Long-range order for antiferromagnetic Potts models

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Long-range order for the three-state antiferromagnetic Potts model may appear at zero temperature as an instability with respect to boundary conditions. It is studied using an approximate correspondence, reminiscent of duality, which links this model with the ferromagnetic Ising model at a particular temperature. The basic idea is to represent entropy constraints in the former in terms of energy increase in the latter. The correspondence can be made exact by modifying the Ising model. The (non)existence of long-range order is then linked to the location of the critical temperature of the modified Ising model with respect to the particular value given by the correspondence.

I. INTRODUCTION

The existence of the different phases occurring in a classical lattice system may be understood as an instability in the equilibrium state under a change of boundary conditions (BC) in large finite volumes, with the instability persisting even in the thermodynamic limit of infinite volume. Often much can be deduced from the behavior of a system at zero temperature. Thus, e.g., in the case of the Ising model, fixing all spins on the boundary of a volume to point up (down) leads unambiguously to a ground state with all spins in the bulk aligned in the same direction. These BC yield at low temperatures (and for a two- or higher- dimensional model) two different phases characterized as a sea of aligned spins with only small islands of the opposite ones. This follows by the Peierls argument from the fact that to introduce an island of opposite spins one must pay with an energy proportional to the boundary of the island.[1]

The situation is much less clear for systems with nonvanishing residual entropy. Even a description of different phases at $T=0$ is a nontrivial problem in this case. As a typical example consider the recently much discussed, three-state antiferromagnetic (AF) Potts model on a square lattice. This is a model with spins σ_i, attached to lattice sites i, taking on $q=3$ values $\sigma_i=1,2,3$, and with the Hamiltonian

$$H=J\sum_{\langle i,j\rangle}\delta_{\sigma_i,\sigma_j},\quad J>0 \qquad (1)$$

that favors nonaligned spins on neighboring sites. $\delta_{\sigma_i,\sigma_j}$ is the Kronecker symbol and the sum is over pairs of nearest neighbors (NN).[2] It has been suggested[3] that at low temperatures there are six different phases called broken-sublattice-symmetry (BSS) states. Divide the square lattice into two sublattices (referring to a chessboard we shall call them the black and the white sublattice). A BSS state is, e.g., that with typical configurations differing only slightly from the ground state with the spin "1" on the black sublattice and a random distribution of the spins "2" and "3" over the white sublattice. Actually, more recent phenomenological[4] and Monte Carlo[5] renormalization-group calculations have indicated that on a square lattice there is only one phase (no BSS), though the situation remains rather unclear for cubic[6,7] or higher-dimensional lattices. It is known that $T=0$ is a critical value for the AF Potts model on a square lattice.[8] This follows from its equivalence with a critical ice model. However, the criticality in principle does not say anything about the (non)existence of BSS states.

The analysis presented in this paper may be applied also to some higher-dimensional models, but for simplicity we shall use as an illustrative example the AF Potts model on a square lattice (our result in this particular case will agree with the conclusion that there is only one phase).

II. CORRESPONDENCE TO THE ISING FERROMAGNET

For models with residual entropy, similarly as for the Ising model, the behavior at $T=0$ should be decisive for existence of order at low temperatures. We shall comment on this statement later, but first we discuss order for the AF Potts model at $T=0$. To analyze whether the BSS states exist we impose the BC shown in Fig. 1 and try to evaluate a relevant order parameter—e.g., the probability $P(\sigma_0=1)$ that the spin on the black site in the center is also "1". All possible configurations at $T=0$ are ground configurations[9] and appear with equal probability. Contrary to the Ising model, where the BC determine the ground configuration in the bulk uniquely, here we have many ground configurations consistent with the BC. $P(\sigma_0=1)$ is just the number of ground configurations consistent with the BC and such that $\sigma_0=1$, divided by

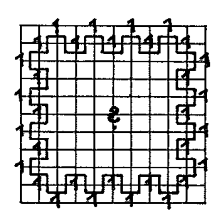

FIG. 1. Volume Λ with a "dented" boundary and the BC on black sublattice sites that enforces the spin 1 on the black sublattice and should lead to a BSS state.

