A Monte Carlo renormalisation group calculation of the dynamical exponent z for the Baxter-Wu model

LETTER TO THE EDITOR

A Monte Carlo renormalisation group calculation of the dynamical exponent z for the Baxter–Wu model

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Abstract. A Monte Carlo renormalisation group technique is used to calculate time correlation functions for the Baxter–Wu model. Initial lattices of size 24×24 and 48×48 are used. The value obtained for the dynamical exponent z is in good agreement with that obtained by means of standard Monte Carlo methods.

Recently, several attempts have been made to calculate the dynamical exponent z for various model systems. Although some calculations have utilised standard Monte Carlo (Stoll *et al* 1973) or renormalisation group (Achiam 1980, Mazenko and Valls 1981) techniques, the most promising results have been obtained using a dynamic Monte Carlo renormalisation group method (DMCRG) developed by Tobochnik *et al* (1981). However, attempts to test the DMCRG method have been hampered somewhat by the lack of model systems for which dynamical exponents have already been obtained. Therefore, with the exception of the three-state Potts model (Tobochnik and Jayaprakash 1982), the DMCRG has so far been applied only to the kinetic Ising model with near neighbour interactions in two and three dimensions (Tobochnik *et al* 1981, Yalabik and Gunton 1982, Katz *et al* 1982). In this note, the DMCRG is applied to obtain the exponent z for the kinetic Ising model with spin-flip (Glauber 1963) dynamics on a triangular lattice with triplet interactions. The results are in good agreement with those obtained for this model by means of standard Monte Carlo techniques (Katz *et al* 1979, Katz and Gunton 1981).

The zero field equilibrium properties of the Ising model on a triangular lattice with triplet interactions have been solved exactly by Baxter and Wu (1973, 1974). The model is described by the reduced Hamiltonian

$$H = K \sum_{\langle ijk \rangle} S_i S_j S_k$$

where the sum is over all elementary triangles of the lattice. The critical temperature is known exactly to be $K_c = \ln(\sqrt{2}+1)/2$. The ground state of this Hamiltonian is fourfold degenerate and the system is believed to belong to the same static universality class as the four-state Potts model. The ground state magnetisation can be either $M = 1$ (a single ferromagnetic state) or $M = -\frac{1}{3}$ (for which there are three possible states). The $M = -\frac{1}{3}$ states have spins up on one triangular sublattice and down on the other two sublattices. A renormalisation group transformation applied to such a

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system must keep the ground states of the system invariant. One such transformation has been used by den Nijs *et al* (1976) in a renormalisation group treatment of the equilibrium statics of this model and yields critical exponents consistent with the exact results. Figure 1 shows the cell division for this transformation. The new cell spin is defined as the sign of the sum of the three spins which compose the cell. Note that some spins are not included in any cell and are simply dropped in the next renormalisation. Because of the three equivalent sublattices and the use of periodic boundary conditions, the linear dimension of any lattice chosen for a Monte Carlo study must be a multiple of 3. Since application of the blocking rule reduces the linear dimension by a factor of $b = 2$ at each iteration, the choice of the initial size of our lattices was severely restricted. We chose lattices of size 24×24 and 48×48 with periodic boundary conditions. Both lattices were renormalised down to a 6×6 lattice, as an examination of figure 1 will reveal that renormalising to a 3×3 lattice would require overlapping cells.
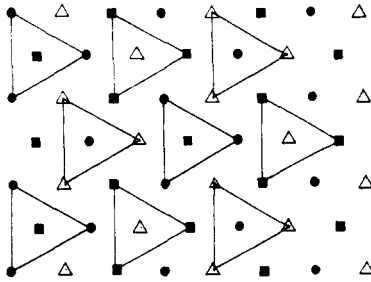

Figure 1. The three sublattices, with the cells indicated by the full lines.

The DMCRG method has been discussed in detail by Tobochnik *et al* (1981), so we will only summarise that method here. We determine z by matching the time correlation functions

$$C(N, m, T_2; t) = C(Nb^d, m+1, T_1; b^z t) \tag{1}$$

where

$$C(N, m, T; t) = (N^m)^{-1} \left\langle \sum_i S_i^{(m)}(t) S_i^{(m)}(0) \right\rangle_{T,N}. \tag{2}$$

The number of spins in the original lattice is N, and $N^{(m)}$ is the number of block spins $S^{(m)}$ after m applications of the blocking rule. Using standard Monte Carlo techniques, we generated a sequence of spin configurations on lattices of size 24×24 and 48×48. Then, using the blocking rule described above, each configuration was blocked down to a 6×6 lattice. The time correlation functions defined in (2) were computed after each blocking. Since we were interested in the fixed point solution we set $T_1 = T_2 = T_c$, where T_c is the critical temperature of the infinite system. We averaged over 301 independent runs of 20 000 Monte Carlo steps per spin (MCS) for each lattice. Also, in each run, 15 000 MCS were eliminated before any averages were taken. Using many different statistically independent runs facilitates the calculation of errors.

