First- and Second-Order Phase Transitions in Potts Models: Renormalization-Group Solution

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A generalization of the Niemeijer–van Leeuwen renormalization-group transformation treating disordered cells of spins as vacancies is introduced and applied to the two-dimensional q-state Potts model. Finite-lattice approximations yield the changeover from continuous to first-order phase transitions predicted by Baxter but not observed in previous renormalization-group calculations. Exact results are conjectured for the tricritical exponents of dilute Potts models.

The two-dimensional q-state Potts model[1] has been the subject of considerable theoretical interest. It is known that the model is related to other systems of unusual interest such as the eight-vertex, Ashkin-Teller, and F models.[2,3] Using the latter equivalence, Baxter[2] showed that the phase transition of the Potts model is continuous for $q \leq q_c$ and first order for $q > q_c$ with $q_c = 4$. Numerous position-space renormalization-group (RG) methods have been applied to this problem and have failed to detect these first-order transitions.[4,5] This deficiency is intriguing because the same calculations give accurate critical exponents for $q \leq 4$.[4] Furthermore, first-order transitions have been successfully described by RG methods in other contexts.[6] The failure indicates either an inherent difficulty with the position-space methods or an incomplete realization of RG ideas by these calculations. In this Letter we demonstrate the latter to be the case by generalizing the Neimeijer–van Leeuwen (NvL) method[7] and applying it to the ferromagnetic q-state Potts model. The new, physically motivated feature of the RG transformation is that disordered configurations of the spins in a cell are assigned to a special cell state corresponding to a vacancy. This RG necessitates an extension of the Hamiltonian space to include lattice-gas terms. We obtain a critical value q_c such that transitions are continuous for $q \leq q_c$ and first order for $q > q_c$. For the simplest approximation $q_c \approx 4.7$. Figure 1 shows the topology of the resulting phase diagram. This topology supports a recent conjecture[3] concerning the critical exponents of the Potts model and enables us to extend it to tricritical exponents as well.

The two-dimensional q-state Potts model is defined by the Hamiltonian[1]

$$-\beta\mathcal{H} = J \sum_{\langle i,j \rangle} \delta_{s_i,s_j}, \tag{1}$$

where the summation is over all nearest-neighbor pairs on a lattice. Each spin variable s_i can assume q values. The transition temperatures of the Potts model, $J_c^{-1}(q)$, are known by duality relations for the square[1] and triangular lattices.[8] As noted above, Baxter[2] inferred for the square lattice that the phase transition is first order for $q > q_c$ and continuous for $q \leq q_c$, where $q_c = 4$. It

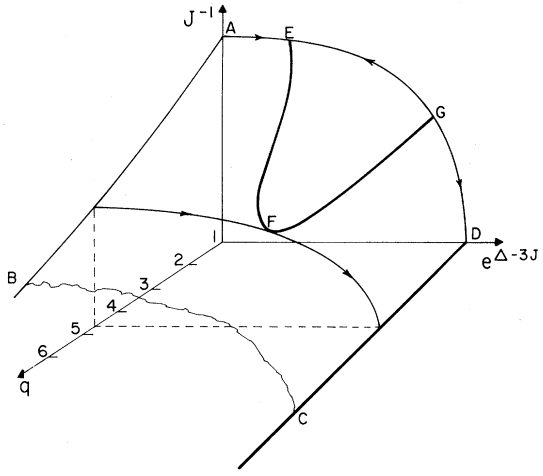

FIG. 1. Phase diagram of the Potts lattice gas in the space of temperature, J^{-1}, fugacity, $e^{\Delta-3J}$, and number of states, q.

is believed that q_c is lattice independent. Recently den Nijs[3] proposed an empirical relation that expresses the thermal Potts exponents for $q \leq 4$ in terms of those of Baxter's[9] eight-vertex model,

$$(y^{\mathrm{p}} - 3)(y^{8v} - 2) = 3, \tag{2}$$

where $y^{8v} = 2\mu/\pi$ with $\cos\mu = \frac{1}{2}\sqrt{q}$. The values for the exponents agree with the exact results for $q = 2$ and $q = 4$,[10] and they are consistent with the predictions from series-expansion and RG methods. Although the RG calculations yielded good exponents, they consistently failed to obtain the known first-order transitions and produced instead continuous transitions for all finite q.

