Finite-Temperature Phase Transition in a Class of Four-State Potts Antiferromagnets

Youjin Deng,1, a Yuan Huang,1, b Jesper Lykke Jacobsen,2,3, c Jesús Salas,4, d and Alan D. Sokol5,6, e
1Hefei National Laboratory for Physical Sciences at Microscale and Department of Modern Physics, University of Science and Technology of China, Hefei, Anhui 230026, China
2Laboratoire de Physique Théorique, École Normale Supérieure, 24 rue Lhomond, 75231 Paris, France
3Université Pierre et Marie Curie, 4 place Jussieu, 75252 Paris, France
4Gregorio Millán Institute, Universidad Carlos III de Madrid, 28911 Leganés, Spain
5Department of Physics, New York University, 4 Washington Place, New York, New York 10003, USA
6Department of Mathematics, University College London, London WC1E 6BT, United Kingdom

(Received 8 August 2011; published 3 October 2011)

We argue that the four-state Potts antiferromagnet has a finite-temperature phase transition on any Eulerian plane triangulation in which one sublattice consists of vertices of degree 4. We furthermore predict the universality class of this transition. We then present transfer-matrix and Monte Carlo data confirming these predictions for the cases of the Union Jack and bisected hexagonal lattices.

DOI: 10.1103/PhysRevLett.107.150601

PACS numbers: 05.50.+q, 11.10.Kk, 64.60.Cn, 64.60.De

The q-state Potts model [1, 2] plays an important role in the theory of critical phenomena, especially in two dimensions [3–5], and has applications to various condensed-matter systems [2]. Ferromagnetic Potts models are by now fairly well understood, thanks to universality; but the behavior of antiferromagnetic Potts models depends strongly on the microscopic lattice structure, so that many basic questions must be investigated case by case. Is there a phase transition at finite temperature, and if so, of what order? What is the nature of the low-temperature phase(s)? If there is a critical point, what are the critical exponents and the universality classes? Can these exponents be understood (for two-dimensional models) in terms of conformal field theory [5]?

One expects that for each lattice L there exists a value \( q_c(L) \) [possibly noninteger] such that for \( q > q_c(L) \) the model has exponential decay of correlations at all temperatures including zero, while for \( q = q_c(L) \) the model has a zero-temperature critical point. The first task, for any lattice, is thus to determine \( q_c \).

Some two-dimensional (2D) antiferromagnetic models at zero temperature can be mapped exactly onto a “height” model (in general vector valued) [6, 7]. Since the height at zero temperature can be mapped exactly onto a “height” theory.

In particular, when the q-state zero-temperature Potts antiferromagnet on a 2D lattice \( L \) admits a height representation, one ordinarily expects that \( q = q_c(L) \). This prediction is confirmed in most heretofore-studied cases: three-state square-lattice [6, 9–11], three-state kagome [12, 13], four-state triangular [14], and four-state on the line graph of the square lattice [13, 15]. The only known exceptions are the triangular Ising antiferromagnet [16] and the three-state model on the diced lattice [18].

Moore and Newman [14] observed that the height mapping employed for the four-state Potts antiferromagnet on the triangular lattice carries over unchanged to any Eulerian plane triangulation (a graph is called Eulerian if all vertices have even degree; it is called a triangulation if all faces are triangles). One therefore expects naively that \( q_c = 4 \) for every (periodic) Eulerian plane triangulation.

Here we will present analytic arguments suggesting that this naive prediction is false for an infinite class of Eulerian plane triangulations, namely, those in which one sublattice consists entirely of vertices of degree 4. More precisely, we predict that on these lattices the four-state Potts antiferromagnet has a phase transition at finite temperature (so that \( q_c > 4 \)); we shall also predict the universality class of this transition. We will conclude by presenting transfer-matrix and Monte Carlo data confirming these predictions for the cases of the Union Jack and bisected hexagonal lattices.