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the number of all ground configurations consistent with the BC. When "gluing" together a central region with, for example, 2 on the black sublattice, with a boundary region where there is 1 on the black sublattice, one pays with a certain "stiffness" in the intermediate region. To compute $P(\sigma_0=1)$ means a rather subtle evaluation of a loss of entropy caused by this stiffness.

This situation reminds one of the Ising model at a finite temperature, in which changing from spin up along the BC to spin down in a central region forces one to pay with energy along a contour (a wall) bordering an island of spin down. We propose to make this analogy a tool for evaluation of $P(\sigma_0=1)$. Consider thus the black sublattice viewed as a new lattice with a NN of distance $\sqrt{2}$ (it is again a square lattice, though turned by $\pi/2$ and scaled by $\sqrt{2}$). If $\{\sigma_i\}$ is a ground configuration in the volume Λ, consistent with the BC in Fig. 1, consider its restriction to the black sublattice Λ_b in Λ and draw an edge (connecting two sites of the white sublattice Λ_w) separating the NN of Λ_b whenever the spins attached to them differ [see Fig. 2(a)]. We shall call the set of these edges the *boundary* and its connected components the *contours* of a configuration $\{\sigma_i\}$. Whenever ∂ is a boundary, we denote $|\partial|$ the number of its contours, and $||\partial||_v$ the number of the white sublattice sites through which ∂ passes. Denoting also $|\Lambda_w|$ the number of sites in Λ_w, we get for the number of ground configurations consistent with the BC.

$$Z_{\text{AF Potts}}(\beta=\infty)=\sum_{\partial} 2^{|\partial|}2^{|\Lambda_w|-||\partial||_v} . \tag{2}$$

Indeed, with a given ∂, one may choose the configuration on Λ_b in $2^{|\partial|}$ different ways, and then the spin on a white site is fixed whenever ∂ passes through it, while it can take on two values if the site does not lie on ∂. As explained in the caption of Fig. 2, we used an obvious restriction on configurations on Λ_b:

(i) There can be no white lattice site such that we find all three values 1, 2, and 3 on its black nearest neighbors.

The restriction also implies that each white lattice site is an end point of an even number (0, 2, or 4) of edges. It means, however, that the boundaries are exactly the same geometrical objects as boundaries for the Ising model on the black sublattice [see Fig. 2(b)]. The partition function of this ferromagnetic (F) Ising model at an inverse temperature β is[10]

$$Z_{\text{F Ising}}(\beta)=\sum_{\partial} e^{\beta E_b-2\beta||\partial||_e} , \tag{3}$$

where E_b is the number of pairs of NN in Λ_b and $||\partial||_e$ is the number of edges in ∂. Denoting $|\partial|_c=||\partial||_e-||\partial||_v+|\partial|$ (the cyclomatic number of ∂ if viewed as a graph), we get from (2)

$$Z_{\text{AF Potts}}(\beta=\infty)=2^{|\Lambda_w|}\sum_{\partial} 2^{|\partial|_c-||\partial||_e} . \tag{4}$$

On the other side, taking a particular temperature $\bar{\beta}=\frac{1}{2}\ln 2$ in (3), we have

$$Z_{\text{F Ising}}(\bar{\beta})=2^{E_b/2}\sum_{\partial} 2^{-||\partial||_e} . \tag{5}$$

The striking similarity of (4) and (5) (taking into account the fact that both partition functions are expressed in terms of the same objects ∂ with a direct geometrical meaning) allows us to compare not only the corresponding partition functions but also the probabilities of particular geometric situations in both ensembles. Since for the Ising model

$$\exp(2\beta_c)=1+\sqrt{2}>2=\exp(2\bar{\beta}) ,$$

we have $\bar{\beta}<\beta_c$ the critical (inverse) temperature. The spontaneous magnetization thus vanishes at $\bar{\beta}$ and from two possible complementary situations shown in Fig. 3, that in Fig. 3(a) takes place. Namely, in a typical configuration any site in a central region is, for Λ large enough encircled by a great number of contours. We shall now conjecture that the same is true also for the AF Potts ensemble (4). This would, however, mean that the middle site has "no way of learning" about the BC, and the $P(\sigma_0=1)$ would approach $\frac{1}{3}$ with $\Lambda\to\infty$, implying that there is no BSS state for the AF Potts model on a square lattice at $T=0$.