In the position-space RG method a Potts Hamiltonian $\mathcal{H}\{s\}$ is mapped by means of a weight factor onto a renormalized Hamiltonian $\mathcal{H}'\{s'\}$ of fewer variables s'. Each such variable is associated with a cell of spins in the original lattice. In the usual approach[7,11] the variables s' are also taken to be Potts spins. This is a sensible choice if all or a majority of spins in a cell are in the same state. It is a questionable choice, however, when many or all of the spins in the cell are in different states. For example, in the latter case a common mapping assigns to the Potts-cell spin each of the different states represented in the cell with equal weight. This suggests that such a cell can interact ferromagnetically with its neighbors, which overestimates the tendency to order. On the contrary, we expect that a completely disordered cell has little aligning influence on neighboring cells. Viewed on the larger scale of the renormalized system it acts much like a vacant site. Therefore, we propose to generalize the weight factor so that disordered configurations are assigned (fully or with a fractional weight) to the empty state or vacancy. With this new prescription, a simple Potts model will be mapped under the RG transformation to a dilute Potts system or Potts lattice gas,[12,13] in which the variables s' consist of a lattice-gas variable $t_i = 0$ (vacant) or 1 (occupied) and, in the latter case, a Potts variable $s_i = 1, 2, \ldots, q$. Thus the RG transformation acts in the parameter space characterized by the nearest-neighbor Hamiltonian

$$-\beta\mathcal{H} = \sum_{\langle i,j \rangle} t_i t_j (K + J\delta_{s_i,s_j}) - \Delta \sum_i t_i. \tag{3}$$

The couplings K and J denote lattice-gas and Potts interaction parameters, respectively, and the chemical potential Δ governs the concentration of vacancies. The pure Potts model corresponds to chemical potential $\Delta = -\infty$ or, equivalently, $K = \infty$. In terms of the variables s_i the Hamiltonian (3) has the symmetry of the q-state Potts model.

We applied these ideas to the q-state Potts model on a triangular lattice for continuous values of q. A two-cell approximation with three spins per cell was employed. In order to guarantee the correct ground-state energies necessary to describe the first-order transition[6] each cell was surrounded by six replicas of the other. *Ab initio* there was little guidance as to the weight factor which determines the relation between cell and site spins. We chose a generalized majority rule: If all spins in a cell are in the same Potts state or if two spins are in the same state and the third is vacant, the cell spin is in that Potts state. All other configurations are assigned to the vacant-cell state. Note that this permits the generation of vacancies even for the Ising model. The calculation yielded continuous transitions for the q-state Potts model for $q \leq q_c$ and first-order transitions for $q > q_c$ with $q_c = 4.73$. The results are discussed in detail below. Variations of the weight factor resulted in larger q_c and poorer values for the exponents. Preliminary investigations of a three-cell approximation yielded similar results.

The following picture emerges from these calculations. Figure 1 shows schematically the topology of the RG flow diagram in the space of temperature, J^{-1}, fugacity, $e^{\Delta - 3J}$, and number of states q. The surface $ABCD$ separates the ferromagnetic and disordered phases. Within this surface there are lines of critical fixed points, EF, and tricritical fixed points, GF, which meet at F for $q = q_c$. CD is a line of discontinuity fixed points.[6] The intersection AB of the surface with the plane $e^{\Delta - 3J} = 0$ corresponding to the pure Potts problem defines the critical temperature $J_c^{-1}(q)$ of the Potts model. The RG trajectories lie in planes of constant q. Thus, flows that begin at the transition temperature of the (pure) q-state Potts model are attracted by the critical fixed line for $q \leq q_c$ and by the first-order fixed line for $q > q_c$. We note that the fixed line EFG is analogous to the fixed line in the Kosterlitz-Thouless description of the XY model.[14] The quantity q_c plays a role analogous to the Kosterlitz-Thouless temperature. In our approximation $q_c = 4.73$ compared to Baxter's exact result $q_c = 4$.[2] Note that the effects of increasing q and of increasing dilution are similar, for both drive the transition first order.

