ELSEVIER

22 May 1995

PHYSICS LETTERS A

Physics Letters A 201 (1995) 252–256

Tricritical behavior of the three-state triangular Potts model

H. Meyer [a], J.C. Anglès d'Auriac [a], J.M. Maillard [b], G. Rollet [c], F.Y. Wu [c]

[a] *CRTBT, 25 Avenue des Martyrs, BP 166X, 38084 Grenoble Cedex, France*

[b] *Laboratoire de Physique Théorique et Hautes Energies, Tour 16, 1er étage, 4 Place Jussieu, 75252 Paris Cedex, France*

[c] *Department of Physics, Northeastern University, Boston, MA 02115, USA*

Received 20 January 1995; accepted for publication 8 March 1995

Communicated by L.J. Sham

Abstract

The phase transition occurring in the three-state Potts model on the triangular lattice with two- and three-spin interactions is studied using Monte Carlo simulations and exact calculations. A tricritical point is found to exist on the self-dual trajectory, and extensive simulations lead to a conjectured location of this point.

1. Introduction

It is now well known that the standard q-state ferromagnetic Potts model in two dimensions exhibits a first-order transition for $q > 4$ and a continuous transition for $q \leqslant 4$ [1,2]. When the interaction is antiferromagnetic, however, the existence of a transition, if any, and the nature of the transition are less clear. This uncertainty is generally related to the existence of a nonzero residual entropy [3]. For this reason, the $q = 3$ antiferromagnetic model on the triangular lattice is of special interest, since it possesses a sixfold degenerate ground state and a zero residual entropy, implying that there is a transition. From a universality consideration one expects the transition to be the same as that of the standard six-state model, namely, one of first order. This first-order transition has indeed been confirmed by series analysis [4]. Thus, depending on the nature of interactions, the transition in the $q = 3$ triangular model can change from continuous to first order. It is therefore of pertinent interest to inquire what happens in models with competing interactions. In this paper we take up this question. As it turns out, we arrive at some unexpected answers which show that the naive universality argument is no longer valid.

We consider the isotropic version ($J_1 = J_2 = J_3$) of the three-state Potts model on the triangular lattice described by the Hamiltonian

$$\mathcal{H} = -\sum_{\text{n.n.}} J_i\, \delta_{\mathrm{Kr}}(s, s') - J \sum_{\Delta} \delta_{\mathrm{Kr}}(s, s')\, \delta_{\mathrm{Kr}}(s', s''), \tag{1}$$

where the first sum is over nearest neighbors consisting of spins $s, s' = 1, 2, 3$, and the second sum over all up-pointing triangles of spins s, s' and s''. Here, $-J_i$, $i = 1, 2, 3$, are the two-site interactions (in the three respective axis directions), and $-J$ the three-site interaction in alternate (say, the up-pointing) triangular faces of the lattice. The interactions are competing if J and J_i are of opposite signs. The lattice is shown in Fig. 1.

When $J = 0$, the Hamiltonian (1) reduces to that of the standard model for which the transition is known to be continuous when $J_i > 0$ [5] and of first order

SSDI 0375-9601(95)00212-X

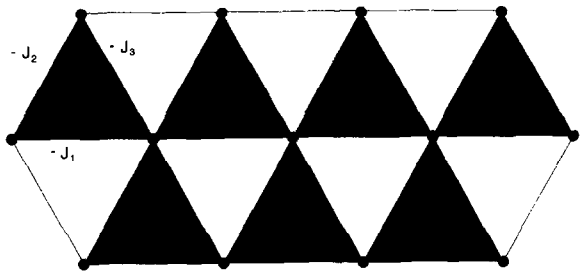

Fig. 1. The triangular Potts lattice. Black circles indicate spins and shaded triangles indicate three-site interactions.

