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Phys. Rev. Lett. **107**, 150601 — Published 3 October 2011

DOI: 10.1103/PhysRevLett.107.150601

Finite-temperature phase transition in a class of 4-state Potts antiferromagnets

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We argue that the 4-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.

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 $\mathcal{L}$ there exists a value $q_c(\mathcal{L})$ [possibly noninteger] such that for $q > q_c(\mathcal{L})$ the model has exponential decay of correlations at all temperatures including zero, while for $q = q_c(\mathcal{L})$ 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 model must either be in a "smooth" (ordered) or "rough" (massless) phase, the corresponding zero-temperature spin model must either be ordered or critical, never disordered. Experience tells us that the most common case is criticality [8]. The long-distance behavior is then that of a massless Gaussian with some (*a priori* unknown) "stiffness matrix" $\mathbf{K} > 0$. The critical operators can be identified via the height mapping, and the corresponding critical exponents can be predicted in terms of $\mathbf{K}$. Height representations thus provide a means for recovering a sort of universality for some (but not all) antiferromagnetic models and for understanding their critical behavior in terms of conformal field theory.

In particular, when the q-state zero-temperature Potts antiferromagnet on a 2D lattice $\mathcal{L}$ admits a height representation, one ordinarily expects that $q = q_c(\mathcal{L})$. This prediction is confirmed in most heretofore-studied cases: 3-state square-lattice [6, 9, 11, 12], 3-state kagome [13, 14], 4-state triangular [15], and 4-state on the line graph of the square lattice [14, 16]. The only known exceptions are the triangular Ising antiferromagnet [17] and the 3-state model on the diced lattice [10].

Moore and Newman [15] observed that the height mapping employed for the 4-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 4-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 [$D(4, 8^2)$] and bisected hexagonal [$D(4, 6, 12)$] lattices.

Exact identities. Let $G = (V, E)$ and $G^* = (V^*, E^*)$ be a dual pair of connected graphs embedded in the plane (Fig. 1a). Then define $\widehat{G} = (V \cup V^*, \widehat{E})$ to be the graph with vertex set $V \cup V^*$ and edges ij whenever $i \in V$ lies on the boundary of the face of G that contains $j \in V^*$ (Fig. 1b). The graph $\widehat{G}$ is a plane quadrangulation: on each face of $\widehat{G}$, 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, $\widehat{G}$ is nothing other than the dual of the medial graph $\mathcal{M}(G) = \mathcal{M}(G^*)$ [19]. Conversely, every plane quadrangulation $\widehat{G}$ arises via this construction from some pair G, G^*.

Now let $\widetilde{G}$ be the graph obtained from $\widehat{G}$ by adjoining a new vertex in each face of $\widehat{G}$ and four new edges connecting this new vertex to the four corners of the face

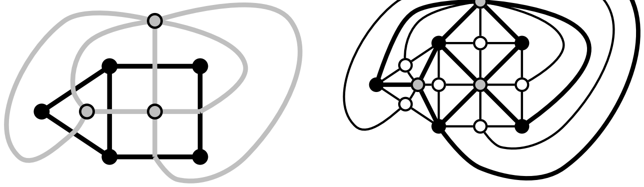

Figure 1: (a) A dual pair G (black dots and lines) and G^* (gray dots and lines). (b) The quadrangulation $\widehat{G}$ (black/gray dots and thick lines) and triangulation $\widetilde{G}$ (all dots and lines).

(Fig. 1b). This graph $\widetilde{G}$ 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 4-state Potts antiferromagnet at zero temperature (= 4-coloring model) on $\widetilde{G}$ can be mapped exactly onto the 9-state Potts *ferro*magnet on G and G^*:

$$Z_{\widetilde{G}}(4,-1) = 4 \cdot 3^{-|V|}\, Z_G(9,3) = 4 \cdot 3^{-|V^*|}\, Z_{G^*}(9,3) \quad (1)$$

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 $\widehat{G}$ or via a completely packed loop model on $\mathcal{M}(G)$.

Height representation [15]. Consider the 4-coloring model on an Eulerian plane triangulation Θ. We can orient the edges of Θ such that the three edges around each face define a cycle (clockwise on one sublattice of Θ^* and counterclockwise on the other). Let $\mathbf{e}_0, \mathbf{e}_1, \mathbf{e}_2$ be unit vectors at angles $0, 2\pi/3, 4\pi/3$ in the plane. Then, to any proper 4-coloring σ of the vertices of Θ, we assign heights $\mathbf{h}_i$ in the triangular lattice such that $\mathbf{h}_j - \mathbf{h}_i = \mathbf{e}_0, \mathbf{e}_1, \mathbf{e}_2$ on an oriented edge $\vec{ij}$ according as $\{\sigma_i, \sigma_j\} = \{1,2\}$ or $\{3,4\}$, $\{1,3\}$ or $\{2,4\}$, $\{1,4\}$ or $\{2,3\}$.

