = 2.02$ was found (Bausch *et al* 1981) in contradiction with these Monte Carlo estimates. In order to calculate a more precise value for z with Jan's method and to settle that controversy we perform MC simulations for Glauber Ising models at $T = T_c$ with large sizes up to 512^3 in three and 8192^2 in two dimensions on a vector computer (CDC Cyber 205 at Bochum University) and analyse their results.

We consider a system in its initial state with all spins parallel, which can be understood as a magnetisation $M = 1$. Using the standard Monte Carlo procedure (Binder 1984), we follow the system's relaxation into equilibrium. As the temperature for the simulation, we choose the critical temperature $T_c = 1/0.221\,655$ (Pawley *et al*

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1984). The process of block spin renormalisation then is used to replace a block of b^d neighbouring spins (in the d-dimensional square or cubic lattice) by one renormalised block spin. Its orientation is determined by the orientation of the majority of the original spins in the b^d cell. These renormalised spins form again another lattice for which a magnetisation M_b can be determined. The magnetisation of the primary spins approaches a fixed value M_1 after a time t; we will find another time t_b, where the magnetisation of the (b^d)-block spin lattice will reach the same value M_1. Using two different block sizes b and b' and comparing the times t_b and $t_{b'}$ at which the magnetisations $(M_b, M_{b'})$ of two (b, b') block spin lattices renormalised from the same system reach the same fixed value M_1, yields the relation (Jan *et al* 1983)

$$t_b/t_{b'} = (b/b')^z, \tag{1}$$

which can be written as

$$z = \log(t_b/t_{b'})/\log(b/b'), \tag{2}$$

to define z for b and $b' \to \infty$.

In comparison with MC simulations on a scalar computer (Zorn *et al* 1981, Kalle and Winkelmann 1982), the implementation of the algorithm on a vector computer requires some profound changes. Starting from an existing program (Wansleben *et al* 1984), our lattice was divided into 2^d interpenetrating sublattices, also to allow for simple vectorisation of the first renormalisation blocking procedure from 2^d primary spins. Instead of the manufacturer-supplied random-number generator RANF, the shift-register method (Tausworthe 1965, Kirkpatrick and Stoll 1981) had to be used for the spin-flip decisions because RANF led to a systematically wrong trend for the magnetisation at long times (Kalle and Wansleben 1984). Further refinement of the program led finally to a speed of about 22×10^6 spin-flip attempts per second, which may be a world record for the Metropolis method on general purpose computers. About 50 hours of central processor time was used in total. The renormalisation part of the program took only about one percent of computer time for the three-dimensional system, as opposed to most other renormalisation methods. A copy of the computer program is available upon request.

In three dimensions, 128^3, 256^3, and 512^3 systems and in two dimensions, 1024^2, 2048^2, 4096^2 and 8192^2 lattices were simulated in many runs with times up to 1000 or 10 000 Monte Carlo steps per spin. (A 1080^3 system was simulated at $T = 1.4T_c$ as a feasability study using a Cyber 176, resulting in relaxation times $\tau_1 = 2.89 \mp 0.01$ and $\tau_2 = 0.55 \mp 0.15$ for the ansatz $M = a_1 e^{-t/\tau_1} a_2 e^{-t/\tau_2}$.) Figure 1 shows the result obtained by 265 runs each up to 1000 steps for the 128^3 system. The Monte Carlo error for each point is smaller than the symbol size. Besides the magnetisation curve for the primary spin lattice ($b = 1$), the curves for the different renormalised lattices ($b = 2$, 4, 8 ...) can be seen. Equation (2) requires that these curves can be made to coincide by a rescaling of time, which corresponds to a shift to the left or right on the logarithmic time scale. As the reader may check by superimposing two copies of this plot, the curves for $b = 1$ and $b = 2$ do not allow for a good match, whereas the others can be made to coincide well (Jan *et al* 1983). To recognise even weak effects of cell size b and trends with the value M used to compare the curves, different intervals in M were chosen to compute the resulting z. Table 1 gives an example of our resulting estimates for z.

