Partial Order and Finite-Temperature Phase Transitions in Potts Models on Irregular Lattices

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We evaluate the thermodynamic properties of the 4-state antiferromagnetic Potts model on the Union-Jack lattice using tensor-based numerical methods. We present strong evidence for a previously unknown, "entropy-driven," finite-temperature phase transition to a partially ordered state. From the thermodynamics of Potts models on the diced and centered diced lattices, we propose that finite-temperature transitions and partially ordered states are ubiquitous on irregular lattices.

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The q-state Potts model has an essential role in the theory of classical critical phenomena and phase transitions [1]. Antiferromagnetic Potts models are rich and complex, displaying many different types of behavior as a function of q and of lattice geometry, and the search for guiding principles continues. Key questions include whether the model has a phase transition, if this occurs at finite temperature, the nature of the low-temperature phase, and the universality class of the transition.

In the Landau theory of phase transitions, these are described by an order parameter. Minimizing the energy at low temperatures requires the order parameter to be finite everywhere. However, in systems with extensive ground-state degeneracy [2], of which the best-known example is ice [3], the nonzero entropy at zero temperature may cause a different type of ordered state. A partial order, involving only some of the lattice sites, is stabilized by minimization of energy in combination with maximization of entropy. This "entropy-driven" transition can occur at a finite temperature. Such partial order is known in both frustrated [4,5] and unfrustrated [6] systems. In the latter case, partial order arises purely due to configurational entropy effects, and the $q = 3$ antiferromagnetic Potts model on the diced lattice provides an excellent example of the associated phase transition [7].

In this Letter we pursue the physical origin of the finite-temperature phase transition in two-dimensional (2D) q-state Potts models. Although these systems have no exact solution for $q > 2$, we employ tensor-based numerical methods to obtain hitherto unavailable thermodynamic quantities. We show that the $q = 4$ Potts model on the Union-Jack lattice exhibits a finite-temperature transition to a state of partial order. We characterize this transition by computing the entropy, specific heat, and magnetization, quantities we also use to provide a complete discussion of the $q = 3$ model on the diced lattice. We propose that finite-temperature transitions and partially ordered states are a general property of Potts models on irregular lattices.

Let the q states of the Potts model for lattice site i be labeled $\sigma_i = 0, 1, \ldots, q-1$. In the Hamiltonian,

$$\mathcal{H} = J\sum_{\langle i,j\rangle}\delta_{\sigma_i\sigma_j} - H\sum_i \delta_{\sigma_i,0}, \tag{1}$$

$J > 0$ corresponds to the antiferromagnetic case and a field H is coupled to one of the q states. We consider only a single coupling J on every bond, and begin with $H = 0$. We employ tensor-based numerical techniques developed recently by a number of authors [8–12] to compute the partition function Z to high accuracy, and hence to obtain the required thermodynamic quantities.

We illustrate the methods by focusing on the Union-Jack lattice [Fig. 1(a)]. The partition function

$$Z = \mathrm{Tr}e^{-\beta\mathcal{H}} = \sum_{\{\sigma_i\}}\prod_{\Box} e^{-\beta\mathcal{H}_\Box}, \tag{2}$$

$\Box$ represents the structural unit [Fig. 2(a)] and

$$\mathcal{H}_\Box^{\mathrm{UJ}} = J(\delta_{\sigma_1\sigma_2} + \delta_{\sigma_2\sigma_3} + \delta_{\sigma_3\sigma_4} + \delta_{\sigma_4\sigma_1})/2 + J(\delta_{\sigma_1\sigma_5} + \delta_{\sigma_2\sigma_5} + \delta_{\sigma_3\sigma_5} + \delta_{\sigma_4\sigma_5}). \tag{3}$$

The tensor $T_\Box = e^{-\beta\mathcal{H}_\Box}$ is defined [8,11] by summing over the C-sublattice sites σ_5 and introducing the bond (or dual-lattice) variables $\alpha = \mathrm{mod}(\sigma_1 - \sigma_2, q)$,