Exact identities.—Let \( G = (V, E) \) and \( G^* = (V^*, E^*) \) be a dual pair of connected graphs embedded in the plane [Fig. 1(a)]. Then define \( \tilde{G} = (V \cup V^*, \tilde{E}) \) to be the graph with vertex set \( V \cup V^* \) and edges \( ij \) whenever \( i \in E \) lies on the boundary of the face of \( G \) that contains \( j \in V^* \) [Fig. 1(b)]. The graph \( \tilde{G} \) is a plane quadrangulation: on each face of \( \tilde{G} \), one pair of diametrically opposite vertices corresponds to an edge \( e \in E \) and the other pair corresponds to the dual edge \( e^* \in E^* \). In fact, \( \tilde{G} \) is nothing other
new vertex in each face of ^tripartition This graph \( \sim \) Potts ferromagnet on model) on
\[ \sim \frac{1}{4} \]
than the dual of the medial graph \( \mathcal{M}(G) = \mathcal{M}(G^*) \) [19]. Conversely, every plane quadrangulation \( \tilde{G} \) arises via this construction from some pair \( G, G^* \).

Now let \( \tilde{G} \) be the graph obtained from \( G \) by adjoining a new vertex in each face of \( G \) and four new edges connecting this new vertex to the four corners of the face [Fig. 1(b)]. This graph \( \tilde{G} \) is an Eulerian plane triangulation, with vertex tripartition \( V \cup V^* \cup C \) where \( C \) is the set consisting of the "new" degree-4 vertices. Conversely, every Eulerian plane triangulation in which one sublattice consists of degree-4 vertices arises in this way.

We will show elsewhere [20] that the four-state Potts antiferromagnet at zero temperature (= four-coloring model) on \( \tilde{G} \) can be mapped exactly onto the nine-state Potts ferromagnet on \( G \) and \( G^* \),

\[
Z_{\tilde{G}}(4, -1) = 4 \times 3^{-|v|} Z_G(9, 3) = 4 \times 3^{-|v|} Z_G^*(9, 3),
\]

(1)

where \( Z_G(q, v) \) denotes the Potts-model partition function with \( v = e^J - 1 \) (\( J \) = nearest-neighbor coupling). The proof passes either via an RSOS model on \( \tilde{G} \) or via a completely packed loop model on \( \mathcal{M}(G) \).

Height representation [14].—Consider the four-coloring model on an Eulerian plane triangulation \( \Theta \). We can orient the edges of \( \Theta \) such that the three edges around each face define a cycle (clockwise on one sublattice of \( \Theta^* \) and counterclockwise on the other). Let \( e_0, e_1, e_2 \) be unit vectors at angles 0, 2\( \pi/3 \), 4\( \pi/3 \) in the plane. Then, to any proper four-coloring \( \sigma \) of the vertices of \( \Theta \), we assign heights \( h_j \) in the triangular lattice such that \( h_j - h_i = e_{\sigma(i)\sigma(j)} \) or \( \sigma(i) \sigma(j) = \{1, 2\} \) or \( \{3, 4\} \) or \( \{1, 3\} \) or \( \{2, 4\} \) or \( \{1, 4\} \) or \( \{2, 3\} \).

Phase transition and universality class.—Let now \( G, G^* \), and \( \tilde{G} \) be infinite regular lattices. Conformal field theory [5] tells us that a \( q \)-state Potts ferromagnet with \( q > 4 \) cannot have a critical point. Therefore the nine-state Potts ferromagnet in (1) is noncritical, suggesting that the four-state Potts antiferromagnet at zero temperature on \( \tilde{G} \) is also noncritical [21]. But since this model has a height representation, it cannot be disordered; therefore it must be ordered. It follows that the four-state Potts antiferromagnet on \( \tilde{G} \) has an order-disorder transition (whether first order or second order) at finite temperature.

