Three-state Potts model with antiferromagnetic interactions: a MFRG approach

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Abstract. The mean-field renormalisation group method is used to study the critical temperature of the three-state Potts antiferromagnet in 3D lattices, as well as the three-state Potts model on the square lattice with ferromagnetic (along x) and antiferromagnetic (along y) interactions, and its quantum version, the 1D Potts antiferromagnet in a transverse field. Comparison is made with other results.

1. Introduction

The antiferromagnetic q-state Potts model on a bipartite lattice is an example of a system with a finite residual entropy. Phase transitions in systems with infinitely degenerate ground states have been the subject of much investigation, due to the variety of low-temperature orderings which can be envisaged. Berker and Kadanoff [1] first suggested the possibility, in these systems, of a low-temperature critical phase with algebraically decaying correlations. The first case to be studied was the three-state Potts antiferromagnet on the square lattice, where indications for this sort of behaviour at non-zero temperature were found by Grest and Banavar [2]. Their interpretation of the Monte Carlo data has since been criticised [3-7] and it is now established [8] that the system exhibits a transition only at zero temperature where, in fact, due to its equivalence to the square-ice model, power-law decay of correlations occurs [9]. The scaling argument of Berker and Kadanoff is, however, not sufficient [7] to rule out other possibilities of low-temperature behaviour, and in fact a continuous phase transition into a phase with long-range order has been found in $d = 3$ for $q = 3$ and $q = 4$ [10-12]. Adding to the evidence obtained by Monte Carlo techniques, the exact solution of this model on a Bethe lattice [13] confirms the existence of a phase transition of the usual second-order kind (which occurs at non-zero temperature for high enough coordination number). In this case, the nature of the ordering is further elucidated by the consideration of an external field.

In what concerns the ordering temperature T_c, the only prediction to which the Monte Carlo estimates can be compared is the one obtained by mean-field approximation [12]. In this work we apply the mean-field renormalisation group technique (MFRG), first developed by Indekeu et al [14], which presents two main advantages: it gives a better approximation than mean field for the phase diagram, and it applies easily to $d = 3$. This method has already been applied to the Potts ferromagnet in a transverse field [15], and to some frustrated systems like the triangular Ising antiferromagnet [16]; even at low temperatures, or in the case of first-order phase transitions,

when the assumption implied by MFRG is less justified, the predicted critical line is found to be in reasonable agreement with other calculations. Our results for the three-state Potts antiferromagnet are presented in § 2, where comparison is also made with available Monte Carlo data. As for the critical behaviour, much information is still missing. An ε-expansion calculation done by Banavar *et al* [11] has led to the argument that the three-state Potts antiferromagnet is in the same universality class as the xy model. The capability of the MFRG method to predict critical exponents is poorer than for estimating critical couplings, at least when small clusters are used, as in the present calculation; the estimate obtained for the critical exponent ν is also included in § 2.

Another related model with an infinitely degenerate ground state is a two-dimensional Potts model with ferromagnetic (J_x) and antiferromagnetic (J_y) interactions in the two respective directions of a square lattice. Kinzel *et al* [17] have given an argument showing that an ordered phase (characterised by a ferromagnetic correlation between alternating ferromagnetic chains) can exist in this model, and obtained an expression for its critical point as a function of $\alpha = -J_y/J_x$. These authors have also carried out a Monte Carlo simulation of the same model, which suggests, however, that one may be in the presence of an unconventional infinite-order transition of the sort found in the square-lattice Potts model with antiferromagnetic nearest-neighbour and ferromagnetic next-nearest-neighbour interactions [2, 3]. In § 3 we again make use of the MFRG method to obtain an estimate of the critical temperature dependence on α, and to compare it with the results of Kinzel *et al*.