The tricritical fixed points for integer q are of

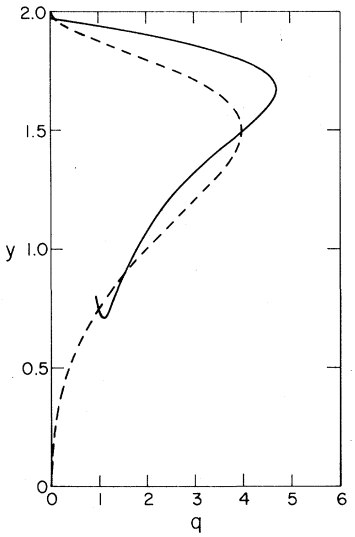

FIG. 2. Critical and tricritical exponents (lower and upper branch, respectively) from the two-cell approximation (solid curve) and the extended conjecture of den Nijs.

physical interest for $q=2$ (Blume-Emery-Griffiths model[12]) and for $q=3$.[13] At these points $q+1$ phases are simultaneously critical, of which q are identical and one is singled out. In general the symmetry is not that of the $(q+1)$-state Potts model. Only for the special value $q=1$ is the tricritical fixed point identical to the $q+1$ (Ising) ferromagnetic critical point. Our results indicate an interesting relation between the exponents of the tricritical points and those of the critical points of the Potts model. In Fig. 2 we show the values of the most relevant exponent, $y=\nu^{-1}$, of the critical and tricritical fixed points as obtained by our two-cell approximation. The lower branch of the dashed line shows the conjecture of den Nijs, Eq. (2), for the critical exponents.[3] According to the topology of our RG, the tricritical exponents should be an analytic continuation thereof and this is shown as the upper branch of the dashed curve. It is noteworthy that we can extend den Nijs's conjecture to the tricritical exponents for the Blume-Emery-Griffiths model ($y=\frac{9}{5}$) and the three-state Potts lattice gas ($y=\frac{12}{7}$). This extended conjecture is supported by the fact that it reproduces the correct Ising exponent for $q=1$, which is $y=\frac{15}{8}$. Table I summarizes the numerical results for the exponents and gives in parentheses the values from the extended den Nijs conjecture. At $q=1$ the approximation fails to map any point of the pure axis towards the critical fixed point. Finally we mention that the behavior of the latent heat exhibits, in the vicinity of q_c, the same essential singularity in q as Baxter's exact result.[2]

TABLE I. Critical temperature J_c^{-1} and exponent $y=\nu^{-1}$ for the pure Potts model and tricritical exponent $y_t=\nu_t^{-1}$ for the dilute Potts model. Exact or conjectured results are shown in parentheses.

q	J_c^{-1}	y	y_t
1		0.74 (0.75)	1.94 (1.875)
2	1.89 (1.82)	1.08 (1)	1.90 (1.8)
3	1.41 (1.59)	1.32 (1.2)	1.86 (1.714)
4	1.22 (1.44)	1.49 (1.5)	1.80 (1.5)
5	1.12 (1.34)	2 (2)	
6	1.05 (1.27)	2 (2)	

In summary, we have generalized on physical grounds the usual RG transformations so that disordered sets of variables are mapped to vacancies. We have applied this idea to the two-dimensional Potts model in a simple approximation and obtained the changeover from continuous to first-order transitions. In addition a strong indication of a relation between critical and tricritical exponents emerged. The basic idea is easily incorporated into common approximation methods and we expect that it can be applied advantageously to a wide variety of problems.

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[1]R. B. Potts, Proc. Cambridge Philos. Soc. 48, 106 (1952).

[2]R. J. Baxter, J. Phys. C 6, L445 (1973).

[3]M. P. M. den Nijs, to be published.

[4]C. Dasgupta, Phys. Rev. B 15, 3460 (1977); M. P. M. den Nijs and H. J. F. Knops, Physica (Utrecht) 93A, 441 (1978); M. P. M. den Nijs, Physica (Utrecht) 95A, 449 (1979).

[5]A. Aharony, J. Phys. A 10, 389 (1977); E. Domany and E. K. Riedel, Phys. Rev. B 19, 5817 (1979); A. N.

