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Propagation of Order in the Dilute Antiferromagnetic Three-State Potts Model

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A recent analysis of the propagation of order in a dilute 3-state Potts antiferromagnetic model on a triangular lattice at zero temperature by Adler *et al.* has shown the importance of nonlocality in the propagation of order. We study a linearized continuous version of this model, which can be mapped onto three independent percolation problems. We discuss the respective roles of nonlocality and nonlinearity, in particular in connection with central-force percolation.

KEY WORDS: Potts model; percolation; central-force percolation.

Much work in statistical mechanics has been concerned with the critical behavior of percolation[1] and other geometrical phase transitions. Two essential properties have been extensively used in these studies, both theoretically and from a computational point of view: *linearity* and *locality*. More recently, the need to consider more complex situations resulted in the study of nonlocal and/or nonlinear problems, such as bootstrap percolation, central-force percolation, damage propagation in cellular automata,[2] etc.

One simple example of this is the propagation of order in the dilute 3-state Potts antiferromagnetic model on a triangular lattice at zero temperature (3-PAFT).[3,4] We introduce here a continuous version of the 3-PAFT and then linearize it. It turns out that the linear model is exactly reducible to three decoupled percolation problems which can be visualized

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in a very simple fashion. Following a suggestion of Adler *et al.*,[4] we consider the relation of this model with the central-force percolation (CFP) problem,[5–7] always treated in its linear approximation. We show that these models differ, although they share many common properties.

Let us consider a triangular lattice where a proportion p of sites chosen at random are occupied and $1-p$ are empty. On each occupied site i, we have a spin σ_i, which can take three values (say A, B, and C). We now introduce a Hamiltonian H defined as

$$H = J \sum \varepsilon_i \varepsilon_j \delta(\sigma_i, \sigma_j) \tag{1}$$

where the sum runs over all pairs of neighboring sites i, j. The value of ε_i is 1 if the site i is occupied and 0 if not; J is a positive constant; and δ is the usual Krönecker symbol [i.e., $\delta(x, y) = 1$ if $x = y$, and 0 if not]. For the complete ($p = 1$) triangular lattice, there exist three ordered ground states with zero energy. The system is not frustrated. Once two adjacent sites are given two different states, a single ground state is selected, and therefore order propagates through the system.

There exists a threshold value of the parameter $p = p^*$ below which order does not propagate.[4] The order parameter of the system is the concentration of sites whose spin state is completely determined in all ground states. This problem has been described at length by Adler *et al.*[4] The determination of p^* is a complex problem due to the fact that only a partial information is transmitted through a single bond: If, for instance, σ_i is in state A, a neighboring occupied site j will have two possible states of zero energy: namely B or C. A spin will be in a completely determined state if at least two independent and compatible pieces of information reach the site (see Fig. 1).

We can now formulate a continuous version of this problem, which is a Heisenberg model. Let us attribute to all sites a unit vector $\mathbf{s}_i$ in a three-dimensional space and introduce the Hamiltonian H_c:

$$H_c = J \sum \varepsilon_i \varepsilon_j (\mathbf{s}_i \cdot \mathbf{s}_j)^2 \tag{2}$$

with the same convention as in the previous Hamiltonian [Eq. (1)]. A single bond between two occupied sites i and j will have a zero energy if the two vectors $\mathbf{s}_i$ and $\mathbf{s}_j$ are orthogonal. Since these vectors are in a three-dimensional space, a single bond will not determine uniquely the vector $\mathbf{s}$ at a given site. This can be seen by fixing the direction of, say, $\mathbf{s}_i$; then, $\mathbf{s}_j$ will only be determined to lie in the plane perpendicular to $\mathbf{s}_i$ by the minimum-energy requirement. The continuous Heisenberg model has all the properties of the initial (discrete) 3PAFT.

