Two-dimensional Potts antiferromagnets with a phase transition at arbitrarily large q

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(Dated: October 22, 2012)

We exhibit infinite families of two-dimensional lattices (some of which are triangulations or quadrangulations of the plane) on which the q-state Potts antiferromagnet has a finite-temperature phase transition at arbitrarily large values of q. This result is proven rigorously using a Peierls argument. Additional numerical data are obtained using transfer matrices, Monte Carlo simulation, and a high-precision graph-theoretic method.

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 about the phase diagram and critical exponents must be investigated case-by-case.

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 (AF) 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, 12, 13], 3-state kagome [14, 15], 4-state triangular [16], and 4-state on the line graph of the square lattice [15, 17]. Until recently the only known exception was the triangular Ising AF [18].

Kotecký, Salas and Sokal (KSS) [10] have observed that the height mapping employed for the 3-state Potts AF on the square lattice [6] carries over unchanged to any plane quadrangulation; and Moore and Newman [16] observed that the height mapping employed for the 4-state Potts AF on the triangular lattice carries over unchanged to any Eulerian plane triangulation (a graph is called Eulerian if all vertices have even degree). One therefore expects naively that $q_c = 3$ for every (periodic) plane quadrangulation, and that $q_c = 4$ for every (periodic) Eulerian plane triangulation.

Surprisingly, these predictions are *false*! KSS [10] proved rigorously that the 3-state AF on the diced lattice (which is a quadrangulation) has a phase transition at finite temperature (see also [20]); numerical estimates from transfer matrices yield $q_c(\text{diced}) \approx 3.45$ [21]. Likewise, we recently [11] provided analytic arguments (falling short, however, of a rigorous proof) that on any Eulerian plane triangulation in which one sublattice consists entirely of vertices of degree 4, the 4-state AF has a phase transition at finite temperature, so that $q_c > 4$. We also presented transfer-matrix and Monte Carlo data confirming these predictions for the union-jack and bisected hexagonal lattices, leading to the estimates $q_c(\text{UJ}) \approx 4.33$ and $q_c(\text{BH}) \approx 5.40$.

These results suggest the obvious question: How large can q_c be on a plane quadrangulation (resp. Eulerian plane triangulation)? The answers are clearly larger than 3 or 4, respectively — but how much larger?

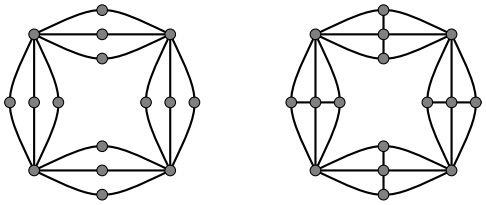


Figure 1. Unit cells of the lattices G_n and H_n for $n = 3$.

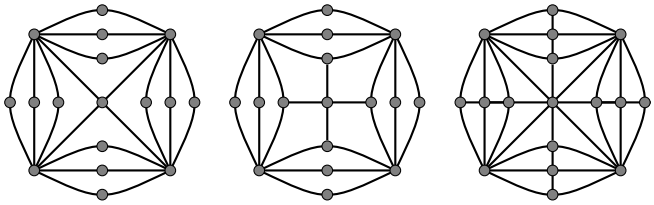


Figure 2. Unit cells of the lattices G'_n, G''_n and H'''_n for $n = 3$.

In this Letter we shall give a rigorous proof of the unexpected answer: we exhibit infinite classes of plane quadrangulations and Eulerian plane triangulations on which q_c can take *arbitrarily large* values. We shall also complement this rigorous proof with detailed quantitative data from transfer matrices, Monte Carlo simulations, and a powerful graph-theoretic approach developed recently by Jacobsen and Scullard [22].

The lattices G_n and H_n. Let G_n be obtained from from the square (SQ) lattice by replacing each edge with n two-edge paths in parallel; and let H_n be obtained from G_n by connecting each group of n "new" vertices with an $(n-1)$-edge path (see Fig. 1). Resumming over the spins on the "new" vertices [23], it is easy to show that the q-state Potts model on G_n or H_n with nearest-neighbor coupling $v = e^J - 1$ is equivalent to a SQ-lattice Potts model with a suitable coupling $v_{\text{eff}}(q, v)$ [24]; moreover, for $q > 2$ (resp. $q > 3$) an AF model ($-1 \le v \le 0$) on G_n (resp. H_n) maps onto a ferromagnetic model ($v_{\text{eff}} \ge 0$) on the SQ lattice. Concretely, for the zero-temperature AF ($v = -1$) we have

$$v_{\text{eff}}^{G_n}(q, -1) \;=\; \Big(\frac{q-1}{q-2}\Big)^n \;-\; 1 \tag{1}$$

$$v_{\text{eff}}^{H_n}(q, -1) \;=\; \frac{q-1}{q-2}\Big(\frac{q-2}{q-3}\Big)^{n-1} \;-\; 1 \tag{2}$$