when $J_1 = J_2 = J_3 < 0$ [4]. The $J \neq 0$ model was first studied by Baxter et al. [5] and later by Wu and Lin [6]. It is found that the partition function possesses a duality relation with the self-dual trajectory

$$x_1 x_2 x_3 x = x_1 + x_2 + x_3 + 1, \tag{2}$$

where $x = \exp(J/kT), x_i = \exp(J_i/kT)$. In the $J = 0$ and $J_1 = J_2 = J_3 > 0$ model, the trajectory (2) yields the exact critical point [7]

$$J_1/kT_c = \ln[2\cos(\pi/9)] = 0.6309.... \tag{3}$$

For $J = 0$, $J_1 = J_2 = J_3 < 0$, the critical point is known from series analysis [4] to occur at

$$J_1/kT_c = -1.59. \tag{4}$$

The model (1) has also been analyzed by Wu and Zia [8], who conjectured on the basis of a uniqueness assumption that the self-dual trajectory (2) is an actual critical frontier. The nature of the transition along (2), however, has not been analyzed.

Here, we study transitions in the isotropic version of the model (1) by means of extensive Monte Carlo simulations on finite lattices of up to 3888 sites in conjunction with exact calculations for a small lattice. As a result, we determine the phase diagram, the nature of transitions, as well as the critical frontiers in both the ferromagnetic and the antiferromagnetic regimes. We verify that the transition in the antiferromagnetic regime is of first order; we also verify the conjecture that the self-dual trajectory is a critical frontier. However, we find that the nature of transition along this latter frontier changes from continuous to first order at a tricritical point, even though the frontier lies in the ferromagnetic regime. This finding is surprising, as a naive universality would imply a continuous transition throughout. On the basis of simulation results, we conjecture the exact location of this tricritical point.

2. The critical frontier and the phase diagram

We first present in this section our main findings. Details of analyses are described in subsequent sections.

From a ground state energy consideration [8], the parameter space of the isotropic model is divided into ferromagnetic ($J + 3J_1 > 0, J + 2J_1 > 0$), antiferromagnetic ($J + 3J_1 < 0, J_1 < 0$), and paramagnetic ($J + J_1 < 0, J_1 > 0$) regimes. The self-dual trajectory (2), which now reads

$$x x_1^3 = 3x_1 + 1, \tag{5}$$

lies entirely in the ferromagnetic regime.

We show in Fig. 2 the critical frontiers determined from simulations in the $(J_1/kT, J/kT)$ plane. Points A, B, C, D, F, G, I, J are data points of the critical point from simulations performed on a 972-site lattice, points P and Q are given respectively by (4) and (3), and other data points are from simulations on 3888-site and 507-site lattices. The frontiers are found to consist of two branches. One branch, shown by the broken curve connecting points C, B, ..., P , is in the antiferromagnetic regime where we find all transitions of first order. The other branch, which is in the ferromagnetic regime, is the self-dual trajectory (5) shown in Fig. 2. It is seen that all data points lie practically on this trajectory, thus confirming the Wu–Zia conjecture that the trajectory is indeed a critical frontier. Furthermore, we find along this frontier transitions of first order for $J_1 < 0$ and continuous for $J_1 > 0$. Our best data provide the bound

$$-0.2 < J_1/kT < 0.2 \tag{6}$$

for the location of the tricritical point[1], the point at which the nature of transition changes. This leads us to conjecture that point T in Fig. 2, namely, the point with coordinates

$$J_1 = 0, \quad J/kT = \ln 4, \tag{7}$$

[1] After the completion of our work, we have been informed by B. Nienhuis [9] that a method corresponding to an approximate calculation of the central charge along (5) also indicates the existence and the locus of a tricritical point in this model.