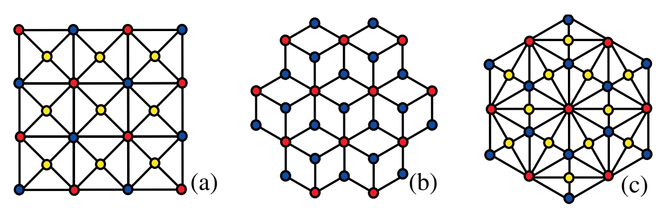

FIG. 1 (color online). (Color online) (a) Union-Jack lattice. Sites in sublattices A (red circles) and B (blue) have coordination numbers $z_A = z_B = 8$, while those in sublattice C (yellow) have $z_C = 4$. (b) Diced lattice. A sites (red) have $z_A = 6$, while B sites (blue) have $z_B = 3$. (c) Centered diced lattice: $z_A = 12$ (red), $z_B = 6$ (blue), and $z_C = 4$ (yellow).

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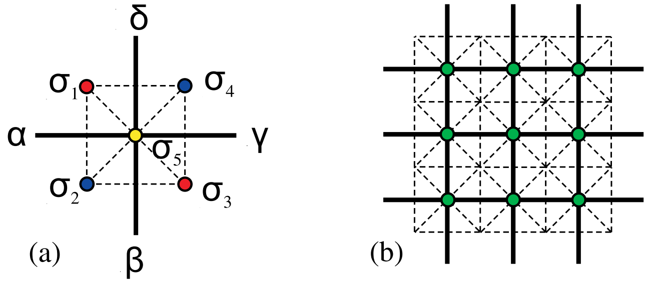

FIG. 2 (color online). (a) Schematic representation of the tensor T, obtained by integrating over the C-sublattice sites and performing the dual transformation. (b) The Union-Jack lattice (dashed lines) is transformed to the dual square lattice (solid lines) on which the tensor T is defined.

$\beta = \mathrm{mod}(\sigma_2 - \sigma_3, q)$, $\gamma = \mathrm{mod}(\sigma_3 - \sigma_4, q)$, and $\delta = \mathrm{mod}(\sigma_4 - \sigma_1, q)$ [Fig. 2(a)]. The partition function

$$Z = \sum_{\alpha\beta\gamma\delta\ldots} T_{\alpha\beta\gamma\delta} T_{\alpha\epsilon\mu\nu} \ldots \tag{4}$$

becomes a product of tensors defined on the square lattice [Fig. 2(b)]. The tensor renormalization group (TRG) [8,10] is a real-space coarse-graining method, in which the precision of the tensor contraction is greatly enhanced by simultaneous renormalization of an "environment" block [10,11]. Infinite time-evolving block-decimation (iTEBD) [12] is a projection method, in which projecting the transfer matrix sufficiently many times on a random vector gives very accurately its largest eigenvalue. Both methods simulate the properties of an infinite system, the truncation being performed in the size D of the rank-4 tensor $T_{\alpha\beta\gamma\delta}$, which thus determines the precision. With an accurate partition function, we then obtain all other thermodynamic information.

One guiding principle for the antiferromagnetic Potts model in 2D concerns the existence of a critical q, $q_c(\mathcal{L})$, for each lattice geometry $\mathcal{L}$. At zero temperature, neighboring sites may not have the same "color" σ_i (Fig. 1), making the model equivalent to a vertex coloring problem. By exploiting the Dobrushin Uniqueness Theorem [13], Salas and Sokal proved [14] that the correlation function decays exponentially at all temperatures (including zero) for sufficiently large q, meaning a disordered ground state and no phase transition. For sufficiently small q, ordered ground states usually exist [7,15]. For $q = q_c(\mathcal{L})$, $T = 0$ is a critical point; this situation is common for many integer q values, including on the square [15], kagome [16] (both $q_c = 3$), and triangular ($q_c = 4$) lattices [17].

In terms of q_c, the diced lattice [Fig. 1(b)] is anomalous. Despite an average coordination number of 4, the model with $q = 3$ has a finite-temperature phase transition, hence $q_c > 3$. This transition is driven [7] by the entropy available from the irregular nature of the lattice, meaning that there are more sites of one type than of others. The low-temperature phase can be ordered on the A sublattice (for example, $\sigma_i = 0$) but not on B ($\sigma_i = 1$ or 2), creating a partially ordered state. We investigate the hypothesis that such behavior is generic for irregular lattices. We do this both by seeking an explicit new example of a finite-temperature transition, which leads us to consider the Union-Jack lattice, and by analyzing in detail the thermodynamic properties of irregular lattices.