In § 4, we study the one-dimensional Potts antiferromagnet in a transverse field Γ, which, at $T = 0$, constitutes [18] the quantum version of the two-dimensional Potts model with ferromagnetic (J_x) and antiferromagnetic (J_y) interactions. This quantum model has been investigated by finite-size scaling and phenomenological renormalisation by Herrmann *et al*, who found indications of a massless low-temperature behaviour with an essential singularity for values of $\lambda = -\Gamma/J_y$ below a certain value λ_c. We obtain an estimate for the value of λ at which the zero-temperature transition occurs, which is very close to the one found by those authors. In fact, the method of MFRG is closely related to phenomenological renormalisation; it is nevertheless remarkable that the same result can be achieved by a comparison of just one- and two-spin clusters. An estimate for the critical exponent of the classical equivalent model is also included in § 4; the result obtained within this approximation gives an indication but does not allow a definitive conclusion about the nature of the singularity discussed by Herrmann *et al*.

We conclude in § 5 with a brief discussion of the results.

2. Three-state Potts antiferromagnet

We consider two interpenetrating sublattices, denoted by A and B, with each A Potts spin being surrounded by z B Potts spins. The ordering scheme suggested by Monte Carlo simulations is the so-called broken-sublattice symmetry (BSS) which consists of having one of the states, say 1, on sublattice A and the other two states distributed randomly on sublattice B. A global order parameter describing this type of ordering may be defined [12]:

$$H(T) = \tfrac{1}{2} \sum_{r=1}^{3} |P_r(A) - P_r(B)|$$

where P_r is the average population per site of state r on the given sublattice. Alternatively we can use the projection operator onto state k, P^k, and define the order parameter as $\langle P_A^1 \rangle - \langle P_B^1 \rangle$, where $P_{A(B)}^1$ refers to sublattice $A(B)$ and $\langle\ \rangle$ means a thermodynamical average.

Now the main idea of MFRG is to compare the behaviour 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 start by considering the Hamiltonian for one Potts spin located on site i belonging to sublattice A:

$$\mathcal{H}_1^{(A)} = -zJ'[P_{iA}^1 C_{1B} + \tfrac{1}{2}(P_{iA}^2 + P_{iA}^3)(1 - C_{1B})]$$

where J' is the antiferromagnetic coupling and C_{1B} denotes the mean-field probability for state 1 in sublattice B.

We then have

$$\langle P_{iA}^1 \rangle = \frac{\exp(zK'C_{1B})}{\exp(zK'C_{1B}) + 2\exp[\tfrac{1}{2}zK'(1 - C_{1B})]} \qquad K' = \beta J'. \tag{2.1}$$

We have an analogous equation for one Potts spin located on site j belonging to sublattice B:

$$\mathcal{H}_1^{(B)} = zJ'[P_{jB}^1 C_{1A} + \tfrac{1}{2}(P_{jB}^2 + P_{jB}^3)(1 - C_{1A})]$$

$$\langle P_{jB}^1 \rangle_1 = \frac{\exp(zK'C_{1A})}{\exp(zK'C_{1A}) + 2\exp[\tfrac{1}{2}zK'(1 - C_{1A})]}. \tag{2.2}$$

In the disordered phase, $\langle P_{iA} \rangle_1 = \langle P_{jB} \rangle_1 = \tfrac{1}{3}$, in which case equations (2.1) and (2.2) are trivially satisfied. The onset of antiferromagnetic order corresponds to $\langle P_{iA}^1 \rangle_1$ being different from $\langle P_{jB}^1 \rangle_1$. We then write $C_{1A} = \tfrac{1}{3} + \tfrac{1}{2}\Delta_1$, $C_{1B} = \tfrac{1}{3} - \tfrac{1}{2}\Delta_1$ and, assuming Δ_1 to be small (which is true in the vicinity of a second-order transition), we get

$$m_1 = \langle P_{iA}^1 \rangle_1 - \langle P_{jB}^1 \rangle_1 = -\tfrac{1}{3}zK'\Delta_1. \tag{2.3}$$

We consider now the Hamiltonian for a two-spin cluster

$$\mathcal{H}_{II} = -J\sum_k P_{1A}^k P_{2B}^k - (z-1)J[P_{1A}^1 C_{IIB} + \tfrac{1}{2}(P_{1A}^2 + P_{1A}^3)(1 - C_{IIB}) + P_{2B}^1 C_{IIA}$$

$$+ \tfrac{1}{2}(P_{2B}^2 + P_{2B}^3)(1 - C_{IIA})].$$

Writing $C_{IIA} = \tfrac{1}{3} + \tfrac{1}{2}\Delta_{II}$, $C_{IIB} = \tfrac{1}{3} - \tfrac{1}{2}\Delta_{II}$, we get

$$m_{II} = \langle P_{1A}^1 - P_{2B}^1 \rangle_{II} = -3(z-1)K\Delta_{II}\frac{1}{6 + 3\,e^K}. \tag{2.4}$$