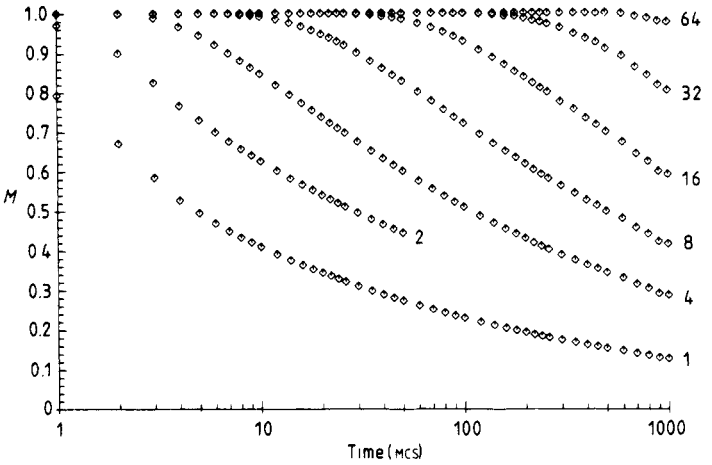

Figure 1. Variation of the original and renormalised magnetisation with time. The number on each curve gives the block spin size b.

Table 1. Exponent estimates for z resulting from simulation of a 1024^2 lattice (250 runs with 1000 MC steps per spin) obtained by averaging over four values M near 0.925, 0.875, 0.825 and 0.775.

b/b'	1	2	4	8	16
2	1.69				
4	2.15	2.38			
8	2.30	2.29	2.16		
16	—	2.15	2.13	2.15	
32	—	2.10	2.09	2.15	2.14

Table 2. Exponent estimates for z resulting from simulation of a 128^3 lattice (265 runs up to 1000 MC steps per spin) obtained by averaging over four intervals M near 0.85, 0.75, 0.65 and 0.55.

b/b'	1	2	4	8	16
2	2.06				
4	2.04	2.00			
8	2.09	2.09	2.17		
16	2.05	2.09	2.13	2.09	
32	—	2.04	2.10	2.07	2.04

An exact value for z in two dimensions with logarithmic corrections was suggested by Domany (1984), which in our case gives

$$z = 2 + x/\log(b).$$

Figure 2 shows a plot of the values z resulting from simulations of the 1024^2 and 2048^2 systems against $1/\log(b)$. There is no obvious trend for z with varying b, and even if such a trend is suggested, the extrapolated z for $b \to \infty$ does not approach $z = 2.00$,

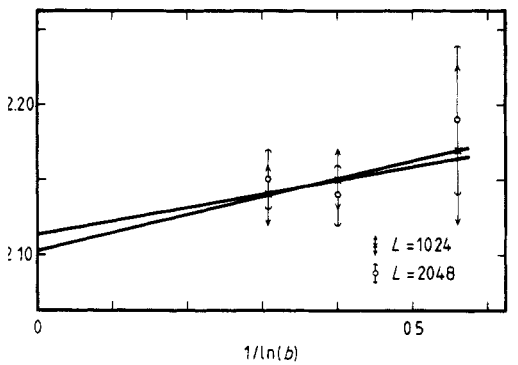

Figure 2. Test for trend in z with increasing b in two dimensions. Resulting values z for different block spin sizes b ($b = 2b'$) are plotted against $1/\ln(b)$. $z(b) = z(b=\infty) + \text{constant}/\ln(b)$; $z(b=\infty, 1024^2) = 2.10 \pm 0.04$; $z(b=\infty, 2048^2) = 2.11 \pm 0.04$.