We can also understand the type of order in the four-coloring model on \( \tilde{G} \), and hence the universality class of the order-disorder transition in case it is second order. If the lattice \( G \) is self-dual, the point \( (q, v) = (9, 3) \) lies on the self-dual curve \( v = \sqrt{q} \), which is expected to be the locus of first-order transitions; so there are phases in which \( G \) is ordered and \( G^* \) is disordered, and vice versa (nine of each). We therefore predict that the four-coloring model on \( \tilde{G} \) has phases in which the sublattice \( V \) is ordered in one of the four possible directions while \( V^* \) and \( C \) are disordered, and the same with \( V \) and \( V^* \) interchanged. The symmetry is \( S_4 \times Z_2 \), so we expect that the transition is in the universality class of a four-state Potts model plus an Ising model (decoupled). On the other hand, if \( G \) is not self-dual, then we expect (barring a fluke) that \( (q, v) = (9, 3) \) does not lie on a phase-transition curve; hence one of the lattices \( G, G^* \) will be ordered (say, \( G \)) while the other is disordered. In this case we predict that the four-coloring model on \( \tilde{G} \) has phases in which the sublattice \( V \) is ordered in one of the four possible directions while \( V^* \) and \( C \) are disordered. The symmetry is \( S_4 \), and the universality class is that of a four-state Potts model.

We recall that the central charge \( c \) and magnetic and thermal exponents \( X_m, X_t \) are \( (c, X_m, X_t) = (\frac{2}{3}, \frac{1}{3}, 1) \) for the Ising model and \( (1, \frac{1}{8}, \frac{1}{2}) \) for the four-state Potts model.

**Union Jack (UJ) lattice.**—The simplest self-dual case is \( G = G^* = \tilde{G} = \) square lattice and \( \tilde{G} = \) Union Jack lattice [Fig. 2(a)]. We computed transfer matrices with fully periodic boundary conditions for even widths \( L \leq 20 \) (\( v = -1 \) [22] and \( L \leq 16 \) (general \( v \)). Estimates of \( c, X_m, X_t \) were extracted from the free energy \( f_L \) and free-energy gaps \( \Delta f_L \) via [5]

\[
f_L = f_\infty - \pi c/(6L^2) + o(1/L^2),
\]

(2)

\[ \begin{array}{ll}
\text{(a)} & \text{(b)} \\
\end{array} \]

**FIG. 2** (color online). (a) Union Jack lattice, \( L = 6 \). (b) Bisected hexagonal lattice, \( L = 8 \). The shaded areas show the minimal unit cells (pink) and the rectangular unit cells used in the row-to-row transfer-matrix computations (blue). The tripartition of the vertex set is shown in black, gray, and white as in Fig. 1.
\[ \Delta f_L = 2\pi X/L^2 + o(1/L^2). \]  

Figure 3 (upper left) shows estimates of \(c(v)\) at \(q = 4\). The maximum at \(v = -0.95\) indicates the transition: finite-size scaling (FSS) yields \(v_c = -0.944(5)\) and \(c = 1.510(5)\), in agreement with our prediction \(c = 1 + \frac{7}{10} = \frac{17}{10}\). The crossings of \(X_m(v)\) and \(X_t(v)\) yield \(v_t = -0.9488(3), X_m = 0.1255(6), \) and \(X_t = 0.51(2)\), in agreement with \(X_m = \frac{8}{9} \) and \(X_t = \frac{1}{2} \) [23].

A similar plot for \(c(q)\) at \(v = -1\) shows the lattice-independent Berker-Kadanoff phase \([c = 1 - \frac{6(t-1)^2}{2}]\) with \(q = 4\cos^2(\pi/t)\) for \(0 < q < q_c\). The maxima of \(c(q)\) [Fig. 3, upper right] yield the estimates \(q_0 = 3.63(2), c = 1.43(1)\) and \(q_c = 4.330(5), c = 1.63(1)\). The crossings of \(X_m(q)\) and \(X_t(q)\) yield \(q_0 = 3.616(6), X_m = 0.0751(3), X_t = 0.88(2)\) and \(q_c = 4.326(5), X_m = 0.134(2), X_t = 0.52(3)\).

The data for \(q_0\) are consistent with \(q_0 = B_{10} = (5 + \sqrt{5})/2 = 3.61803\) [24] and \(c = 7/5, X_m = 3/40, X_t = 7/8\); the underlying conformal field theory could be a pair of \(m = 4\) minimal models [25].