The above conjecture is actually the only nonrigorous part of our argument. Unfortunately contour models [such as, e.g., (3)] are well controlled only when the weight of long contours decreases quickly (β large), when the alternative in Fig. 3(b) takes place.[1] Here we have just

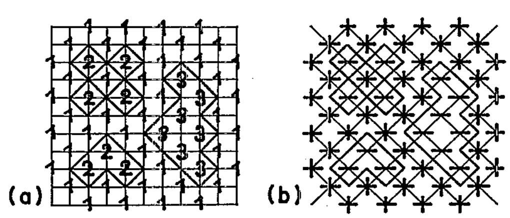

FIG. 2. Contours for (a) the AF Potts model on Λ, (b) the F Ising model on Λ_b (+, − denotes spin up, down, respectively). For the boundary ∂ drawn, it is $|\partial|=3$, $||\partial||_v=34$, $||\partial||_e=38$, $|\partial|_c=7$, and $||\partial||_{v(4)}=4$. Note that for the contour shown in the left upper corner, the restriction (i) implies that the spin 1 in its center is compulsory and that the only different configuration on the black sublattice consistent with it is that with 2 changed to 3 on all four sites.

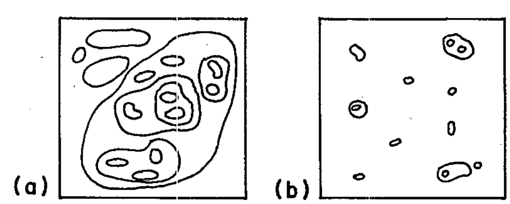

FIG. 3. Large scale view with the lattice suppressed of a typical boundary ∂ for a contour ensemble in alternative situations: (a) Disorder—A site in the center is encircled by many contours and "forgets" the BC; (b) Order—There are only short contours and a large part of the volume is in the state forced by the BC.

the opposite situation. In support of the conjecture, note that

$$\frac{||\partial||_e}{2} \le ||\partial||_v - |\partial| = ||\partial||_e - |\partial|_c \le ||\partial||_e . \qquad (6)$$

The upper bound means that the weight of long boundaries ∂ in (4) is even larger than in (5). However, one could argue that the ensemble (4) favors within the boundaries of a given length those consisting of many different (and, in principle, short) contours. We believe that the lower bound in (6) suggests that in spite of it, long contours occur with a non-negligible probability and the alternative in Fig. 3(a) takes place. To prove it would mean proving certain "correlation inequalities" for "contour models." This problem certainly deserves further study.

III. EXACT CORRESPONDENCES TO MODIFIED ISING AND POTTS FERROMAGNETS

One may proceed even without the above conjecture. Namely, starting from (4) we shall introduce modified Ising and Potts models that give at a particular nonvanishing temperature exactly the same probability of particular geometric situations as expressed in terms of ∂.

A. Ising model with degenerated spins

Consider the following modification of the Ising model on the black sublattice.[11] The spin at each lattice site i can take on four values $\sigma_i \in \{+1_1, +1_2, -1_1, -1_2\}$, the Hamiltonian is that of the Ising ferromagnet[10]

$$H = -\sum_{\langle i,j \rangle} \sigma_i \sigma_j . \qquad (7)$$

The multiplication $\sigma_i\sigma_j$ in the above formula is to be interpreted in the following way:

$$(+1_a)(+1_a)=(-1_a)(-1_a)=1,$$
$$(+1_a)(-1_b)=(-1_a)(+1_b)=-1 , \qquad a,b=1,2$$

and (8)

$$(+1_a)(+1_b)=(-1_a)(-1_b)=-\infty, \quad a\neq b, \quad a,b=1,2 .$$

The latter multiplication rule is actually a hard-core condition forcing the two nearest-neighbor spins not to take on values of the same sign but with different subscripts. The contours of a configuration are constructed in the same way as for the usual Ising model by simply ignoring the subscripts.