Phase transition and universality class. Let now G, G^* and $\widetilde{G}$ 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 9-state Potts ferromagnet in (1) is noncritical, suggesting that the 4-state Potts antiferromagnet at zero temperature on $\widetilde{G}$ 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 4-state Potts antiferromagnet on $\widetilde{G}$ has an order-disorder transition (whether first-order or second-order) at finite temperature.

We can also understand the type of order in the 4-coloring model on $\widetilde{G}$, 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 4-coloring model on $\widetilde{G}$ 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 4-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 4-coloring model on $\widetilde{G}$ 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 4-state Potts model.

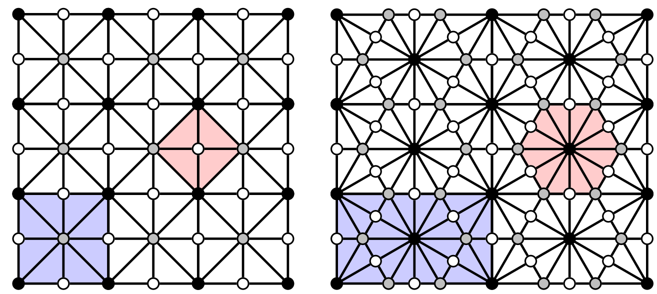

Figure 2: (a) Union-jack lattice, $L = 6$. (b) Bisected hexagonal lattice, $L = 8$. The shaded areas show the minimal unit cells (pink) and the rectangular unit cells used in the row-to-row transfer-matrix computations (blue). The tripartition of the vertex set is shown in black/gray/white as in Fig. 1.

We recall that the central charge c and magnetic and thermal exponents X_m, X_t are $(c, X_m, X_t) = (\frac{1}{2}, \frac{1}{8}, 1)$ for the Ising model and $(1, \frac{1}{8}, \frac{1}{2})$ for the 4-state Potts model.

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

$$f_L = f_\infty - \pi c/(6L^2) + o(1/L^2) \quad (2)$$

$$\Delta f_L = 2\pi X/L^2 + o(1/L^2) \quad (3)$$

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

A similar plot for $c(q)$ at $v = -1$ shows the lattice-independent Berker–Kadanoff phase [$c = 1 - 6(t-1)^2/t$ with $q = 4\cos^2(\pi/t)$] for $0 \le q < q_0$ and a noncritical phase for $q_0 < q < q_c$. The maxima of $c(q)$ [Fig. 3, upper

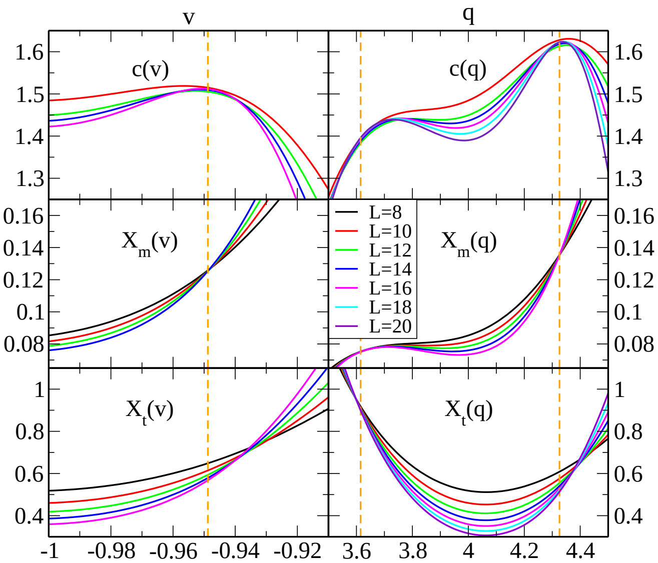

Figure 3: Estimates for central charge c and critical exponents X_m, X_t for the UJ lattice, as a function of v at $q = 4$ (left) and as a function of q at $v = -1$ (right). Dashed vertical lines indicate our best FSS estimates of v_c, q_0 and q_c. Fits used Eqs. (2)/(3) with $o(1/L^2)$ replaced by A/L^4,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

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 $q_0 = B_{10} = (5 + \sqrt{5})/2 \approx 3.61803$ [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 4-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 endpoint of this curve, in which case the model could be driven there to some sort of multicritical behavior: for instance, a 4-state Potts model plus a *tricritical* Ising model (decoupled), which would have $c = 1+\frac{7}{10} = \frac{17}{10}$ 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 $8 \le L \le 512$. We measured the sublattice magnetizations $\mathcal{M}_A, \mathcal{M}_B, \mathcal{M}_C$, the nearest-neighbor correlations $\mathcal{E}_{AB}, \mathcal{E}_{AC}, \mathcal{E}_{BC}$ and the next-nearest-neighbor correlations $\mathcal{E}_{AA}, \mathcal{E}_{BB}, \mathcal{E}_{CC}$. We then computed the 3×3 sublattice susceptibility matrix and the 6×6 specific-heat matrix; from their eigenvalues we can extract the magnetic and thermal critical exponents. The leading susceptibility eigenvalue diverges with the predicted exponent $\gamma/\nu = 2 - 2X_m = 7/4$ (Fig. 4a), and FSS analysis yields the estimate $v_c = -0.9485(1)$. Likewise, the leading specific-heat eigenvalue diverges with exponent $\alpha/\nu = 2 - 2X_t = 1$ [23] (Fig. 4b), 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 4-state Potts model. The second susceptibility eigenvalue diverges as $L^{3/2}$, probably with a multiplicative logarithm (Fig. 4c), while the second specific-heat eigenvalue tends to a finite constant; we have no theoretical understanding of these behaviors.