The main idea behind MFRG is that Δ_1 and Δ_{II} must scale like m_1 and m_{II}. Imposing this scaling relation for Δ_1 and Δ_{II}, we arrive at the renormalisation recursion relation for K' and K. The fixed-point equation associated with it is

$$\tfrac{1}{3}z = (z-1)/(2 + e^{K_c}). \tag{2.5}$$

The simple cubic lattice is a bipartite with $z = 6$; in this case (2.5) gives $-1/K_c = 1.44$, to be compared with 2.0 from mean field and 1.28 from Monte Carlo [12]. For $z = 8$, which describes the BCC lattice, we get $-1/K_c = 2.12$, whereas the Monte Carlo data of Banavar *et al* [11] give an estimate of 1.8.

According to (2.5), $T_c = 0$ for $z = 3$, whereas it is known that $T_c = 0$ already [19] for $z = 4$, i.e. the square lattice. This disagreement is not surprising as we cannot expect very good results from MFRG at low temperatures, when the relevant correlations are not appropriately accounted for by the assumptions which led to equations (2.3) or (2.4).

The temperature range for which the correlations are almost trivial decreases with increasing cluster size. We have performed a similar calculation involving the comparison of two- and four-spin clusters. Equation (2.5) is then replaced by

$$(z-2)\frac{4\,e^{2K_c} + 4\,e^{K_c} + 10}{3\,e^{4K_c} + 36\,e^{2K_c} + 24\,e^{K_c} + 18} = (z-1)\frac{2}{3(e^{K_c} + 2)}.$$

This gives $-1/K_c(z=6) = 1.40$ and $-1/K_c \to 0$ when $z \to 3.5$, which constitutes an improvement on the previous result, but still misses the exact result $T_c(z=4) = 0$.

Critical indices can be obtained by linearisation of the renormalisation recursion relation around a fixed point. We have calculated the critical exponent ν, defined here as $dK'/dK = 2^{1/\nu d}$. For the simple cubic lattice we get $\nu^{(MFRG)} = 1.7$. This is not a good estimate if one compares it with the value $\nu = \frac{2}{3}$ predicted for the 3D XY model [20]. We recall however that, within a similar approximation, the value obtained for the 3D Ising model is $\nu_{Ising}^{(MFRG)} = 1.5$ [15]; so $\nu^{(MFRG)} > \nu_{Ising}^{(MFRG)}$, which is still compatible with the argument of Banavar *et al* [11].

As we have said, the method gives better results for the critical couplings than for the critical exponents; a comparable accuracy in the latter can only be achieved by the use of considerably bigger clusters.

3. 2D Potts model with ferromagnetic (J_x) and antiferromagnetic (J_y) interactions

We now continue by considering the two-dimensional Potts model with ferromagnetic interactions along the x axis and antiferromagnetic interactions along the y axis. The square lattice is seen here as a sequence of alternating A and B chains (figure 1).
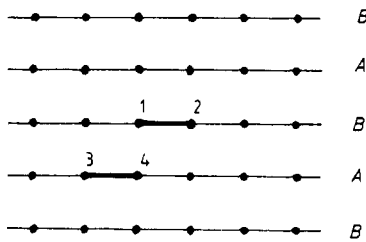

Figure 1. Two-site clusters on A and B chains.

For the one-site clusters, we can use (2.5) with $2(K'_y - K'_x)$ instead of zK'. We then consider a two-site cluster of the type indicated in figure 1, and write its Hamiltonian:

$$\mathcal{H}_{11}^{(B)} = -J_x \sum_k P_{1B}^k P_{2B}^k - (J_x C_{11B} + 2J_y C_{11A})(P_{1B}^1 + P_{2B}^1) - [\tfrac{1}{2}J_x(1 - C_{11B}) + \tfrac{1}{2}J_y(1 - C_{11A})]$$

$$\times (P_{1B}^2 + P_{1B}^3 + P_{2B}^2 + P_{2B}^3).$$

The Hamiltonian $\mathcal{H}_{11}^{(A)}$ for a two-spin cluster belonging to A can be written analogously.