Our results for the static energy

$$E(t = 0) = \sum_{\langle ijk \rangle} S_i S_j S_k \tag{3}$$

are shown in table 1. We note that matching occurs in the last iteration to within one standard deviation. We note also that in spite of the large number of Monte Carlo runs used (a total of 6×10^6 MCS for each lattice), the standard deviations for the static averages are quite large.

Table 1. Results for the energy as defined in (3). N is the number of spins in the original lattice and m is the number of renormalisation transformations performed.

	2^m	$N = 24 \times 24$		2^m	$N = 48 \times 48$
$E(0)$	1	1.5502 ± 0.0026	$E(0)$	1	1.5129 ± 0.0039
	2	1.4865 ± 0.0045		2	1.4217 ± 0.0067
	4	1.5574 ± 0.0060		4	1.4663 ± 0.0094
				8	1.5508 ± 0.0128

The results of our calculation of the time correlation functions $C(N, m, T; t)$ are given in table 2. For large times the data for $C(t)$ can be represented by exponential decay,

$$C(N, m, T; t) = A_m^{(N)} \exp(-t/\tau_m). \tag{4}$$

Figure 2 is a plot of $C(t)$ against t after renormalisation down to a 6×6 lattice. Since we are at the fixed point, we would expect to find $A_m^{(N)} = A_{m+1}^{(Nb^d)}$. However, an

Table 2. Results for the correlation function $C(t)$ as defined in (2). The time unit is Monte Carlo steps per spin.

	2^m	$N = 24 \times 24$		2^m	$N = 48 \times 48$
$C(10)$			$C(80)$	1	0.5694 ± 0.0043
	1	0.7009 ± 0.0019		2	0.6502 ± 0.0047
	2	0.7852 ± 0.0020		4	0.7435 ± 0.0050
	4	0.8606 ± 0.0019		8	0.8336 ± 0.0051
$C(20)$			$C(120)$	1	0.5543 ± 0.0046
	1	0.6643 ± 0.0023		2	0.6335 ± 0.0051
	2	0.7499 ± 0.0024		4	0.7264 ± 0.0055
	4	0.8356 ± 0.0023		8	0.8195 ± 0.0056
$C(30)$			$C(160)$	1	0.5445 ± 0.0048
	1	0.6463 ± 0.0025		2	0.6226 ± 0.0053
	2	0.7314 ± 0.0026		4	0.7149 ± 0.0058
	4	0.8204 ± 0.0026		8	0.8094 ± 0.0059
$C(40)$			$C(200)$	1	0.5371 ± 0.0049
	1	0.6346 ± 0.0026		2	0.6144 ± 0.0055
	2	0.7191 ± 0.0028		4	0.7062 ± 0.0060
	4	0.8094 ± 0.0028		8	0.8014 ± 0.0063
$C(50)$			$C(240)$	1	0.5315 ± 0.0051
	1	0.6260 ± 0.0027		2	0.6081 ± 0.0057
	2	0.7100 ± 0.0029		4	0.6993 ± 0.0062
	4	0.8011 ± 0.0029		8	0.7950 ± 0.0065
$C(60)$			$C(280)$	1	0.5268 ± 0.0052
	1	0.6194 ± 0.0028		2	0.6028 ± 0.0058
	2	0.7029 ± 0.0030		4	0.6936 ± 0.0064
	4	0.7943 ± 0.0031		8	0.7895 ± 0.0067

Figure 2. A plot of ln $C(t)$ against time for 24×24 (crosses) and 48×48 (open circles) lattices after blocking down to a 6×6 lattice.

examination of figure 2 indicates this is not the case. A least squares fit to our data, assuming ln $C(t) \sim A + Bt$, yields $A_{24} = -0.1793$, $B_{24} = 0.000850$ and $A_{48} = -0.1843$ and $B_{48} = -0.000186$. Since $A_{24} \neq A_{48}$, the value of z obtained would be dependent on the points chosen for matching. The values of z range from $z = 2.01$ ($t = 50$ and $b^z t = 201.6$) to $z = 2.19$ at $t = \infty$. If, on the other hand, we require that the amplitudes A_{24} and A_{48} be equal at the fixed point, the values of z range from $z = 2.03$ to $z = 2.05$. These values are in good agreement with values obtained by means of a Monte Carlo study of the relaxation of the energy–energy and magnetisation–magnetisation time correlation functions. This study yielded a value of $z = 1.95$ with an estimated error of 10%. It should be noted that the standard Monte Carlo method yields an effective exponent, because one cannot be certain of the size of the asymptotic dynamical critical region. However, the calculation by means of DMCRG is performed at the critical point and such considerations are therefore unimportant. It should also be noted that the accuracy of the DMCRG method depends upon the assumption that the number of renormalisations performed is sufficient to eliminate the effect of irrelevant operators. Since matching is achieved for the static correlation function it is likely, but not a certainty, that this is the case. Finally, we point out that it is possible that a different choice of blocking rule would lead to a faster convergence.

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