Concerning \(q_c\), we have seen that at \((q, v) = (4, v_c)\) the critical behavior is that of a four-state Potts model plus an Ising model (decoupled), and it is compelling to think that this behavior will persist along a curve in the \((q, v)\) plane passing through \((q, v) = (q_c, -1)\). However, it is possible that \((q_c, -1)\) might be the end point of this curve, in which case the model could be driven there to some sort of multicritical behavior: for instance, a four-state Potts model plus a tricritical Ising model (decoupled), which would have \(c = 1 + \frac{2}{10} = \frac{17}{10}\) and \(X_m = X_{1/2,0} = 21/160 = 0.13125\) [25]. Alternatively, the critical exponents along the transition curve may vary continuously with \(q\).

We also simulated the \(q = 4\) model, using a cluster Monte Carlo (MC) algorithm, on periodic \(L \times L\) lattices with \(8 \leq L \leq 512\). We measured the sublattice magnetizations \(M_A, M_B, M_C\), the nearest-neighbor correlations \(E_{AA}, E_{AC}, E_{BC}\) and the next-nearest-neighbor correlations \(E_{AA}, E_{BB}, E_{CC}\). We then computed the \(3 \times 3\) sublattice susceptibility matrix and the \(6 \times 6\) specific-heat matrix; from their eigenvalues we can extract the magnetic and thermal critical exponents. The leading susceptibility eigenvalue diverges with the predicted exponent \(\gamma/v = 2 - 2X_m = 7/4\) [Fig. 4(a)], and FSS analysis yields the

![FIG. 3](color online). Estimates for central charge \(c\) and critical exponents \(X_m, X_t\) for the UJ lattice, as a function of \(v\) at \(q = 4\) (left) and as a function of \(q\) at \(v = -1\) (right). Dashed vertical lines indicate our best FSS estimates of \(v_c, q_0, \) and \(q_c\). Fits used Eqs. (2) and (3) with \(o(1/L^2)\) replaced by \(A/L^4\), for three (respectively two) consecutive values of \(L\).

![FIG. 4](color online). Monte Carlo data for the UJ lattice at \(q = 4\). (a) Leading susceptibility eigenvalue \(\lambda_1(\chi)\) divided by \(L^{7/4}\). (b) Leading specific-heat eigenvalue \(\lambda_1(C)\) divided by \(L\). (c) Second susceptibility eigenvalue \(\lambda_2(\chi)\) divided by \(L^{5/2}(\log L)^{-1/4}\). Lines are meant only to guide the eye.
estimate \( v_c = -0.9485(1) \). Likewise, the leading specific-heat eigenvalue diverges with exponent \( \alpha / v = 2 - 2L_c = 1 \) [23] [Fig. 4(b)], and FSS analysis yields the estimate \( v_c = -0.9483(2) \). It is curious that we do not see here the multiplicative logarithms that are expected [26] for the four-state Potts model. The second susceptibility eigenvalue diverges as \( L^{3/2} \), probably with a multiplicative logarithm [Fig. 4(c)], while the second specific-heat eigenvalue tends to a finite constant; we have no theoretical understanding of these behaviors.

A transition in this model was recently predicted by Chen et al. [27], who found \( v_c = -0.9477(5) \) by a tensor renormalization-group method; they also gave an entropy-counting argument predicting the type of order. However, in their approximation the specific heat was nondivergent, exhibiting a jump discontinuity.

**Bisected hexagonal (BH) lattice.** The simplest non-self-dual case is \( G = \text{triangular lattice} \) and \( G^* = \text{hexagonal lattice} \), yielding \( \hat{G} = \text{diced lattice} \) and \( \hat{G} = \text{bisected hexagonal lattice} \) [Fig. 2(b)]. We computed transfer matrices with fully periodic boundary conditions for the same widths as for the UJ lattice, except that \( L \) must now be a multiple of 4 to be compatible with the periodic boundary conditions [see Fig. 2(b)]. FSS analysis of \( c(v) \) at \( q = 4 \) yields the estimates \( v_c = -0.8281(1) \) and \( c = 1.0005(5) \), in agreement with our prediction \( c = 1 \). The crossing of \( X_m(v) \) and the minimum of \( X_c(v) \) yield \( v_c = -0.8280(1), X_m = 0.15(1), X_c = 0.65(10) \), which are compatible with \( X_m = \frac{1}{8} \) and \( X_c = \frac{1}{2} \) although rather imprecise.