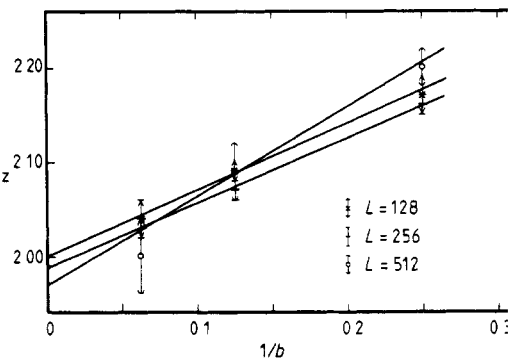

Figure 3. Test for systematic trend with increasing b in three dimensions. For all three simulated system sizes, the results z are plotted against $1/b$. $z(b) = z(b=\infty) + \text{constant}/b$; $z(b=\infty, 128^3) = 2.00 \pm 0.03$; $z(b=\infty, 256^3) = 1.99 \pm 0.03$; $z(b=\infty, 512^3) = 1.97 \pm 0.05$.

but tends to about $z = 2.11$. The influence of the simulated system size was found to be marginal, So our data does not support Domany's hypothesis. Averaging over all treated system sizes and pairs b, b' with $b = 2b'$ leads to a value

$$z = 2.14 \qquad (d = 2) \tag{3}$$

with a probable error of about 0.02.

The simulations done for the three-dimensional model revealed systematic trends overlooked in the earlier paper (Jan *et al* 1983), which in view of the computer power involved in this work is not surprising. As in the two-dimensional case, one finds that the values z obtained with block spin lattices $b = 1$ and $b = 2$ are not reliable. Detailed analysis again shows no clear systematic trend in z for decreasing magnetisation M or increasing system size. Jan *et al* could not detect a trend in z for increasing block spin size b. To test our results for such a trend, we plot in figure 3 the values z resulting from our three-dimensional data for all three system sizes against the block spin size $b = 2b'$ used to determine them. These points clearly suggest a systematic trend to lower values z for increasing b. Assuming the ansatz $z = z_{b=\infty} + \text{constant}/b$ we can extrapolate as in figure 3 by a best fit:

System size	128^3	256^3	512^3
$z_{b=\infty}$	2.00	1.99	1.97
$\Delta z_{b=\infty}$	0.03	0.03	0.05

(Note that if one would average over all estimated values for z, as Jan *et al* did, a mean of 2.12 ∓ 0.02 would result, which is comparable with their result $z = 2.11 \mp 0.03$.) The influence of system size again can be considered marginal; so a weighted mean

$$z = 1.99 \mp 0.03 \qquad (d = 3), \tag{4}$$

can be regarded as an estimate for z in three dimensions using the above ansatz. (The

analysis of the original magnetisation for the primary spins using the relation $M \propto t^{-\beta/\Delta}$ and $z = \Delta/\nu$ yields with $\beta/\nu = (1+\eta)/2 = 0.515$ (Pawley 1984) a value $z = 2.04 \mp 0.04$ which supports the extrapolated z.)

A more general ansatz for the trend of z for increasing b is

$$z = z_{b=\infty} + \text{constant } b^{-\Omega}.$$

Figure 4 shows the estimated z with different exponents Ω. Assuming $0.5 < \Omega < 1.5$ ($\Omega > 2$ seems incompatible with our data), our final estimate is

$$z = 1.95 \mp 0.10 \qquad (d = 3). \tag{5}$$

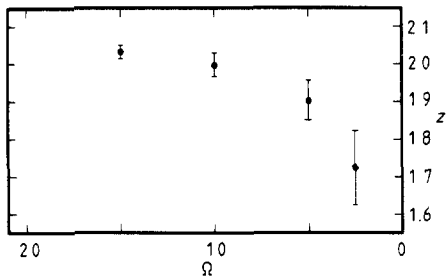

Figure 4. For the ansatz $z = z_{b=\infty} + \text{const } b^{-\Omega}$, estimates of z_∞ for different Ω are shown. A reasonable interval for Ω is $0.5 < \Omega < 1.5$.

This number is obviously different from the results given in some earlier papers (2.11, 2.17, 2.08; see introduction). By investment of much computer power it was possible for the first time to notice the trend of z for increasing block size b in three dimensions (as opposed to two dimensions) and so our z systematically shifts away from earlier values obtained with less computer time. However, our $d = 3$ result neatly fits with within the theoretically obtained value $z = 2.02$ of Bausch *et al.* More details are found in Kalle (1984).

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