Berker and S. Ostlund, to be published; S. J. Shenker, L. P. Kadanoff, and A. M. M. Pruisken, to be published.
[6]B. Nienhuis and M. Nauenberg, Phys. Rev. B 11, 4152 (1975), and Phys. Rev. Lett. 35, 477 (1975).
[7]Th. Niemeijer and J. M. J. van Leeuwen, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, London, 1976), Vol. 6, p. 425.
[8]D. Kim and R. I. Joseph, J. Phys. C 7, L167 (1974); L. Mittag and M. J. Stephen, J. Phys. A 7, L109 (1974).
[9]R. J. Baxter, Ann. Phys. (N.Y.) 70, 193 (1972).
[10]Symmetry arguments indicate that the four-state Potts model is in the same universality class as the Baxter-Wu model [R. J. Baxter and F. Y. Wu, Phys. Rev. Lett. 31, 1294 (1973)], for which $y = 1.5$. See also I. G. Enting, J. Phys. A 8, L35 (1975).
[11]L. P. Kadanoff, A. Houghton, and M. C. Yalabik, J. Stat. Phys. 14, 171 (1976); L. P. Kadanoff, Ann. Phys. (N.Y.) 100, 359 (1976).
[12]M. Blume, V. J. Emery, and R. B. Griffiths, Phys. Rev. A 4, 1071 (1971).
[13]A. N. Berker, S. Ostlund, and F. A. Putnam, Phys. Rev. B 17, 3650 (1978).
[14]J. M. Kosterlitz, J. Phys. C 7, 1046 (1974).

Numerical Estimates of the Hausdorff Dimension of the Largest Cluster and Its Backbone in the Percolation Problem in Two Dimensions

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We present numerical estimates of the Hausdorff dimension D of the largest cluster and its "backbone" in the percolation problem on a square lattice as a function of the concentration p. We fine that D is an approximately linear function of p in the region near $p = p_c$ ($\simeq 0.59$) with a dimension about equal to that of a self-avoiding walk when $p = 0.455$. The dimension of the backbone, or biconnected part, of the largest cluster equals that of the self-avoiding walk when $p \simeq p_c$. At $p = p_c$ the dimension of the largest cluster equals the anomalous dimension introduced by Stanley *et al*.

In analysis of experiments on magnetic systems Birgeneau *et al*.[1] and Stanley *et al*.[2] recently suggested a self-avoiding random walk (SAW) as a model for the largest cluster in a percolating net. Qualitative arguments were presented suggesting that the geometrical properties of the clusters were similar to those of the SAW. Here we study this interesting suggestion by estimating the dimension of each of the two structures numerically.

The dimension which we estimate is the Hausdorff-Besicovitch[3] dimension D_H which is defined so that a particular structure is covered by a minimum of $N(\eta)$ disks of radius η and $\lim_{\eta \to 0} N(\eta)\eta^{D_H}$ is finite. We have checked that direct application of this definition to numerically estimate D_H for a self-avoiding walk (SAW) in two dimensions gave results consistent with the value[4] $D_{SAW} = 1.33$ obtained by finding the mean end-to-end distance $\langle r^2 \rangle$ as a function of the number of steps n. (Writing $\langle r^2 \rangle = n^{2\nu_s}$ it is easy to show that $D_{SAW} = 1/\nu_s$.) We have also checked the value $D_{SAW} = 1.33$ by application of the second method.

In the percolation system we estimate D_H from the relation of the average size n_c of the largest cluster to the total size n^2 of the percolating net. We find empirically that n_c varies with n as $n_c = Kn^{2y}$ where K and y are constants (see Fig. 1). (This relation is expected when na is less than the coherence length ξ.) We note that n_c can also be regarded as an upper bound on the number of disks of size $\eta = a$ required to cover the largest cluster in a net of size n^2. For fixed a and for each n we introduce a change of length scale $x' = x/na$. In terms of this length scale the covering of the largest cluster in the net of size n^2 is by disks of radius $\eta' = \eta/na = 1/n$. Thus each value of n corresponds to a different covering. Using $n_c = Kn^{2y}$ we have $N(\eta') = n_c = Kn^{2y} = K(\eta')^{-2y}$ or $D = 2y$. By the argument just given, these D's are an upper bound on the Hausdorff dimension. We do not have a quantitative estimate of the error involved in treating D as an estimate for D_H. We have two indications that the error in using D as