In the vicinity of the transition one then gets

$$\langle \tfrac{1}{2}(P_{3A}^1 + P_{4A}^1)\rangle_{11} - \langle \tfrac{1}{2}(P_{1B}^1 + P_{2B}^1)\rangle_{11} = (K_2 - 2K_y)\Delta_{11}\frac{2\,e^{K_x}+1}{3\,e^{K_x}+6}.$$

The fixed-point equation obtained by imposing the scaling relation implied by the renormalisation is now

$$2(K_x - K_y) = (K_x - 2K_y)\frac{2\,e^{K_x}+1}{e^{K_x}+2}. \tag{3.1}$$

In figure 2 we plot T_c as a function of $\alpha = -J_y/J_x$. The curve which corresponds to the relation $(1+e^{K_z})(1-e^{K_y}) = 3$, predicted by Kinzel *et al* [17], is also drawn for comparison.
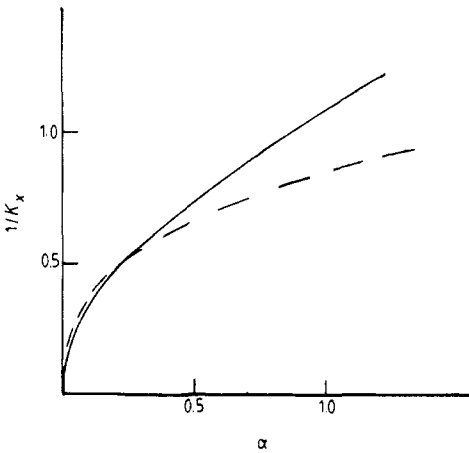

Figure 2. $1/K_x$ as a function of $\alpha = -(J_y/J_x)$ (———, MFRG, equation (3.1); - - -, [17]).

4. 1D Potts antiferromagnet in a transverse field

We now apply the MFRG method to the one-dimensional Potts antiferromagnet in a transverse field.

$\mathcal{H}_1^{(A)}$ and $\mathcal{H}_1^{(B)}$ can then be written:

$$\mathcal{H}_1^{(A)} = -2J_y'[P_{iA}^1 C_{1B} + \tfrac{1}{2}(P_{iA}^2 + P_{iA}^3)(1 - C_{1B})] - \Gamma'\psi_{iA}$$

$$\mathcal{H}_1^{(B)} = -2J_y'[P_{jB}^1 C_{1A} + \tfrac{1}{2}(P_{jB}^2 + P_{jB}^3)(1 - C_{1A})] - \Gamma'\psi_{jB}$$

where $\psi = \Sigma_{s=0}^2 \psi^{(s)}$, $\psi^{(s)}$ being the 'ladder operator' for the Potts states $|\alpha\rangle$.

Using the methods of [15], one easily obtains

$$\langle P_{iA}^1\rangle_1 - \langle P_{jB}^1\rangle = -J_y'\Delta_1 F_1(K_y', \lambda')$$

$$F_1(K_y', \lambda') = \frac{12}{27}\frac{-(1/\lambda')\exp(-3\lambda'K_y') + (1/\lambda') + \tfrac{3}{2}K_y'}{\exp(-3\lambda'K_y') + 2} \qquad \lambda' = -\Gamma'/J_y'.$$

We next consider the Hamiltonian for a two-site cluster:

$$\mathcal{H}_{11} = -J_y \sum_k P^k_{1A} P^k_{2B} - J_y [P^1_{1A} C_{11B} + \tfrac{1}{2}(P^2_{1A} + P^3_{1A})(1 - C_{11B}) + P^1_{2B} C_{11A}$$

$$+ \tfrac{1}{2}(P^2_{2B} + P^3_{2B})(1 - C_{11A})] - \Gamma(\psi_{1A} + \psi_{2B})$$

and, again following [15], we get

$$\langle P^1_{1A} - P^1_{2B} \rangle_{11} = -J_y \Delta_{11} F_{11}(K_y, \lambda)$$

($F_{11}(K_y, \lambda)$ is given in the appendix).