The partition function of this model is

$$Z_{\text{MF Ising}}(\beta)=\sum_{\partial} e^{\beta E_b - 2\beta||\partial||_e} 2^{|\partial|_c} , \qquad (9)$$

the factor $2^{|\partial|_c}$ giving the number of possible choices of subscripts to an Ising-model configuration in accordance with the hard-core condition. Thus, considering the model at the temperature $\bar{\beta}=\frac{1}{2}\ln 2$, we get *exactly the same* probability distribution of contours as for the AF Potts model. Hence the (non)existence of BSS states is equivalent to (non)existence of a spontaneous magnetization in our model and thus depends on the fact of whether its critical inverse temperature is below (above) $\bar{\beta}$. Although $\beta_c > \bar{\beta}$ for the usual Ising model, our modification may effectively lower the critical temperature below $\bar{\beta}$. While we do not know if this is the case, it is a question that could be answered, e.g., by probing the model by a Monte Carlo experiment. The advantage is that the AF Potts model at $T=0$ (i.e., the temperature on the boundary of the region $\beta \le \infty$) is mapped to a model included *inside* a one-parameter family (9).

Note that our model is also equivalent to the Ashkin-Teller model in a limit of infinite couplings. Indeed, identify first the degenerated spin σ_i with a pair of spins (s_i, S_i) in the following way:

$$+1_1 \to (s_i=+1, S_i=+1), \quad +1_2 \to (s_i=+1, S_i=-1) ,$$
$$-1_1 \to (s_i=-1, S_i=+1), \quad -1_2 \to (s_i=-1, S_i=-1) .$$

Then one reproduces (7) by

$$H=\tfrac{1}{4}(\alpha+1)\sum_{\langle i,j\rangle}\left\{-s_is_jS_iS_j - S_iS_j + \left[1-\frac{4}{\alpha+1}\right]s_is_j + 1\right\} \qquad (10)$$

in the limit $\alpha\to\infty$. One may close the logical circle by observing that the model described by Eq. (10) at the temperature $\bar{\beta}$ is equivalent to the ice model and hence to the AF Potts model at $T=0$. To see it we first note that considering equivalently s_iS_i and S_i as independent spins we have in the limit $\alpha\to\infty$ an isotropic Ashkin-Teller model with the edge weights[12]

$$\omega_0=e^{\beta}, \quad \omega_1=e^{-\beta}, \quad \omega_2=e^{-\beta}, \quad \omega_3=0 . \qquad (11)$$

This model is equivalent to an alternating eight-vertex model[13] which is critical whenever

$$\omega_0=\omega_1+\omega_2+\omega_3 . \qquad (12)$$

In view of (11) the critically condition $e^{\beta}=2e^{-\beta}$ yields just $\beta=\frac{1}{2}\ln 2$. Taking into account the symmetry of the model with respect to permutations of (11) we get for the parameters of the alternating eight-vertex model corresponding to the temperature $\bar{\beta}$

$$a=\frac{1}{\sqrt{2}}e^{\bar{\beta}}=1, \quad b=\frac{1}{\sqrt{2}}(e^{-\bar{\beta}}-e^{-\bar{\beta}})=0 ,$$
$$c=\frac{1}{\sqrt{2}}(e^{-\bar{\beta}}+e^{-\bar{\beta}})=1, \quad d=\frac{1}{\sqrt{2}}e^{\bar{\beta}}=1 , \qquad (13)$$

obtaining thus just the ice model.

B. Potts model with a triangular hard core

Another possibility is to modify the F Potts model on Λ_b. Namely, consider the usual Hamiltonian (1) with $J<0$ by adding three-site and four-site interaction terms.

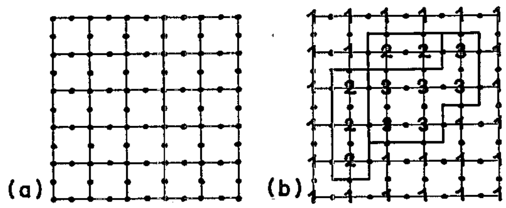

FIG. 4. (a) Decorated square lattice and (b) ground configuration of the AF Potts model restricted to the black sublattice with its boundary ∂; $||\partial||=21$, $N(\partial)=2$.