Setting v_{eff} equal to the SQ-lattice ferromagnetic critical point $v_c(\text{SQ}) = \sqrt{q}$ [3, 25], we obtain q_c for G_n and H_n; they have the large-n asymptotic behavior

$$q_c(G_n) \;\approx\; q_c(H_n) \;\approx\; \frac{2n}{W(2n)} \;+\; O\big((n/\log n)^{1/2}\big) \tag{3}$$

where $W(x) \approx \log x - \log\log x + o(1)$ is the Lambert W function [26]. We have thus exhibited two infinite families of periodic planar lattices on which the Potts AF has arbitrarily large q_c as $n \to \infty$ [27]. These lattices are not triangulations or quadrangulations, but they can be modified to be such and retain the phase transition, as we now show.

The modified lattices. Starting from G_n or H_n, insert a new vertex into each octagonal face and connect it either to the four surrounding vertices of the original SQ lattice, to the four "new" vertices, or to all eight vertices; call these modifications $'$, $''$ and $'''$, respectively. In particular, G'_n and G''_n are quadrangulations, and H'''_n is an Eulerian triangulation (Fig. 2).

If we integrate out the spins at the vertices placed into the octagonal faces, we obtain the model on G_n or H_n perturbed by a 4-spin or 8-spin interaction. When q is large, this interaction is weak (of order $1/q$) because its Boltzmann weight is bounded between a maximum value of q and a minimum value of $q-4$ or $q-8$. We therefore expect that the new edges will have a negligible effect on the phase transition when q is large, and that all the modified lattices will have $q_c(n)$ whose large-n behavior is essentially identical to Eq. (3). Let us now sketch a rigorous proof [28] of this assertion.

Proof of phase transition. Recall first how one proves, using the Peierls argument, the existence of ferromagnetic long-range order (FLRO) at low temperature in the q-state Potts ferromagnet on the SQ lattice. The Peierls contours are defined as the connected components of the union of all bonds on the dual SQ lattice that separate unequal spins. A Peierls contour γ of length $|\gamma|$ and cyclomatic number $c(\gamma)$ comes with a weight that is bounded above by $(q-1)^{c(\gamma)}(1+v)^{-|\gamma|}$: here $(q-1)^{c(\gamma)}$ is a bound on the number of colorings of the SQ lattice consistent with the contour γ. Further, on the SQ lattice we have $c(\gamma) \le |\gamma|/2$, and the number of contours of length n surrounding a fixed site can be bounded by $(n/2)16^n$. Standard Peierls reasoning then shows that for any pair of sites x, y one has

$$\text{Prob}(\sigma_x \neq \sigma_y) \;\le\; \sum_{n=4}^{\infty} (n/2)16^n (q-1)^{n/2}(1+v)^{-n}\,, \tag{4}$$

which is $\le 5/16$ whenever $1 + v \ge 32\sqrt{q}$. This proves FLRO (the constant 32 is of course suboptimal). The foregoing argument is valid for fixed boundary conditions (e.g., $\sigma = 1$) in the plane, but with suitable modifications it can also be carried out for periodic boundary conditions (i.e., on a torus).

Let us now consider the Potts antiferromagnet on one of the six modified lattices $G'_n, \ldots, H'''_n$. Since our goal is to show FLRO on the SQ sublattice, we define Peierls contours exactly as we did for the SQ-lattice ferromagnet, ignoring the spin values at all other sites. Although we no longer have any simple explicit formula for the contour weights, it is nevertheless possible to prove an

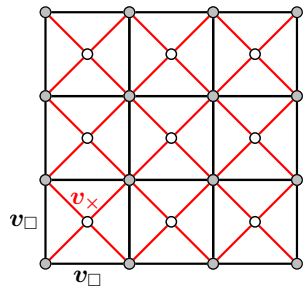
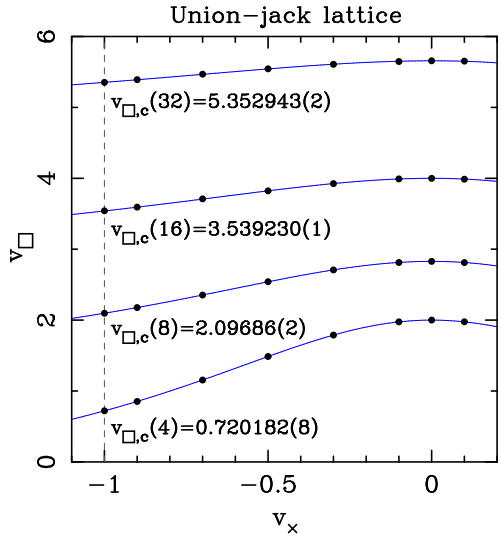