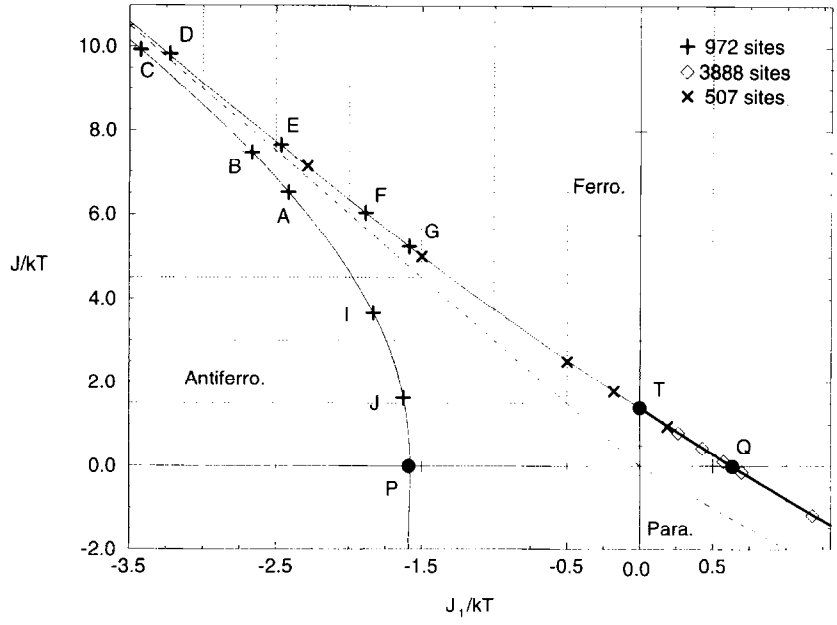

Fig. 2. The critical frontiers in the $(J/kT, J_1/kT)$ space. Thin lines denote trajectories of first order transitions and fat line denotes the trajectory of continuous transitions. The line in the ferromagnetic regime is the self-dual trajectory (5). Points P and Q are given by (4) and (3), and T is the conjectured tricritical point given by (7).

Table 1
Simulation results of a 972-site lattice

	Point								
	A	B	C	D	E	F	G	I	J
$J/\|J_1\|$	2.70	2.80	2.90	3.05	3.10	3.20	3.30	2.00	1.00
$\|J_1\|/kT$	2.42	2.67	3.43	3.23	2.47	1.89	1.59	1.83	1.63
J/kT	6.52	7.47	9.93	9.84	7.65	6.04	5.24	3.67	1.63
$kT/\|J_1\|$	0.414	0.375	0.292	0.310	0.405	0.530	0.630	0.545	0.615

is the actual tricritical point.

It is of interest to consider the phase diagram, and the phase diagram for $J_1 < 0$ is shown in Fig. 3. Here, points labelled by letters are the same as those in Fig. 2. In addition, the solid lines represent the "phase diagram" obtained from the maxima of the specific heat computed from an exactly enumerated partition function for a lattice of 27 sites [10]. Also shown in a broken curve is the self-dual trajectory (5) representing the phase boundary in the ferromagnetic regime. The dotted line connecting points A, B, C, H indicates the approximate location of the phase boundary in the antiferromagnetic regime. We remark that while D, E, F, G are self-dual points under the duality transformation [5,6], the duals of A, B, C, I, J, P on the antiferromagnetic branch lie in an unphysical regime.

3. Monte Carlo simulations

Our simulations are performed on finite lattices of 3888, 972, and 507 sites, or of size $3L^2$ for L = 36, 18, 13, with a twisted periodic boundary condition as described in Ref. [10]. Simulations are performed for the internal energy E and the specific heat C_V for fixed values of $|J/J_1|$. The results are then plotted against the temperature T. We identify the critical point as the temperature where C_V peaks, and the na-

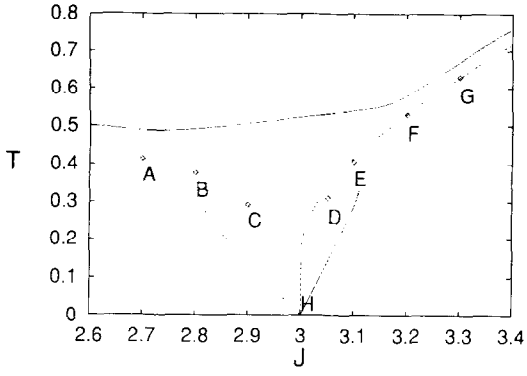

Fig. 3. The phase diagram for $J_1 < 0$, with J in units of $|J_1|$ and T in units of $|J_1|/k$. Data points are those determined from simulations as tabulated in Table 1. Solid lines represent the loci of maxima of the specific heat computed from an exact enumeration of the partition function for a 27-site lattice, broken and dotted lines are the phase boundaries.

