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LETTER TO THE EDITOR

A Monte Carlo study of the three-states antiferromagnetic Potts model in two dimensions

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Abstract. Using Monte Carlo methods we study the two-dimensional three-states Potts model with antiferromagnetic nearest neighbours and ferromagnetic next-nearest neighbours couplings on a square lattice. We focus on the case with only antiferromagnetic coupling: from the analysis of the data we gathered, we find evidence that this system shows critical behaviour only at $T = 0$.

It has been recently suggested by Berker and Kadanoff (1980) that systems with antiferromagnetic (AF) coupling and non-zero ground-state entropy per particle may show an interesting critical behaviour. In particular they may have nontrivial fixed points with algebraic decay of the correlation functions. The simplest of such systems is the AF q-states Potts model.

For the $q = 3$ AF Potts model at zero temperature such a critical behaviour has been proved to be true by using the identity between this model and the six vertex model (Baxter 1970).

Let us briefly review the argument of Berker and Kadanoff (1980) which allows for fixed points at non-zero temperature: suppose S_i, $i = 1, \ldots, q$ is the spin on the ith lattice site of a d-dimensional square lattice. In order to minimise the energy we can divide our original lattice into two sublattices, A and B, so that any site on either sublattice has its nearest neighbour on the other sublattice. We can minimise the energy if we take all the spins, on one sublattice, in a well defined state (let us say 1, for example), while the spins on the other sublattice are in the other $q - 1$ possible states. We may set up many other ground states that respect the constraint of having zero energy.

Let us now consider four spins along the same direction $(S_i, \ldots, S_{i+3})$. If we rescale the system, eliminating the spins between the first one (S_i) and the last one (S_{i+3}), we are left with two cases: the first spin (S_i) is equal or different to the last one (S_{i+3}). These cases have a weight given by the number of configurations that the spins between the first and the last can assume in order to give the final results. This corresponds to a renormalisation of the temperature away from $T = 0$. In fact, after the scaling transformation we may have a lattice in which the nearest neighbours are equal: the energy of such a configuration is different from zero. The guess is that if the connectivity of the lattice is big enough, the renormalisation trajectory originating at $T = 0$ may flow to a stable fixed point at non-zero, non-infinite temperature.

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Using Monte Carlo simulations and ε-expansion techniques (Banavar *et al* 1980) it has been found that the three-dimensional $q = 3$ and $q = 4$ AF Potts models on a simple cubic lattice exhibit a continuous transition. Nevertheless, phenomenological and Monte Carlo renormalisation group computations (Nightingale and Schick 1982, Jayaprakash and Tobochnick 1982, den Nijs *et al* 1982) show that the $q = 3$, two-dimensional AF system has critical behaviour only at $T = 0$, while other computations find Kosterlitz–Thouless type transitions at finite temperature (Cardy 1981). Up to now Monte Carlo simulations for this Potts model have been inconclusive (Grest and Banavar 1981).

The aim of this letter is the study, using Monte Carlo techniques, of the $q = 3$ AF Potts model in two dimensions on a square lattice. This study is implemented by measuring the decay of magnetisation with distance, on a lattice with a magnetic field at the boundary, following a method already used for the study of the XY model (Fucito 1983). Our model is defined by

$$-H/T = T^{-1} \sum_{\langle ij \rangle} \delta_{\sigma_i \sigma_j} + (k/T) \sum_{\langle ij \rangle}{}' \delta_{\sigma_i \sigma_j}, \tag{1}$$

where $\sigma_i = 0, \frac{2}{3}\pi, \frac{4}{3}\pi$ are the three states (or colours) of the Potts model, the first sum runs over nearest neighbours and the primed sum over next-nearest neighbour pairs and K is a coupling. We use periodic boundary conditions in one direction, while in the other direction we constrain the spins at the boundary along one of the three allowed states, creating in this way a magnetic field. Our starting configuration is obtained dividing our lattice into two sublattices A and B as previously described: all the spins in the A lattice have colour σ_1 while the spins on the sublattice B have colour σ_2 or σ_3 with equal probability. We thermalise this configuration at a certain temperature and we compute the average magnetisation, for the sublattice A only, at various distances. For temperatures different from the first one, our starting configuration is always one which has already thermalised at a different temperature. Then we try to fit the functional forms

$$\langle m(x) \rangle \sim A/(x)^{\delta} + A/(L-x)^{\delta} \qquad \langle m(x) \rangle \sim -x/\xi \tag{2}$$

where the first form keeps in account the periodic boundary conditions along the direction of x.

