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COMMENT

Mean-field renormalisation group study of antiferromagnetic q-state Potts models

M C Marques

Laboratório de Física, Faculdade de Ciências, Universidade do Porto, 4000 Porto, Portugal

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Abstract. The MFRG method is used to study the critical behaviour of the q-state Potts antiferromagnet in three dimensions. The q dependence of the critical temperature T_c as well as the exponent ν are derived, and the results are compared with Monte Carlo data and predictions of mean-field theory.

The antiferromagnetic Potts models in three dimensions have a highly degenerate ground state for $q \geqslant 3$. According to Berker and Kadanoff [1] this could lead to a low-temperature critical phase with algebraically decaying correlations, as is now thought to be the case for the three-state Potts antiferromagnet on the square lattice, at $T = 0$ [2, 3]. However, for the simple cubic lattice and $q < q_0$ there is now conclusive evidence from Monte Carlo computer simulations [4-6] of a continuous transition into a phase with long-range order corresponding to the sites of two interpenetrating sublattices (A and B) being preferentially occupied by two sets of Potts states; from these Monte Carlo results q_0 is estimated as being between 5 and 6.

For general q, there is no theory other than mean-field [5, 6] with which the values of the critical temperature $T_c(q)$ can be compared. T_c given by mean-field theory is generally much above the Monte Carlo estimate [7]; on the other hand, the disappearance of order for $q > q_0$ (finite) is not predicted by mean-field theory.

In this work we extend to general q our MFRG calculation for the three-state Potts antiferromagnet [8]; as with other models treated before [9-12], one advantage of this method is that it improves considerably the phase diagram obtained by the mean-field approximation.

The ordering scheme suggested by Monte Carlo simulations [6] consists of having a set of the Potts states, say states $1, 2, \ldots, (q-1)/2$ (q odd), distributed randomly on sublattice A, and the remaining states on sublattice B. A global order parameter describing this type of ordering may be defined as $\langle \Pi_A \rangle = \langle P_A^1 + P_A^2 + \ldots + P_A^{(q-1)/2} \rangle - (q-1)/2q$, where P^k is the projection operator onto state k, subscript A refers to sublattice A and $\langle\ \rangle$ means a thermodynamical average. (A similar assumption can be carried out for q even.)

Now the idea behind MFRG [9] is a comparison of two clusters of different size; the interactions within the clusters are treated exactly and the effect of surrounding spins is simulated by a mean field which is supposed to scale in the same way as the ordering parameter of the cluster.

We first consider the Hamiltonian for one Potts spin located on sublattice A

$$\mathcal{H}_1^A = -C_1 \Pi_A$$

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where $C_1 = J'zb'$ represents the effective field acting on spin 1 as a result of the interactions with its z nearest neighbours. In the vicinity of a second-order phase transition, b' can be assumed small, and

$$m_1 = \langle \Pi_A \rangle = \frac{q^2-1}{4q^2} \beta' C_1.$$

The Hamiltonian for a two-spin cluster is

$$\mathcal{H}_{II} = -J \sum_{K=1}^{q} P_{1A}^K P_{2B}^K - C_{II}(\Pi_{1A} - \Pi_{2B})$$

with $C_{II} = J(z-1)b$.

We then obtain

$$m_{II} = \frac{\langle \Pi_{1A} - \Pi_{2B} \rangle}{2} = \frac{(q^2-1)}{4[q e^K + q(q-1)]} \beta C_{II}.$$

The main assumption of MFRG is to impose the same scaling relation between m_1, m_{II} and b', b. By doing this we arrive at the renormalisation group recursion relation for $K' = \beta' J'$ and $K = \beta J$. The associated fixed point equation is

$$\frac{z}{q} = \frac{z-1}{e^{K_c} + q - 1}. \tag{1}$$

In figure 1 we have plotted $-1/K_c \propto T_c(q)$ against q, as given by equation (1) for $z = 6$.

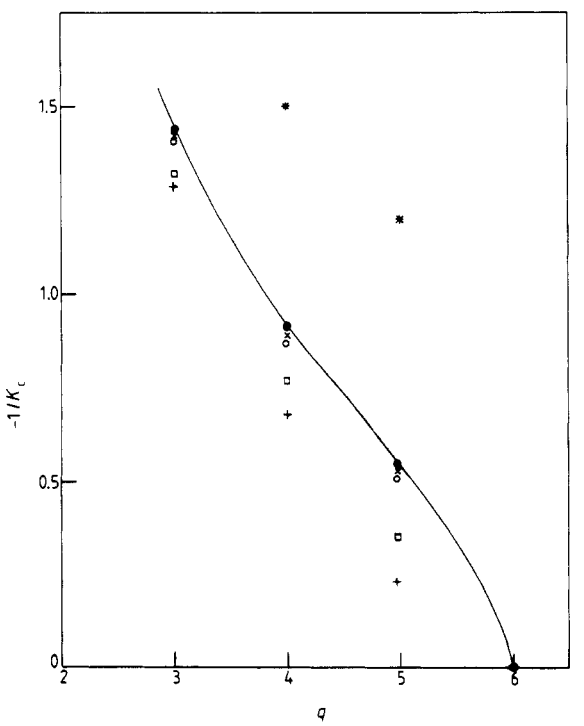

Figure 1. Plot of $-1/K_c$ against q: Monte Carlo data (+); mean-field predictions (*); MFRG results for comparison of two clusters having $N' = 1$, $N = 2$ (●), $N' = 2$, $N = 4$ (○) and $N' = 1$, $N = 4$ (×) and for comparison of three clusters $N'' = 1$, $N' = 2$, $N = 4$ (□). The curve is predicted by equation (1).