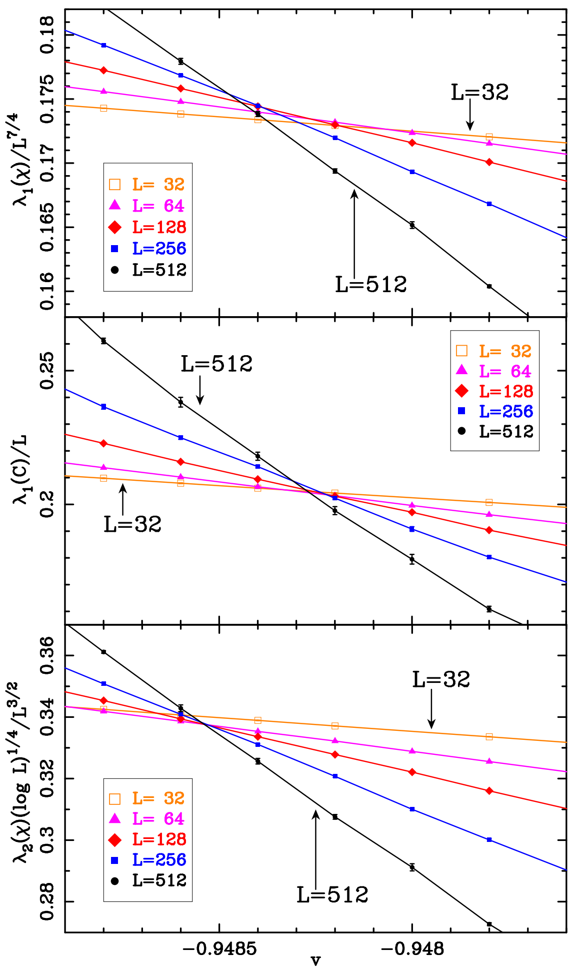

Figure 4: Monte Carlo data for the UJ lattice at $q = 4$. (a) Leading susceptibility eigenvalue $\lambda_1(\chi)$ divided by $L^{7/4}$. (b) Leading specific-heat eigenvalue $\lambda_1(C)$ divided by L. (c) Second susceptibility eigenvalue $\lambda_2(\chi)$ divided by $L^{3/2}(\log L)^{-1/4}$. Lines are meant only to guide the eye.

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 non-divergent, exhibiting a jump discontinuity.

Bisected hexagonal (BH) lattice. The simplest non-self-dual case is G = triangular lattice and G^* = hexagonal lattice, yielding $\widehat{G}$ = diced lattice and $\widetilde{G}$ = bisected hexagonal lattice (Fig. 2b). 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. 2b). FSS analysis of $c(v)$ at $q = 4$ yields the estimates $v_c = -0.8281(1)$ and $c = 1.000(5)$, in agreement with our prediction $c = 1$. The crossing of $X_m(v)$ and the minimum of $X_t(v)$ yield $v_c = -0.8280(1)$, $X_m = 0.15(1)$ and $X_t = 0.65(10)$, which are compatible with $X_m = \frac{1}{8}$ and $X_t = \frac{1}{2}$ although rather imprecise.

The maximum of $c(q)$ yields $q_c = 5.395(10)$, $c = 1.20(5)$. The crossing of $X_m(q)$ and the minimum of $X_t(q)$ yield $q_c = 5.397(5)$, $X_m = 0.15(1)$, $X_t = 0.6(1)$.

We also did MC simulations for $q = 4$ and $8 \le L \le 512$. 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 4-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 *5-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 $v'_c = -0.9513(1)$, $c = 1.17(5)$, $X_m = 0.16(1)$, $X_t = 0.56(4)$. Preliminary MC results are $v'_c = -0.95132(2)$, $X_m = 0.113(4)$, $X_t = 0.495(5)$. 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 4-state Potts universality class.

Conclusion. We have given: (a) an analytical existence argument for a finite-temperature phase transition in a class of 4-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 10975127, the Chinese Academy of Sciences, French grant ANR-10-BLAN-0414, the Institut Universitaire de France, Spanish MEC grants FPA2009-08785 and MTM2008-03020, and NSF grant PHY–0424082.

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