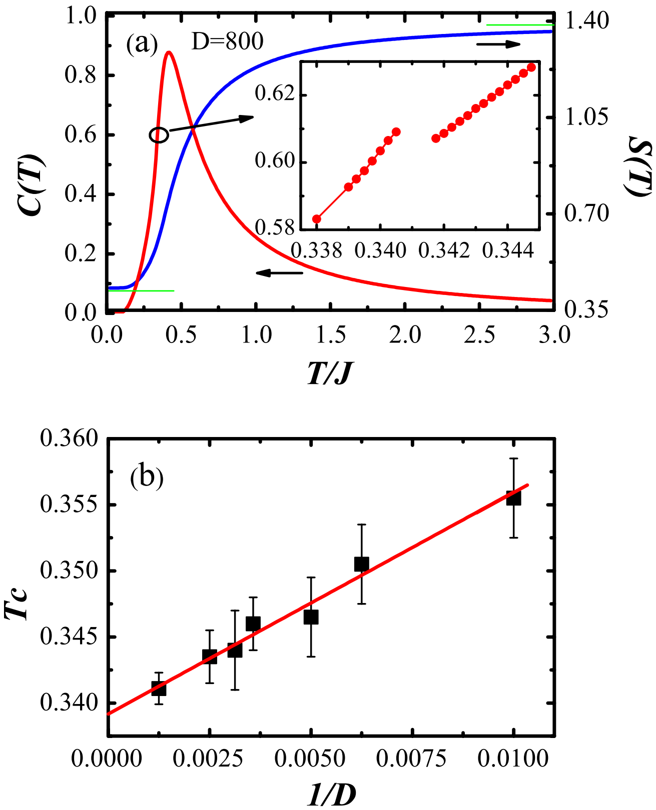

FIG. 3 (color online). (a) Entropy and specific heat for the $q = 4$ Potts model on the Union-Jack lattice, computed with $D = 800$. Thin, green lines denote the zero- and infinite-temperature limits of the entropy. Inset: specific-heat discontinuity near T_c. (b) Linear fit of T_c with $1/D$, which extrapolates to $T_c(\infty) = 0.339(1)$. The error bar denotes the upper and lower temperatures at the discontinuity.

We begin by considering the $q = 4$ Potts model on the Union-Jack lattice. This centered square lattice is tripartite [Fig. 1(a)]. While the $q = 2$ (Ising) model shows partial order and the $q = 3$ model is perfectly ordered, the $q = 4$ model may be expected from its average coordination ($z = 6$) to have zero-temperature order. To address the question of a phase transition occurring instead at finite temperature due the irregular nature of the lattice, we focus directly on the specific heat, shown in Fig. 3(a). The small but clear gap in the curve [inset, Fig. 3(a)] indicates a discontinuous second derivative of the free energy, and hence a second-order phase transition. We have performed detailed calculations to delineate the nature of the discontinuity over a range of D values, and exploit the linear scaling behavior of the matrix-product state with $1/D$ [18], shown in Fig. 3(b), to obtain the precise result $T_c = 0.339(1)$. Thus the $q = 4$ model on the Union-Jack lattice does indeed possess a finite-temperature phase transition, becoming only the second known Potts model in this category.

This transition was to our knowledge neither known beforehand nor even predicted. It underlines directly the importance of the irregular nature of a 2D lattice in promoting a finite zero-temperature entropy and partial order in the ground state. Our result is connected to several other models in statistical mechanics. First, some Potts models may be mapped to a height model, and when this mapping exists the system is critical or ordered at zero temperature [7,15]. As expected from our result, such a height map does exist for the $q = 4$ Union-Jack lattice [17]. Second, at zero temperature, the $q = 4$ Potts model on the Union-Jack lattice can be mapped directly to the 3-bond-coloring problem on its dual, the 4–8 lattice [17]. The total number of states on the 4–8 lattice is known [19], and hence the zero-temperature entropy of the Union-Jack lattice should be $S^{\rm UJ}(0) = 2\ln W_{4-8} = 0.430\,997$, with $W_{4-8} = 1.24\,048$. Our numerical result is 0.430 999 [Fig. 3(a)].