The first problem we have to cope with, in order to fit the functional form (equation (2)), is which error we have to assign to our Monte Carlo data is strongly correlated, and this fact makes it impossible to decide which one of the functional forms of equation (2) fits our results best. To overcome this problem we divide our data at each temperature into various subsets and for each subset we compute the average. We then compute the statistical error as the mean square deviation of these averages. With the statistical error computed in this way we can decide the form of the best fit.

The second, and more serious, problem is to decide about the validity of this kind of analysis. Suppose we want to compute the susceptibility for a system which undergoes a continuous phase transition at a certain temperature T_c. The correlation length is infinite only at $T = T_c$, and only at this temperature should we have algebraic decay of the correlations. But what is shown by Monte Carlo data is a bump at T_c rather than an infinite peak, so that we should expect to have algebraic decay of correlations also in the neighbourhood of T_c. How is it possible to distinguish the fake algebraic decay from the true one? The method we use is to compute the

susceptibility at various lattice volumes and determine in which region we have the same behaviour regardless of the volume. Then we can try a fit of the type

$$X \sim a/(T - T_c)^{\nu} \tag{3}$$

and try to estimate the critical temperature T_c. The data used to fit the functional form in equation (3) are extracted out of the region in which we do not feel volume effects. A similar analysis has already been used for the study of O(2) and O(3) models (Solomon *et al* 1982 and references therein).

We are now ready to discuss our results, starting from the pure AF case with no next-nearest neighbour interaction ($K = 0$).

All these data were obtained with a 63×62 lattice. In figure 1 we show the internal energy against temperature in the region we explored. In figures 2, 3 there are a couple of typical fits of the functional forms of equation (2). We explored the temperatures in the range $0.1 \leqslant T \leqslant 0.8$ and before fitting the data we performed 25 000–30 000 Monte Carlo steps at each temperature. For $T < 0.4$ the data follow an exponential decay. From this naive kind of analysis we would estimate the temperature of the 'transition' to be around $T = 0.4$.

Let us now look at the susceptibility which is plotted against temperature in figure 4. These data were obtained for three different lattice volumes: 62×62, 50×50, 42×42. For this analysis we used periodic boundary conditions in all the directions of the plane. For each temperature and each different volume we performed 10 000–30 000 Monte Carlo steps. Up to $T = 0.4$ finite volume effects seem to dominate. In figure 5 we show the fit of the functional form of equation (3) with the data obtained from the 62×62 lattice. T_c is one of the parameters of the fit and the result is $T_c = 0$.

We now summarise our results for the AF Potts model: from the analysis of the decay of magnetisation with distance, the AF Potts model seems to undergo a transition at $T = 0.4$ from a phase with exponential decay of correlations (low temperature). However, looking at the susceptibility we understand that the results we have for

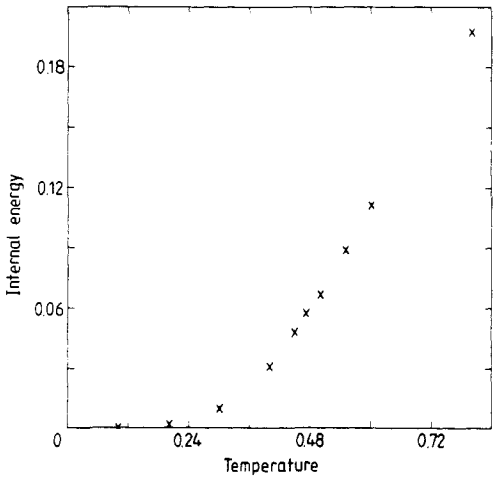

Figure 1. Internal energy against temperature for the AF Potts model. No error bars are shown because they are smaller than the mark of the points.

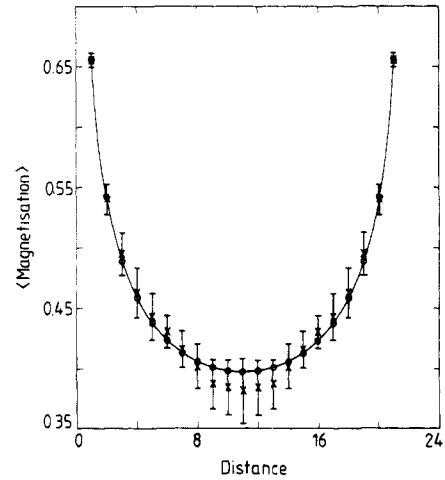

Figure 2. Algebraic decay fit of the average magnetisation against distance for $T = 0.3$. The crosses denote experimental data and the circles theoretical data.

