Calculation of the dynamical exponent z for the three-state Potts model

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We have found using the dynamic Monte Carlo renormalization-group method that the dynamic critical exponent z for the three-state Potts model on a square lattice has the value 2.7 ± 0.4.

Recently, the dynamic critical exponent, z, has been computed for the one- and two-dimensional kinetic Ising model using a dynamic Monte Carlo renormalization-group (DMCRG) method.[1] We have chosen to look at the three-state Potts model to see if we could discern any difference in its value of z from that of the Ising model. Currently, there exists only one estimate of z for this model and that was by Forgacs *et al.*[2] who found using the Migdal RG transformation that $z=2.25$ for $q=3$, and $z=2.065$ for the Ising model. As far as we know there are no estimates from series calculations or numerical simulations.

Before proceeding to our calculation we will comment on the reliability of the DMCRG method. Recently, Mazenko and Valls (MV)[3] have claimed that none of the current methods including those not utilizing RG techniques were reliable for obtaining the dynamic critical exponent, z. MV's criticism of DMCRG consisted of claiming that it was not sensitive enough and that good static results and good one-dimensional (1D) results, were not sufficient checks on the method. They claim that the dynamic scaling regime may be very narrow in 2D.

However, we believe the DMCRG is reliable. The errors in Monte Carlo calculations can be reasonably well assessed, and thus its accuracy can be determined, and so far it has been found to be sufficient to make reasonable estimates for z. The possibility that the dynamic scaling regime is very narrow does not hinder the use of DMCRG since this calculation is made right at T_c which is known exactly for the q-state Potts models. In the DMCRG method the correlation length can be many times the size of the system simulated. The only requirement for the method to work is that the irrelevant variables die out quickly upon blocking. Also, Monte Carlo treats all dimensions on the same footing, unlike other methods which exploit certain simplifying features of 1D systems. Thus, a good result in 1D does carry weight in increasing the validity of the method in higher dimensions. The power of the DMCRG and static MCRG is that it allows one to obtain information on the infinite lattice by a clever use of Monte Carlo simulations of finite lattices. We will summarize the method below.

The reduced Hamiltonian for the Potts model[4] is defined as:

$$H = K \sum_{\langle ij \rangle} \delta_{s_i,s_j}, \quad s_i = 1,\ 2,\ \text{or}\ 3\ .$$

The sum is over nearest-neighbor spins on a square lattice. The dynamics of the model is given by the usual Metropolis rule where the transition probability equals $\min(e^{-\delta H}, 1)$ where δH is the change in the reduced energy in going from an old state to a new state by changing the value of one spin chosen at random.

We now review the DMCRG method. First we create a sequence of spin configurations using standard Monte Carlo methods at a coupling $K = J/k_B T$. From these configurations we construct a sequence of block spin configurations, where each block spin is formed out of four spins by the majority rule. Ties are broken by a random choice. From the block spin configurations we construct another sequence of block spins in the same way as above. This procedure is continued until we have reached a 2×2 lattice of block spins. At each blocking iteration, all length scales have been reduced by a factor of $b=2$. Thus, the correlation length has been reduced by a factor of 2 and the correlation time by a factor of b^z or 2^z. This is how the dynamic exponent z is defined. Any static average over the block spin system is an average of block spins weighted by the Boltzmann probability of the renormalized Hamiltonian. If the $l \times l$ block spin lattices of two spin systems have the same static averages then they must have the same Hamiltonian and the same correlation length. If we had to iterate m times on an N spin lattice and $m+1$ times on an Nb^d spin lattice at the same temperature to match static averages, then one block spin lattice

has a correlation length of ξ/b^m and the other $\xi/b^{(m+1)}$. Since they must have the same correlation length, ξ must equal infinity and we are at the critical temperature. Similarly, if a time-dependent average $E(t)$ of one block lattice and $E(t')$ of the second are equal then $t/t'=b^z$. In this way z can be determined. For our calculations we used the quantity:

$$E(K,t,m,N)=(1/N_m)\sum_{\langle ij\rangle} S_i^{(m)}(t)S_j^{(m)}(0) \ ,$$

where $S_i^{(m)}$ is a block spin after the mth iteration, N_m is the size of the block spin lattice, t is time measured in passes through the lattice, K is the reduced coupling, and N is the number of spins in the original lattice. The sum is over all nearest-neighbor pairs of spins or block spins. To verify K_c we check that

$$E(K_c,0,m,N)=E(K_c,0,m+1,4N)$$

for m sufficiently large. To determine z we find

$$E'(K_c,t,m,N)=E'(K_c,t',m+1,4N) \ ,$$

where

$$E'(K_c,t,m,N)\equiv E(K_c,t,m,N)/E(K_c,0,m,N) \ .$$

Dividing through by the static average will eliminate some of the error due to static quantities not matching exactly either because of statistical uncertainties or the remainder of small effects due to irrelevant operators or finite size effects.