Third, the bond-coloring problem on the 4–8 lattice is further equivalent to a fully-packed loop (FPL) model (on the same lattice), obtained by considering all configurations of noncrossing closed loops. The FPL partition function is $Z = \sum_G n^{N_L}$, where n is a loop fugacity (weight), N_L is the number of loops, and G denotes all loop configurations. Like the FPL model on the square and honeycomb lattices, $n = 2$ for the 4–8 lattice, but unlike these cases the 4–8 lattice is not critical [20]. This is again consistent with our demonstration that long-range order is present at finite temperatures. Finally, the 3-bond-coloring model on the 4–8 lattice is also equivalent to a three-vertex coloring model on the square-kagome lattice [17], and thus the $q = 3$ Potts model on the square-kagome lattice is equivalent at zero temperature to the $q = 4$ Potts model on the Union-Jack lattice.

For a full understanding of the finite-temperature transition and the partially ordered ground state, we turn to the thermodynamic quantities extracted from the partition function. For a heuristic understanding of the partially ordered state, we begin with the entropy. The $q = 3$ Potts model on the diced lattice [Fig. 1(b)] is the prototypical model in this class for a ground state with partial order (Ref. [7] and references therein). As above, if the minority sites order, the majority sites would have two remaining degrees of freedom (d.o.f.s), giving an entropy per site $S_0^D(0) = 2\ln 2/3 = 0.462\,098$. The entropy we compute is shown in Fig. 4, and its low-temperature limit is $S^D(0) = 0.473\,839$. This minor deviation indicates that an ideal A-sublattice order is rather close to the true ground state, with only small contributions from states of imperfect A order. This partial order is destroyed at T_c by thermal fluctuations, and at high T, where all sites may explore all three d.o.f.s, the entropy approaches ln 3.

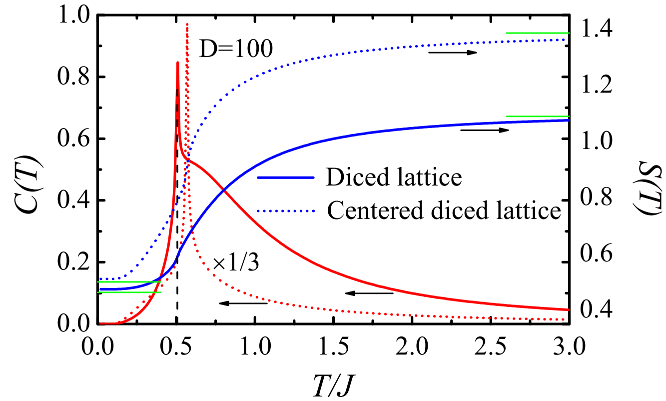

FIG. 4 (color online). Solid lines: entropy $S(T)$ and specific heat $C(T)$ for the $q = 3$ Potts model on the diced lattice, calculated with $D = 100$. The dotted line marks the result of Ref. [7]. Thin, green lines mark the low- and high-T entropy bounds. Dashed lines: results for the $q = 4$ Potts model on the centered diced lattice.

Analogous considerations for the Union-Jack lattice give again a maximum entropy if the high-coordination (minority) sites order. This order may involve sublattices A, B, or both A and B simultaneously. In the last case, if $\sigma_A = 0$ and $\sigma_B = 1$, the d.o.f. in $\sigma_C = 2, 3$ yields a total of $2^{N/2}$ states. If only A sites are ordered ($\sigma_A = 0$, σ_B, $\sigma_C = 1, 2, 3$), the B and C sublattices form a $q = 3$ Potts model on the decorated square lattice. Let the zero-temperature entropy of this model be $S^{\rm DSL}(0) = \ln\zeta$, then the number of states with partial order on A only is $\zeta^{3N/4}$, and these will dominate the total if $\zeta > 2^{2/3} = 1.587\,401$. We have calculated separately the value $S^{\rm DSL}(0) = 0.561\,070$, whence $\zeta = 1.752\,547$. Thus the ground state is indeed composed primarily of states with one ordered sublattice. The discrepancy between $3S^{\rm DSL}(0)/4 = 0.420\,802$ and our result [Fig. 3(a)], $S^{\rm UJ}(0) = 0.430\,999$, can be ascribed to states with neither A nor B order. The high-T entropy approaches ln 4.