The critical line is obtained by setting $F_1(K_y, \lambda) = F_{11}(K_y, \lambda)$. The λ axis is intersected at the 'quantum' fixed point $(-K^*_y = \infty)$; in our calculation $\lambda^* = 0.2$, which agrees very well with the value found by Herrmann and Martin [18].

Not all the points on the critical line are actually fixed points of a completely specified RG procedure. For example, in the 1D Potts ferromagnet in a transverse field there is the 'classical' fixed point at $\lambda^* = 0$, $K^* = \infty$, in addition to the 'quantum' fixed point. The one-dimensional Potts antiferromagnet with $\Gamma = 0$ is disordered at zero temperature (equation (2.5) has no solution for $z = 2$), so there is not, in this case, a classical fixed point with $\lambda^* = 0$. On the other hand, and similar to what was encountered in the 1D Potts ferromagnet [15], we find a (probably) spurious solution $\lambda(T) \neq 0$ in a narrow temperature range around zero; only a free energy calculation would enable a clarification of this point, but this method is obviously not suitable for that.

As discussed by Herrmann and Martin [18], the critical behaviour at the 'quantum' fixed point of this model is equivalent to that of the two-dimensional Potts model with ferromagnetic and antiferromagnetic interactions in the two directions of a square lattice. We have also calculated the exponent y_λ, defined by $d\lambda'/d\lambda|_{K^*_y = -\infty; \lambda = \lambda^*} = 2^{y_\lambda}$. An estimate for the critical exponent ν of the classical equivalent model is then obtained, $\nu = 1/y_\lambda = 2.8$. The high value found for ν within this approximation may in fact be indicative of the essential singularity discussed by Herrmann et al, which will probably show more clearly in a calculation involving bigger clusters.

5. Conclusions

In conclusion, once again MFRG has proved useful for the determination of critical temperatures, improving the mean-field estimates for the three-dimensional three-state Potts antiferromagnets and comparing well with other existing results for the square-lattice Potts model with ferromagnetic and antiferromagnetic interactions. This can be achieved, in the simplest version (when the comparison is made between one- and two-spin clusters), with a small amount of computational work compared to that usually involved in related finite-size or phenomenological scaling methods. As shown with other systems, the capability of the method to predict exponents is poor, although one expects a convergence towards better results for larger clusters. Within this approximation we could not expect to distinguish a low-temperature phase with algebraically decaying correlations; even so we were able to detect, in one case, an increase in the exponent ν which can be indicative of the vicinity of an infinite-order phase transition (where $\nu = \infty$). However, this only occurs at low temperature, where the method can be deficient.

Extensions of this work to general q-state Potts antiferromagnets are presently being studied, as well as the consideration of different sorts of competing interactions.

The use of larger clusters would certainly be desirable for an improvement in the calculation of critical exponents.

Appendix

The Hamiltonian for the isolated two-spin cluster is

$$\mathcal{H}_{11}^0 = -\Gamma(\psi_{1A} + \psi_{2B}) - J_y \sum_k P_{1A}^k P_{2B}^k$$

and has eigenvalues (degeneracy g)

$$E_0 = -\tfrac{1}{2}J_y(1 - 6\lambda + \theta) \qquad g_0 = 1$$

$$E_1 = -\tfrac{1}{2}J_y(1 - 3\lambda + \bar{\theta}) \qquad g_1 = 2$$

$$E_2 = 3J_y\lambda \qquad g_2 = 2$$

$$E_3 = -\tfrac{1}{2}J_y(1 - 3\lambda - \bar{\theta}) \qquad g_3 = 2$$

$$E_4 = -\tfrac{1}{2}J_y(1 - 6\lambda - \theta) \qquad g_4 = 1$$

$$E_5 = 0 \qquad g_5 = 1$$

where $\theta = (1 + 36\lambda^2 + 4\lambda)^{1/2}$, $\bar{\theta} = (1 + 9\lambda^2 - 2\lambda)^{1/2}$.