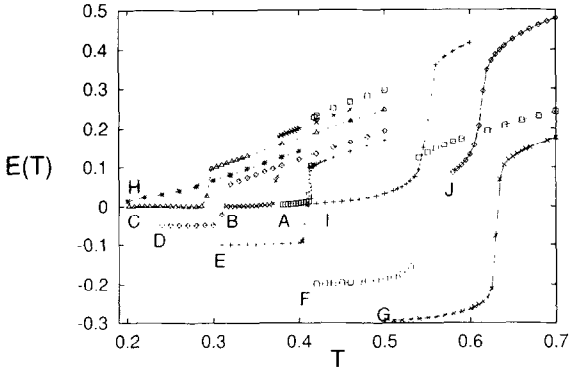

Fig. 4. The internal energy E as a function of the temperature, with E in units of $|J_1|$ and T in units of $|J_1|/k$. Plot H is for $J/|J_1| = 3$ and the other plots are for corresponding points in Figs. 2, 3, and Table 1.

ture of the transition from the energy plot. Results of the internal energy $E(T)$ for $J_1 < 0$ are shown in Fig. 4 with the values tabulated in Table 1. These results are from simulations on the 932-site lattice which is sufficient for the purpose of identifying the nature of the transition being of first order, since in this regime one always observes a jump discontinuity in the energy. Furthermore, the location of the discontinuity coincides well with the associated specific heat maximum, a fact confirming the internal consistency of our simulations. Also shown in Fig. 2 are data points from simulations on lattices of 507 and 3888 sites.

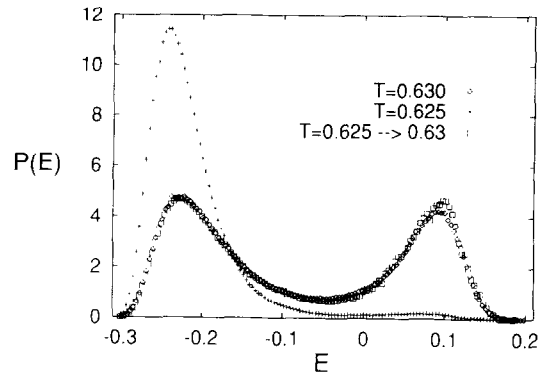

Fig. 5. Probability distribution of the internal energy E for $J/|J_1| = 3.30$ corresponding to point G . Diamonds and pluses are the original simulation data, squares are the extrapolation of the plus-distribution to the temperature of the diamond-distribution.

Simulations on a larger lattice help us to ascertain the transition is continuous.

A typical probability distribution $P(E)$, that of $J/|J_1| = 3.30$ corresponding to point G , is shown in Fig. 5. The onset of the doubly-peaked distribution in $P(E)$ again signifies the occurrence of a first-order transition. The first-order transition has also been confirmed by a cumulant analysis [11] which we have carried out, the details of which are not given in this paper. Finally, we have checked the consistency of our simulations by using the histogram method of Refs. [11, 12] to extrapolate the distribution $P(E)$ at temperature T from the $P(E)$ of another temperature, and compare the results with simulations at T. As shown in Fig. 5, the coincidence of the two is very good.

4. Small lattice calculations

We have also computed numerically the specific heat using the exact enumeration of the partition function for a 27-site ($L = 3$) lattice [10]. As before, we identify the maximum, or the first maximum in case there are two peaks, of the specific heat as the transition temperature. The results are shown by the solid lines in Fig. 3. Considering the smallness of the lattice size, the critical temperature derived from the exact specific heat agrees fairly well with those from simulations, and this agreement becomes even better in the $J \gg 3$ region not shown.