Figure 3. The union-jack (UJ) lattice.

upper bound on the probability of occurrence of a contour γ by using the technique of reflection positivity and chessboard estimates [29]. Without going into details of the needed adaptations of this standard technique for our case (see [28]), we mention only that the final bound on the probability of occurrence of a contour γ is $(\kappa\sqrt{q-1})^{|\gamma|}$, where κ is the probability that the spins on the SQ sublattice follow a fixed checkerboard pattern (say, 1 on the even sublattice and 2 on the odd sublattice) raised to the power 1/volume. This latter probability is easy to bound explicitly, yielding $\kappa \le [1+v_{\text{eff}}(q,v)]^{-1}[q/(q-5)]^{1/2}$, where $v_{\text{eff}}(q,v)$ is the one for the corresponding unmodified lattice G_n or H_n. This implies that, for all the lattices $G'_n, \ldots, H'''_n$, there is FLRO on the SQ sublattice whenever $6 \le q \le q_c(G_n) - O(1)$ [cf. Eq. (3)] and v is close to -1 (low temperature).

Let us also remark that the lattice G''_2 is covered by the general theory of [20], where it is proven that $q_c > 3$; moreover, a minor modification proves the same result for G''_n for all $n \ge 2$.

Data for lattices G'_n and H'_n. The lattices G'_n and H'_n for all n can be reduced to the union-jack (UJ) lattice (Fig. 3) with $v_\times = v$ and $v_\square =$ a suitable $v_{\text{eff}}(q,v)$ [cf. Eqns. (1)/(2) when $v = -1$]; of course the same reduction holds for G_n and H_n by setting $v_\times = 0$. We obtained high-precision estimates of the phase boundary of the UJ model in the $(v_\times, v_\square)$-plane by using the Jacobsen–Scullard (JS) method [22] with untwisted square bases of size up to 6×6 (216 edges) [30]. We checked these results for $q = 4, 8, 16, 32$ by Monte Carlo simulations using a cluster algorithm [31]. The estimated phase boundaries from both methods are shown in Fig. 4a, along with the numerical estimates of $v_{\square,c}$ at $v_\times = -1$. The resulting estimates of $n_c(q)$ [the inverse of the function $q_c(n)$] from Eqns. (1)/(2) are shown in Fig. 4b, where they are compared with the predicted large-q asymptote $n_c(q) \approx \frac{1}{2} q \log q$ from Eq. (3). The functions $q_c(n)$ divided by their large-n asymptote $2n/W(2n)$ are plotted in Fig. 4c. Note that $q_c(G'_n) > q_c(G_n)$ and $q_c(H'_n) > q_c(H_n)$, in accordance with the intuitive idea that the AF edges associated to the modification $'$ *enhance* the ferromagnetic ordering on the SQ sublattice [32].



q	$n_c(G_n)$ (exact)	$n_c(G'_n)$ (JS)	$n_c(H_n)$ (exact)	$n_c(H'_n)$ (JS)	$\frac{1}{2}q\log q$ (asymp.)
4	2.70951	1.33779(2)	2	1.19760(1)	2.77259
8	8.70871	7.33299(6)	7.51762	6.35447(5)	8.31777
16	23.32760	21.92628(1)	21.78650	20.48190(1)	22.18071
32	57.81205	56.38695(1)	55.94903	54.57066(1)	55.45177

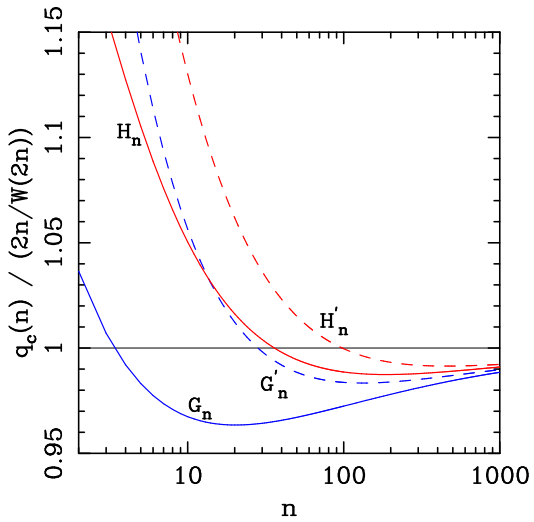


Figure 4. (a) Estimated phase boundaries for $q = 4, 8, 16, 32$ from the Jacobsen–Scullard method (blue curve and numerical values of $v_{\square,c}$ at $v_\times = -1$) and Monte Carlo simulations (black points). (b) Estimates of $n_c(q)$, and their large-q asymptote from Eq. (3). (c) Plots of $q_c(n)$ divided by their large-n asymptote $2n/W(2n)$.