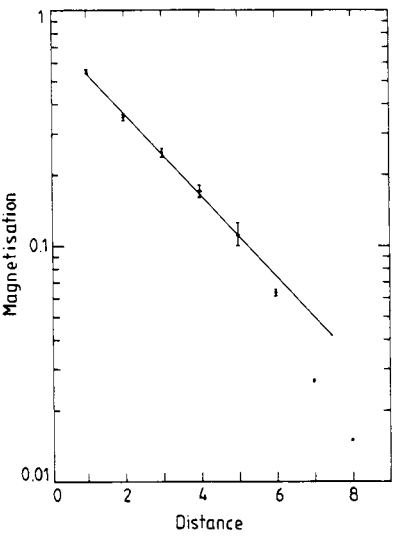

Figure 3. Exponential decay of the average magnetisation against distance from our data at $T = 0.45$. The line is drawn to help the reader.

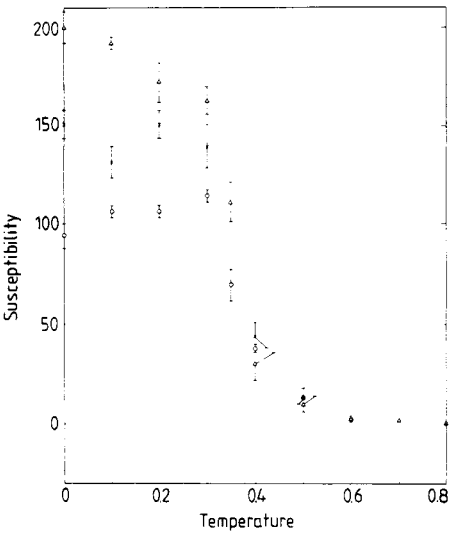

Figure 4. Plot of the susceptibility against temperature for three different lattice volumes; $\triangle = 62$, $\times = 50$, $\bigcirc = 42$.

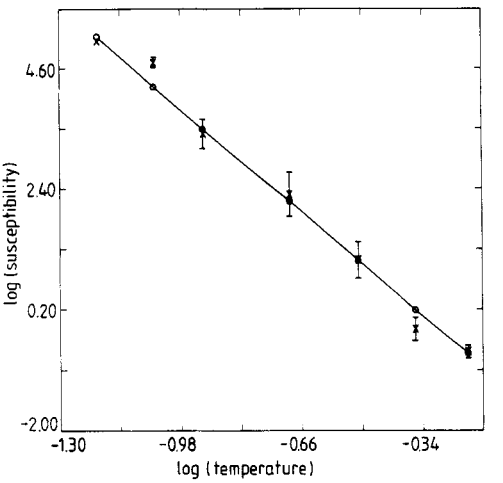

Figure 5. Fit of the functional form of equation (3) with the data obtained for the 62×62 lattice. As a result of the fit $T_c = 0$. The crosses denote experimental data and the circles theoretical data.

$T = 0.4$ may be pure lattice artifacts. This is why we believe the model to be critical just at $T = 0$.

We would now like to comment on our results for the AF Potts model with the addition of a next-nearest neighbour coupling. All of our data has been obtained from a 63×62 lattice with $k = 0.1$. We looked again at the decay of magnetisation with distance starting from a configuration in which all spins in sublattice A had a

colour a, and all spins in sublattice B had colour b, with $a \neq b$. At the boundaries we put a magnetic field in the a colour direction for the sublattice A, and one along the b colour direction for the sublattice B. We explored various temperatures in the range $0.1 \leqslant T \leqslant 0.9$. For $T \leqslant 0.3$ the magnetic field is too strong to detect any decay on such a small lattice. For $T > 0.3$ we can detect a power law decay for both sublattices and at $T = 0.9$ the exponential decay is already very well set up. For $T = 0.7$ and in the neighbourhood of this temperature, our data fit both behaviours. These data suggest this to be the region of the eventual transition. However, for computer CPU time reasons, we were not able to look at the behaviour of the susceptibility.

The whole work required approximately 200 hours of VAX11/780 CPU time.

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