To further check the accuracy of our simulations,

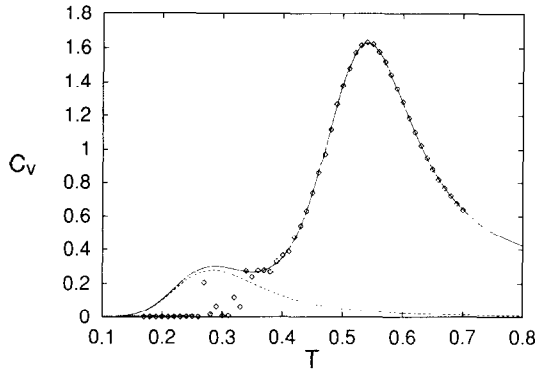

Fig. 6. The specific heat, in units of k, of a 27-site lattice for $J/|J_1| = 3.10$ corresponding to point E . Diamonds are data points from simulations. The solid line is the exact calculation, the broken line the contribution of the ground state and the first three energy levels, and the dotted line the contribution of higher energy states.

we have carried out simulations on the 27-site lattice, and compared the simulated specific heat with that from exact calculations. The example of $J/|J_1| = 3.10$, point E , is shown in Fig. 6. Generally, as shown in Fig. 6, the two specific heats agree remarkably well except at low temperatures. The low temparature discrepancy can be explained by a lack of ergodicity of the Metropolis algorithm. Indeed, the first excited states of the 27-site lattice can be identified as the configurations having exactly three times more violating bonds than violating triangles. Using a single spin-flip algorithm it is easy to see that the cost in energy to go from the ground state to these excited states is prohibitive. This is illustrated in Fig. 6, where the broken line shows the "partial" specific heat with only the ground state and the first three excited levels (561 states) taken into account. Also shown by the dotted line is the "partial" specific heat with all states higher than the first three excited ones taken into account. It is seen that the major contribution comes from that of the higher states. The low temperature satellite peak is a finite size effect which disappears in the thermodynamical limit.

5. Summary and discussions

We have presented results of Monte Carlo simulations and exact numerical calculations for the isotropic triangular model (1), which establish the existence of two critical frontiers, one in the antiferromagnetic and one in the ferromagnetic regime. We confirm that the transition in the antiferromagnetic regime is of first order, and that the critical frontier in the ferromagnetic regime coincides with the self-dual trajectory. In addition, our results indicate the existence of a tricritical point on the ferromagnetic frontier. On the basis of simulation results, we conjecture that the tricritical point is located at (7). We remark that this conjecture is supported by an analysis of the infinite symmetry group associated with the triangular Potts model (1). In this consideration [13], it can be shown that (7) belongs to a variety which is stable and along which the group becomes finite. Thus, (7) is a special point.

Acknowledgement

This work is supported by the CNRS and by the NSF grants INT-9113701 and DMR-9313648. One of us (GR) acknowledges the support of a Lavoisier grant from the Ministère des Affaires Etrangères. JMM would like to thank V. Dotsenko for discussions concerning the tricritical point. FYW and JMM are grateful to B. Nienhuis for the hospitality extended to them at the University of Amsterdam where a part of this research was carried out.

References

[1] R.J. Baxter, J. Phys. C 6 (1973) L445.
[2] F.Y. Wu, Rev. Mod. Phys. 54 (1982) 235.
[3] J.R. Banavar and F.Y. Wu, Phys. Rev. B 29 (1984) 1511.
[4] I. Enting and F.Y. Wu, J. Stat. Phys. 28 (1982) 351.
[5] R.J. Baxter, H.N.V. Temperley and S.E. Ashley, Proc. R. Soc. A 358 (1978) 535.
[6] F.Y. Wu and K.Y. Lin, J. Phys. A 13 (1980) 629.
[7] A. Hintermann, H. Kunz and F.Y. Wu, J. Stat. Phys. 19 (1978) 623.
[8] F.Y. Wu and R.K.P. Zia, J. Phys. A 14 (1981) 721.
[9] Y.M.M. Knops, B. Nienhuis and H.W.J. Blöte, The O(n) model on the triangular lattice, to be published.
[10] J.C. Anglès d'Auriac, J.M. Maillard, G. Rollet and F.Y. Wu, Physica A 206 (1994) 441.
[11] K. Binder, ed., in: Topics in applied physics, Vol. 71. The Monte Carlo method in condensed matter physics (Springer, Berlin, 1992).
[12] M. Ferrenberg and R.H. Swendsen, Phys. Rev. Lett. 58 (1988) 2635.
[13] J.M. Maillard and G. Rollet, J. Phys. A 27 (1994) 6963.