Usually, in Monte Carlo simulations one takes a configuration and runs it for as long as possible to obtain an equilibrium average, and sometimes starts out with one or two other configurations to see if one gets the same results. We have found that after averaging over about 10 to 50 thousand passes there is no change in the average value obtained if the two systems started from the same configuration. However, if a different starting configuration was used a slightly different value was obtained (a fraction of a percent different). This is because there are very long correlation times at the transition and thus the system tends to stay in the same region of phase space. To get around this we used 100 different starting configurations where the spins had random values and ran each for 24 000 passes skipping the first 8000 passes for the purpose of equilibration. In addition to sampling more of phase space, this method has the advantage that when you compute standard deviations (SD) over the 100 data points you really have independent measurements and thus this computation is a reliable estimate of the error bars.

In Table I we show the results for lattices of 16, 64, and 256 spins. The static quantities appear to

TABLE I. DMCRG results. Column under N_m labels the size of the spin or block spin lattice over which averages were computed. The first column of z values is based on matching from the 256 spin lattice to the 64 spin lattice and the second column, matching the 64 to the 16 spin lattice. $E(t=0)$ and $E'(t)$, which are defined in the text, are listed under the columns specifying the original number of spins N.

	N_m	$N=256$	z	$N=64$	z	$N=16$
$E(t=0)$						
	256	0.8114 ±0.0005				
	64	0.8244 ±0.0008		0.8269 ±0.0005		
	16	0.8551 ±0.0013		0.8544 ±0.0007		0.8535 ±0.0007
	4	0.9172 ±0.0017		0.9106 ±0.0006		0.9066 ±0.0008
$E'(t)$		$t=80$		$t=20$		$t=5$
	256	0.839 ±0.002				
	64	0.909 ±0.003	2.7 ±0.4	0.898 ±0.002		
	16	0.965 ±0.003	2.6 ±0.3	0.954 ±0.002	1.8 ±0.2	0.956 ±0.002
	4	0.992 ±0.004	2.7 ±0.4	0.981 ±0.002	2.2 ±0.2	0.977 ±0.002
$E'(t)$		$t=160$		$t=40$		$t=10$
	256	0.822 ±0.002				
	64	0.888 ±0.003	2.6 ±0.3	0.870 ±0.002		
	16	0.946 ±0.004	2.6 ±0.3	0.927 ±0.003	2.0 ±0.2	0.927 ±0.003
	4	0.974 ±0.004	2.7 ±0.2	0.951 ±0.002	2.0 ±0.2	0.951 ±0.003

match on almost three levels for 256 matched to 64 spins. For $m=0$ (on a 64 spin lattice) there is matching within two standard deviations, for $m=1$ they match well within one SD, and for $m=2$ they are about three SD's off. We might expect the averages not to match for $m=0$ since the effects of irrelevant operators would be most prevalent here. For $m=2$ we would expect matching, if there was matching for $m=1$. The problem may be due to statistical fluctuations. Runs $\frac{1}{10}$ as long for the 64 spin lattice and $\frac{1}{2}$ as long for the 256 spin lattice matched within one SD and had averages intermediate between those shown in Table I. Thus, we may have unluckily hit the outskirts of each lattice's statistical bounds. Two other possibilities are the very small effects of irrelevant operators that have not quite died to zero after two iterations of the RG, and the RG being slightly different for the two lattices of different size. In any event the effect is very small and we can at least partially cancel it in our dynamic analysis by dividing the dynamic averages by their static counterparts. The same degree of matching on two levels is found when considering the 64 and 16 spin lattices.

We now compare the dynamic quantities. In Table I we show results for $E'(t)$ for $t=5$ and 10 for the 16 spin lattice, 20 and 40 for the 64 spin lattice and 80 and 160 for the 256 spin lattice. If there were perfect matching z would have the value 2. Since there is not we must interpolate to find z. The results for matching from the 256 spin lattice onto the 64 spin lattice is that $z=2.6$ or 2.7 plus or minus about 0.4. The error bars are based on making the largest change in both the $E'(t)$'s from each lattice. The fact that the same value of z occurs for any pair of $E'(t)$'s used gives us confidence that the method is working and that we are indeed looking at the scaling behavior of the model. We also note that when we match averages from the 16 spin lattice onto those from the 64 spin lattice we obtain the classical value $z=2$ which gives further evidence that we are seeing effects due to critical fluctuations which have not appeared on the smaller lattice. To determine whether our estimate of z is in fact the asymptotic value we would have to look at larger lattices. However, the computer time required to obtain the same accuracy would be an order of magnitude greater for a 1024 spin lattice.

We see the same trend for z as a function of q ($q=2$ is the Ising model) as Forgacs *et al.*,[2] namely, that z increases with q. Also, the DMCRG results clearly show a difference between the results for the Ising model where $z=2.17$ and the three-state Potts model where $z=2.6-2.7$. Both these results are distinct from the classical value of $z=2$.

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