For the three-site interaction we take a "hard core" which will exclude configurations not complying with the restriction (i) (yielding thus the same set of boundaries ∂). Moreover, for each quadruple of black NN of a white site we add the term J to the Hamiltonian if there are four edges of ∂ ending in that white site (and 0 otherwise). Denoting $||\partial||_{v(4)}$ the number of "four-edges" vertices in ∂ we have for the modified (M) F Potts model

$$Z_{\text{MF Potts}}(\beta)=\sum_{\partial} 2^{|\partial|} e^{\beta E_b-\beta||\partial||_e+\beta||\partial||_{v(4)}} . \tag{14}$$

Observing that $||\partial||_e-||\partial||_{v(4)}=||\partial||_v$ we obtain for $\tilde{\beta}=\ln 2$ (up to a constant factor) *exactly* the sum (2). $P(\sigma_0=1)$ thus exactly equals a similar probability for the MF Potts model on Λ_b. The only problem then again is that our modification could effectively force β_c to be less than $\tilde{\beta}$ in spite of the relation $e^{\beta_c}=1+\sqrt{3}>e^{\tilde{\beta}}=2$ valid for the usual F Potts model.

IV. HIGHER-DIMENSIONAL LATTICES

AF Potts models on other lattices, including higher-dimensional ones, may be treated in a similar way. Concerning, e.g., a simple cubic lattice we would get an almost equivalent F Ising or modified F Potts model on a face-centered cubic lattice (built up from the black sublattice). A future publication will be devoted to an analysis of this case.

There is a lattice for which our correspondence is exact in all dimensions d and may be actually used to establish both disorder for $d=2$ and order for $d\geq 3$. Namely, consider the AF Potts model on a decorated hypercubic (DHC) lattice[14–16] [shown in Fig. 4(a) for the case $d=2$]. Taking the original (HC) lattice for the black sublattice and the set of decoration sites for the white one, we get the same set of boundaries for both, the AF Potts model on a DHC lattice [see Fig. 4(b)] and the F Potts model on a (HC) lattice. Denoting $||\partial||$ the number of $(d-1)$-dimensional elementary faces (each through one white lattice site) from ∂ and $N(\partial)$ the number of configurations (on the black sublattice) consistent with ∂, we obtain for $\tilde{\beta}=\ln 2$

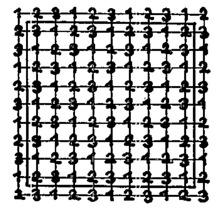

FIG. 5. Rigid ground state.

$$2^{-|\Lambda_w|}Z_{\text{AF}}^{\text{DHC}}(\infty)=2^{-E_b}Z_F^{\text{HC}}(\tilde{\beta}) =\sum_{\partial} N(\partial)2^{-||\partial||} .$$

The $P(\sigma_0=1)$ is thus identical for both systems, since the same geometrical situations contributing to it have the same weight. As already mentioned, $\beta_c>\tilde{\beta}$ for $d=2$. On the other side, numerical estimates indicate that $\beta_c<\tilde{\beta}$ for $d\geq 3$ [$e^{\beta_c}\approx 1.74$ ($d=3$), ≈ 1.47 ($d=4$)—see, e.g., the review of Wu[16]]. Thus for $d=2$ the order parameter vanishes, while for $d\geq 3$ it does not vanish and there exist three different BSS states.

V. CONCLUSION

The preceding analysis was concerned with zero temperature. It should be relevant also for small $T>0$,[17] since a typical configuration should differ only slightly from a ground configuration because one pays for any deviation from it with an energy proportional to the extent of the deviation. Nevertheless, one should be aware that only the states with the highest entropy, existing at $T=0$, will survive to $T>0$.[18] As an example consider the BC shown in Fig. 5, which determines uniquely a ground configuration (we call it a rigid ground state) in the considered volume Λ. At any $T\neq 0$ the system in Λ under this BC will favor a change within a strip around the boundary of Λ to, for example, a BSS state. The energy paid for this change will be outweighed by the gain of an entropy in the bulk.

In conclusion we note that, since our correspondence uses certain contours to relate AF Potts model to F Ising or Potts model, it reminds one of duality. A novel feature is not only the fact that the zero temperature of the former is linked with a nonzero temperature of the latter, but also the possibility of comparing directly typical configurations of both models. This should be useful whenever the correspondence is not exact. Note also that in constructing our contours from a configuration on the black sublattice, we made in some sense a rescaling transformation which according to Berker and Kadanoff[19] renormalizes the system away from $T=0$.

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