The corresponding eigenvectors $|\varphi_i\rangle$ can be obtained after some algebra.

In order to calculate $\langle P_{1A}^1 - P_{2B}^1 \rangle_{\mathcal{H}_{11}}$, where

$$\mathcal{H}_{11} = \mathcal{H}_{11}^0 - \tfrac{3}{4}J_y\Delta_{11}(P_{2B}^1 - P_{1A}^1)$$

we use a perturbation expansion in powers of Δ_{11}, as developed in [15].

Defining

$$A_{ji} = \sum_{r=1}^{g_j} \sum_{s=1}^{g_i} |\langle \varphi_j^r | P_{2B}^1 - P_{1A}^1 | \varphi_i^s \rangle|^2$$

the expressions for the non-vanishing elements are

$$A_{20} = \frac{4}{3} \frac{B^2}{1 + 2B^2} \qquad A_{21} = \frac{4}{3} \frac{A^2}{1 + 2A^2} \qquad A_{51} = \frac{4A^2}{(1 - 2A)^2 + 2(1 + A)^2}$$

$$A_{23} = \frac{4}{3} \frac{(A')^2}{1 + 2(A')^2} \qquad A_{24} = \frac{4}{3} \frac{(B')^2}{1 + 2(B')^2} \qquad A_{53} = \frac{2}{(1 - 2A)^2 + 2(1 + A)^2}$$

where

$$A = \frac{-1 - 3\lambda + \bar{\theta}}{2(1 - 3\lambda + \bar{\theta})} \qquad B = \frac{-1 - 6\lambda + \theta}{1 - 6\lambda + \theta}$$

$$A' = \frac{-1 - 3\lambda - \bar{\theta}}{2(1 - 3\lambda - \bar{\theta})} \qquad B' = \frac{-1 - 6\lambda - \theta}{1 - 6\lambda - \theta}.$$

The linearisation of $\langle P_{1A}^1 - P_{2B}^1 \rangle_{\mathscr{H}_{11}}$ in terms of Δ_{11} then gives

$$\langle P_{1A}^1 - P_{2B}^1 \rangle_{\mathscr{H}_{11}} = -\tfrac{3}{2} J_y \Delta_{11} \mathscr{J} / \mathscr{D}$$

where

$$\mathscr{D} = e^{-\beta E_0} + 2\,e^{-\beta E_1} + 2\,e^{-\beta E_2} + 2\,e^{-\beta E_3} + e^{-\beta E_4} + 1$$

$$\mathscr{J} = e^{-\beta E_0}\left(\frac{A_{20}}{3\lambda + \tfrac{1}{2}(1 - 6\lambda + \theta)}\right) + e^{-\beta E_1}\left(\frac{A_{21}}{3\lambda + \tfrac{1}{2}(1 - 3\lambda + \bar{\theta})} + \frac{A_{51}}{\tfrac{1}{2}(1 - 3\lambda + \bar{\theta})}\right)$$

$$+ e^{-\beta E_2}\left(\frac{A_{20}}{-3\lambda - \tfrac{1}{2}(1 - 6\lambda + \theta)} + \frac{A_{21}}{-3\lambda - \tfrac{1}{2}(1 - 3\lambda + \bar{\theta})}\right.$$

$$\left. + \frac{A_{23}}{-3\lambda - \tfrac{1}{2}(1 - 3\lambda - \bar{\theta})} + \frac{A_{24}}{-3\lambda - \tfrac{1}{2}(1 - 6\lambda - \theta)}\right)$$

$$+ e^{-\beta E_3}\left(\frac{A_{23}}{3\lambda + \tfrac{1}{2}(1 - 3\lambda - \bar{\theta})} + \frac{A_{53}}{\tfrac{1}{2}(1 - 3\lambda - \bar{\theta})}\right) + e^{-\beta E_4}\left(\frac{A_{24}}{3\lambda + \tfrac{1}{2}(1 - 6\lambda - \theta)}\right)$$

$$+ \frac{A_{51}}{-\tfrac{1}{2}(1 - 3\lambda + \bar{\theta})} + \frac{A_{53}}{-\tfrac{1}{2}(1 - 3\lambda - \bar{\theta})}.$$

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