We now return to the specific heat and to the phase transition. Results for the $q = 3$ model on the diced lattice are shown in Fig. 4. The transition point may be obtained with high precision and we find $T_c = 0.505(1)$, a value consistent with the alternative approach used in Ref. [7]. The peak feature is much more pronounced than in Fig. 3. This reflects the relative lack of competition between different types of partially ordered state in the diced lattice (A order only) as compared to the Union-Jack lattice (A or B order). We note that both transitions occur near the peak of the specific-heat curve at $T \sim J/2$, which is the characteristic energy scale of the system, and we suggest that this behavior is generic: a finite-temperature transition must occur at a value $T_c/J \sim O(1)$, and cannot occur arbitrarily close to $T = 0$.

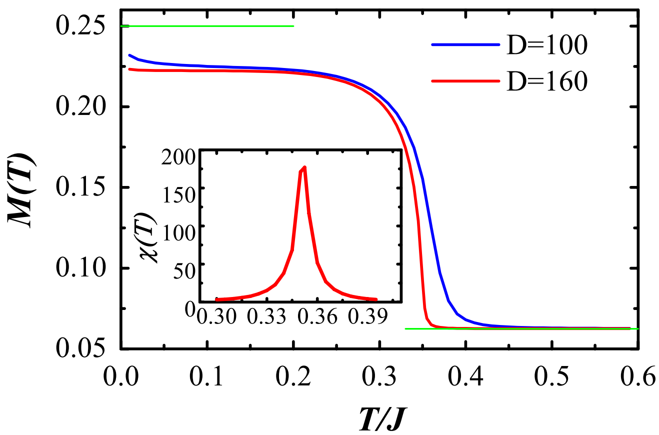

FIG. 5 (color online). Magnetization $M(T)$ of sublattice A for the $q = 4$ Potts model on the Union-Jack lattice, calculated for an applied field of 0.000 025. Thin green lines indicate the low- and high-T bounds. Inset: magnetic susceptibility $\chi(T)$.

The other thermodynamic quantities we illustrate here are the magnetization and susceptibility. By considering finite fields H in the Hamiltonian of Eq. (1), we deduce the spontaneous magnetization on sublattice A of the Union-Jack lattice [red circles in Fig. 1(a)], $M = \sum_{i\in A}\delta_{\sigma_{i=0}}/N$, from the expression

$$M = -\frac{\partial}{\partial H}\lim_{N\to\infty}\frac{1}{N}\ln Z, \qquad (5)$$

computed with a very small external field ($H = 0.000\,025$). The results (Fig. 5) show a clear step around T_c. The high-T limit of M for a completely disordered state is $M^{\rm UJ}(\infty) = \frac{1}{4}\times\frac{1}{4} = \frac{1}{16}$. The low-$T$ limit for a state of perfect A-sublattice order would be $M_0^{\rm UJ}(0) = \frac{1}{4}$, and in fact this value must be obtained for temperatures below the energy from the applied field. However, it is clear from our entropy calculation that the ground state is not one of perfect A order. We find that the magnetization exhibits a related zero-temperature deviation, tending towards the value $M^{\rm UJ}(0) = 0.2232$. This deviation is somewhat smaller for the diced lattice, where the ideal magnetization would be $1/3$ and our numerical result is 0.3192. Returning to the transition, our calculations show the same behavior as in Fig. 3(b), that T_c falls slowly with increasing D. The best qualitative indication of the transition is provided by the magnetic susceptibility, $\chi = \partial M/\partial H$, which has a robust peak (inset, Fig. 5). The critical exponents of these quantities may also be computed by the same techniques, but the highly numerically demanding task of obtaining adequate precision remains in progress.