Data for lattices G''_n and H'''_n. We studied the lattices G''_n and H'''_n for $n = 1, 2, 4, 8, 16, 32, 64$ (note that $G''_1 =$ SQ [6] and $H'''_1 =$ UJ [11]) at $v = -1$, using transfer matrices with cylindrical boundary conditions on widths $L = 1, 2, 3, 4$ unit cells (Fig. 5). The computational complexity is linear in n. We estimated the location of the

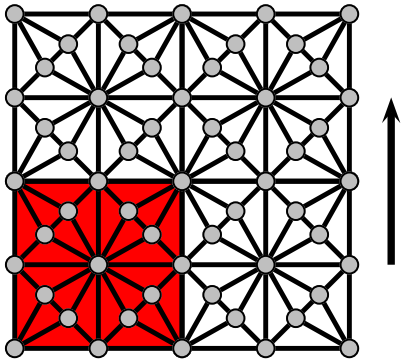


Figure 5. The lattice H_2''' (rotated 45° from Fig. 2) with $L = 2$; a unit cell is shown in red, and the transfer direction is indicated with an arrow.

phase transition (which we expect to be first-order whenever $q_c > 4$) using the crossings of the energies $E_L(q)$ [33]: the results are shown in Fig. 6a.

For H_n''' we checked these results by Monte Carlo: for three integer values of q below the estimated q_c we simulated the model at finite temperature and estimated the transition point $v_c(q)$; we then performed linear and quadratic extrapolations to locate the point q_c where $v_c = -1$. The results are shown in Fig. 6a,b and agree well with the transfer-matrix estimates. For $q \gtrsim 8$ the specific heat diverges at the transition point like $L^{\approx 2}$, in agreement with the finite-size-scaling prediction for a first-order transition; for $4 < q \lesssim 8$ the transition is presumably also first-order but with a large correlation length ξ, so that we are unable to observe the true $L \gg \xi$ asymptotic behavior.

This work was supported in part by NSFC grants 10975127 and 11275185, the Chinese Academy of Sciences, French grant ANR-10-BLAN-0414, the Institut Universitaire de France, Spanish MEC grants FPA2009-08785 and MTM2011-24097, Czech GAČR grant P201/12/2613, and US NSF grant PHY–0424082.

n	$q_c(G_n'')$ (TM)	$q_c(H_n''')$ (TM)	$q_c(H_n''')$ (MC)	$2n/W(2n)$ (asymp.)
1	3	4.31(3)		2.34575
2	3.63(2)	5.27(1)	5.26(2)	3.32732
4	5.02(1)	6.68(1)	6.67(3)	4.98190
8	7.60(1)	9.21(1)	9.21(7)	7.79274
16	12.18(2)	13.73(2)	13.73(10)	12.62134
32	20.29(3)	21.76(3)	21.76(32)	21.01608
64	34.70(5)	36.10(5)	36.14(8)	35.78022

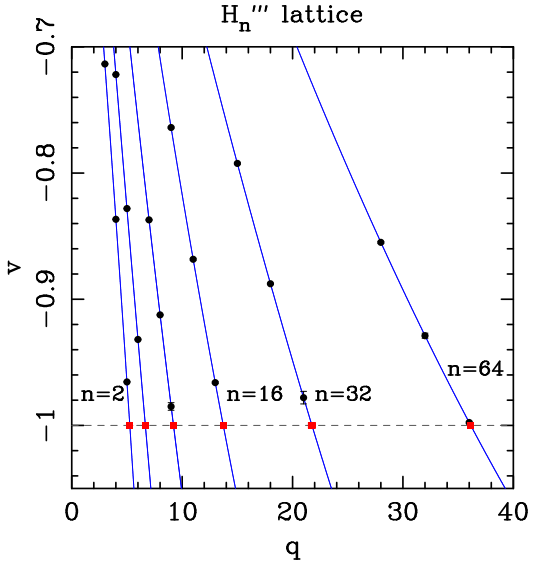


Figure 6. (a) Estimates of q_c from transfer matrices and Monte Carlo, and their large-n asymptote from Eq. (3). (b) Monte Carlo estimates of v_c for H_n''' (black points) and their quadratic fit (blue curves), together with the extrapolated values q_c (red squares).

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