The maximum of \( c(q) \) yields \( q_c = 5.3951(10) \), \( c = 1.20(5) \). The crossing of \( X_m(q) \) and the minimum of \( X_c(q) \) yield \( q_c = 5.3975(5), X_m = 0.15(1), X_c = 0.65(1) \). We also did MC simulations for \( q = 4 \) and \( 8 \leq L \leq 512 \). The leading susceptibility eigenvalue diverges as expected as \( L^{7/4} \) [possibly with a multiplicative \( \log L \)^{-1/8}] and yields \( v_c = -0.828066(4) \). The leading specific-heat eigenvalue is compatible with the four-state Potts behavior \( L(\log L)^{-3/2} \).

A transition in this model was also conjectured in [27]. Our result \( q_c > 5 \) suggests that there will be a finite-temperature transition also in the *five-state* model. Quite surprisingly, we find this transition to be second order, despite the absence of an obvious universality class (since \( q > 4 \)); however, it is also conceivable that the transition is weakly first order, with a correlation length that is finite but very large. Preliminary results from transfer matrices are \( v_c' = -0.9513(1), c = 1.17(5), X_m = 0.16(1), X_c = 0.56(4) \). Preliminary MC results are \( v_c' = -0.95132(2), X_m = 0.113(4), X_c = 0.495(5) \). More detailed data will be reported separately [28].

Taking into account the likely corrections to scaling, our data for \( (q, v) = (4, v_c), (5, v_c') \), and \( (q_c, -1) \) are compatible with all three models being in the four-state Potts universality class.

**Conclusion.** We have given (a) an analytical existence argument for a finite-temperature phase transition in a class of four-state Potts antiferromagnets; (b) a prediction of the universality class; (c) large-scale numerics, using two complementary techniques, to determine critical exponents; (d) determination of \( q_0 \) and \( q_c \) as well as \( v_c \); and (e) the surprising prediction of a finite-temperature phase transition also for \( q = 5 \) on the BH lattice [28].

This work was supported in part by NSFC Grant No. 10975127, the Chinese Academy of Sciences, French Grant No. ANR-10-BLAN-0414, the Institut Universitaire de France, Spanish MEC Grants No. FPA2009-08785 and No. MTM2008-03020, and NSF Grant No. PHY-0424082.
[18] R. Kotecký, J. Salas, and A. D. Sokal, Phys. Rev. Lett. 101, 030601 (2008).
[19] C. Godsil and G. Royle, Algebraic Graph Theory (Springer-Verlag, New York, 2001), Sec. 17.2.
[20] J. L. Jacobsen and A. D. Sokal (to be published).
[21] This suggestion could possibly be made rigorous if (1) could be generalized to an identity for suitable correlation functions.
[22] Here we exploit the algorithm of J. L. Jacobsen, J. Phys. A 43, 315002 (2010).
[23] The four-state Potts value $X_t = \frac{1}{2}$ is more relevant than the Ising value $X_t = 1$ and hence dominates.
[24] The nth Beraha number is $B_n = 4\cos^2(\pi/n)$.
[25] The mth minimal model [5] has central charge $c = 1 - 6/[m(m + 1)]$ and critical exponents $X_{rs} = [(r(m + 1) - sm^2 - 1)/[2m(m + 1)]$ for integer (and sometimes half-integer [7]) $r, s$. It is the continuum limit both of the $q = B_{m+1}$ critical Potts ferromagnet and of the $q = B_m$ tricritical Potts ferromagnet.
[26] J. Salas and A. D. Sokal, J. Stat. Phys. 88, 567 (1997).
[27] Q. N. Chen et al., arXiv:1105.5030 [Phys. Rev. Lett. (to be published)].
[28] Y. Deng, Y. Huang, J. L. Jacobsen, J. Salas, and A. D. Sokal (to be published).