When the discussion of 2D antiferromagnetic Potts models is framed in terms of $q_c(\mathcal{L})$, the diced lattice is the only known system with an average z of 4 but $q_c > 3$. The Union-Jack lattice is now revealed as the only system known with an average z of 6 but $q_c > 4$. In fact this is the largest value known for any planar lattice. Phase transitions in different Potts models belong in general to different universality classes. While the universality class for the $q = 4$ Potts model on the Union-Jack lattice remains under investigation, the partial order we find breaks both the 4-state (Potts) symmetry and the (Ising-like) sublattice symmetry between A and B.

We end this discussion with the logical extension of our analysis. The 11 regular lattices (all sites equivalent) obtained by tiling the plane with regular polygons are known as Archimedean. Among their dual lattices, three are regular and the other eight are irregular. This is the set of Laves lattices, which includes the diced and Union-Jack lattices. We propose that for each Laves lattice with an integral average coordination number, there exists a Potts model with integral q that would feature a zero-temperature transition on a regular lattice of the same coordination, but has a finite-temperature transition, to a state of partial order, on this irregular lattice. As an example we cite the $D(4, 6, 12)$ lattice, or centered diced lattice, shown in Fig. 1(c). This tripartite lattice has an average coordination $z = 6$. Indeed we find (Fig. 4) that a $q = 4$ Potts model on this lattice has a very robust finite-temperature phase transition to a state of predominantly A-sublattice order. Demonstrating the existence of the same physics on a third lattice in this class very strongly reinforces our proposal.

To conclude, we have demonstrated the existence of a previously unknown, finite-temperature phase transition in the $q = 4$ Potts model on the Union-Jack lattice. This establishes the essential property that the presence of inequivalent sites, leading to a nontrivial entropy, drives the finite-temperature transition and confers unusually high values on q_c. We find this type of transition on other irregular lattices in two dimensions. Our analysis underlines the utility of tensor-based numerical methods in investigating the physics of classical statistical mechanical models.

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[1] F. Y. Wu, Rev. Mod. Phys. **54**, 235 (1982).
[2] R. Shrock and S. H. Tsai, Phys. Rev. E **56**, 4111 (1997).
[3] L. Pauling, *The Nature of the Chemical Bond* (Cornell University Press, Ithaca, 1960).
[4] A. Lipowski and T. Horiguchi, J. Phys. A **28**, 3371 (1995).
[5] R. Igarashi and M. Ogata, arXiv:0907.3812 (unpublished)
[6] N. G. Parsonage and L. A. K. Staveley, *Disorder in Crystals* (Oxford University Press, New York, 1978).
[7] R. Kotecky, J. Salas, and A. D. Sokal, Phys. Rev. Lett. **101**, 030601 (2008).
[8] M. Levin and C. P. Nave, Phys. Rev. Lett. **99**, 120601 (2007).
[9] H. C. Jiang, Z. Y. Weng, and T. Xiang, Phys. Rev. Lett. **101**, 090603 (2008).

[10] Z. Y. Xie *et al.*, Phys. Rev. Lett. **103**, 160601 (2009).
[11] H. H. Zhao *et al.*, Phys. Rev. B **81**, 174411 (2010).
[12] G. Vidal, Phys. Rev. Lett. **98**, 070201 (2007); R. Orus and G. Vidal, Phys. Rev. B **78**, 155117 (2008).
[13] R. L. Dobrushin, Theory Probab. Appl. **13**, 197 (1968); R. L. Dobrushin, Theory Probab. Appl. **15**, 458 (1970).
[14] J. Salas and A. D. Sokal, J. Stat. Phys. **86**, 551 (1997).
[15] J. Salas and A. D. Sokal, J. Stat. Phys. **92**, 729 (1998).
[16] D. A. Huse and A. D. Rutenberg, Phys. Rev. B **45**, 7536 (1992).
[17] C. Moore and M. E. J. Newman, J. Stat. Phys. **99**, 629 (2000).
[18] L. Tagliacozzo, R. de Oliveira, S. Iblisdir, and J. I. Latorre, Phys. Rev. B **78**, 024410 (2008).
[19] J. O. Fjaerestad, J. Stat. Mech. (2010) P01004.
[20] J. L. Jacobsen, J. Phys. A **32**, 5445 (1999).