It is clear that this presents a much better approximation to the Monte Carlo results when compared with the mean-field predictions.

We can see from equation (1) that $T_c \to 0$ when $z=6$, $q \to q_0 = 6$. Monte Carlo results [6] give a value of q_0 below 6, but are not conclusive whether q_0 is in fact above 5. The determination of q_0 implies a careful study at low temperatures when some relevant correlations are not appropriately accounted for by the MFRG assumption; once the temperature range for which the correlations are almost trivial decreases with increasing cluster size, the use of bigger clusers is expected to improve the results. When a similar calculation is performed with two- and four-spin clusters, equation (1) is substituted by

$$\frac{z-1}{e^{K_c}+q-1} = \frac{(z-2)[2e^{2K_c}+2(q-2)e^{K_c}+q^2-2q+2]}{e^{4K_c}+6(q-1)e^{2K_c}+4(q-1)(q-2)e^{K_c}+(q-1)(q^2-3q+3)}. \tag{2}$$

For $z=6$, this gives $q_0 = 5.8$.

Another approximation which is known to improve the results involves the comparison of three different clusters [13]. We have done that for one-, two- and four-spin clusters. The result, together with the predictions of equation (2), is also shown in figure 1: clearly a good approximation to the Monte Carlo data is obtained.

In general, this method gives better results for the critical couplings than for the critical exponents. In figure 2 we have plotted the exponent ν as obtained by linearisation of the RG recursion relation around the fixed point, equation (1). We have used a new definition of the length scaling factor, as suggested by Slotte [14]: for one- and

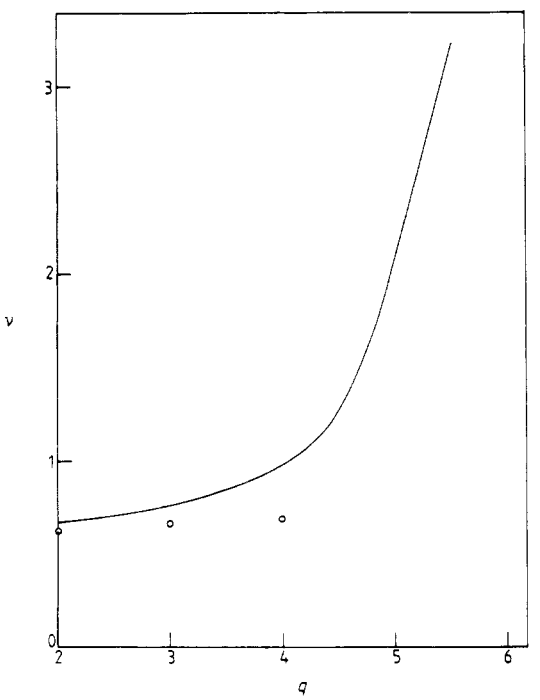

Figure 2. Plot of ν against q comparing the MFRG data (curve) for one- and two-spin clusters with series expansion values (○) for the equivalent $(q-1)$-component Heisenberg models.

two-spin clusters $l = 3(3/22)^{1/2}$ and

$$\nu = \ln l \left[\ln \left(\frac{\mathrm{d}K'}{\mathrm{d}K} \bigg|_{K_c} \right) \right]^{-1}.$$

These results for ν although quantitatively not very accurate may indeed give a good qualitative picture of the dependence of critical exponents on q. In particular $\nu \to \infty$ when $q \to q_0$, which is indicative of an essential singularity. The Monte Carlo results [7] do not seem to distinguish very clearly between a power law or an exponential for the inverse correlation length in this range of temperatures; a slightly better fit to the exponential when $q = 5$ would be indicative of this essential singularity or, at least, a high value of ν.

There is an argument by Banavar *et al* [4], based on ε-expansion calculations, according to which a continuous transition in the q-state Potts antiferromagnet, if it exists, is characterised by the critical exponents of the $(q-1)$-component Heisenberg model. The argument is justified to order ε and $q \leqslant 5$. In figure 2 we have also plotted the estimates obtained from Monte Carlo data [7] and the series expansion values for the equivalent $(q-1)$-component Heisenberg models [15]. The MFRG method clearly overestimates ν, as it does in other models [9, 10], at least when small clusters are used as here. If indeed $\nu \to \infty$ when $q \to q_0$, then the argument by Banavar *et al* fails for $q \to q_0$ and $d = 3$. Our estimate for $\nu(q=5)/\nu(q=4) = 2.2$ is certainly much above the ratio $\nu(n=4)/\nu(n=3)$ obtained from series expansions. It is possible that the high value of $\nu(q=5)$ obtained by this method is just an artefact of the MFRG method due to its limitations at low temperatures. In any case, if an essential singularity does indeed occur when $q \to q_0$, then a sudden increase in ν should appear for q between 5 and q_0; of course, only integer values of q are accessible to Monte Carlo experiments.

The present results for the simple cubic lattice ($z = 6$) can be easily extended to another bipartite lattice, the body-centred cubic ($z = 8$), as was already done for the $q = 3$ antiferromagnet [8]. In this case, and according to equation (2), $q_0 \leqslant 8$. Monte Carlo simulations, however, seem to indicate that order is already absent for $q \geqslant 6$; but the interpretation of the results is difficult in this temperature range and it would be desirable to analyse this system by using the same procedure followed by Hoppe and Hirst [6, 7] which permits the study of a two-ion correlation function.

We think that the use of the present method with bigger clusters and full three-dimensional symmetry is likely to increase the accuracy of the results. In any case, a considerable improvement on the predictions of mean-field theory is already achieved by these simple versions of the method.

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