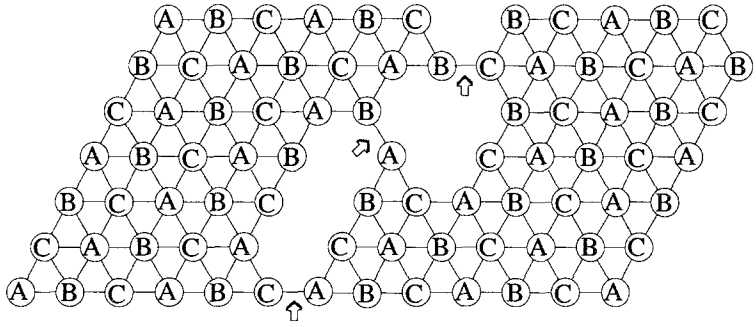


Fig. 1. An example of a lattice where order is transmitted from left to right in the discrete 3PAFT. The spins of the sites at the left border are fixed in the pattern *ABCABC...*, and the ground-state requirement dictates the values of all other spins in the network. If any site is removed so that one of the three bonds marked with arrows is broken, the state of the cluster to the right will only be partially ordered.

However, with the continuous version, we can quantify the ability of the system to transmit order. Suppose we have a square-shaped triangular lattice $MNPQ$. On one side of it, say MN, we set all vectors $\mathbf{s}$ to an ordered state $ABCABCABC...$ [for instance, $A=(1, 0, 0)$, $B=(0, 1, 0)$, and $C=(0, 0, 1)$]. At the opposite end, QP, we fix the vectors $\mathbf{s}$ to another ordered state, $A'B'C'A'B'C'...$, deduced from the previous by a rotation R in the three-dimensional space, i.e., $A'=RA$, $B'=RB$, and $C'=RC$. This rotation can be parametrized by the three Euler angles (φ, θ, ψ). Let us now compute the minimum energy of the lattice as a function of these angles. If the absolute minimum (zero energy) is obtained *only* for $\varphi=\theta=\psi=0$ (modulo symmetries), then order propagates through the system. If other values of φ, θ, and ψ result in a zero energy, then the system is either partially ordered or not ordered at all. When the system is ordered, then there can exist many local minima in the energy as a function of the Euler angles. The absolute minimum value of these energy minima which do not correspond to the reference state $\varphi=\theta=\psi=0$ is a measure of the ability of the system to transmit an order.

In this present form, the continuous model is not simpler to solve than the discrete one. We are thus led to consider the linear version of it. Let us consider an ordered state, e.g., the one imposed by one end of the lattice, and label for simplicity $A=(1, 0, 0)$, $B=(0, 1, 0)$, and $C=(0, 0, 1)$. This will constitute the *reference* state we will refer to. We now introduce a *small perturbation* of this order. If a site had an ordered vector $\mathbf{s}=(1, 0, 0)$, then the perturbed vector will be $\mathbf{s}'=(1, \alpha_2, \alpha_3)$ with $\alpha \ll 1$. The first component can remain 1, for its perturbation would show up in higher order only. If this site is connected to a neighboring one where $\mathbf{s}''=(\beta_1, 1, \beta_3)$, then to

the first order, the scalar product reads $\mathbf{s}' \cdot \mathbf{s}'' = \beta_1 + \alpha_2$, and therefore the energy of the bond will be

$$E = J(\beta_1 + \alpha_2)^2 \tag{3}$$

With this procedure, we obtain a quadratic Hamiltonian for the lattice. We see here that the information transmitted through a bond is partial, since E does not depend on α_1 nor β_2.

It turns out that this linearized model is exactly solvable. However, it differs significantly from both the original 3PAFT and the continuous (Heisenberg) model.

Let us focus on one particular occupied site i whose perturbed vector is $\mathbf{s}' = (1, \alpha_2, \alpha_3)$ (its unperturbed state is A). This site is a neighbor of three sites j (see Fig. 1) whose reference vector is in state **B**. The energy of these three bonds is

$$E_{AB} = J \sum \varepsilon_j (\beta_1^j + \alpha_2)^2 \tag{4}$$

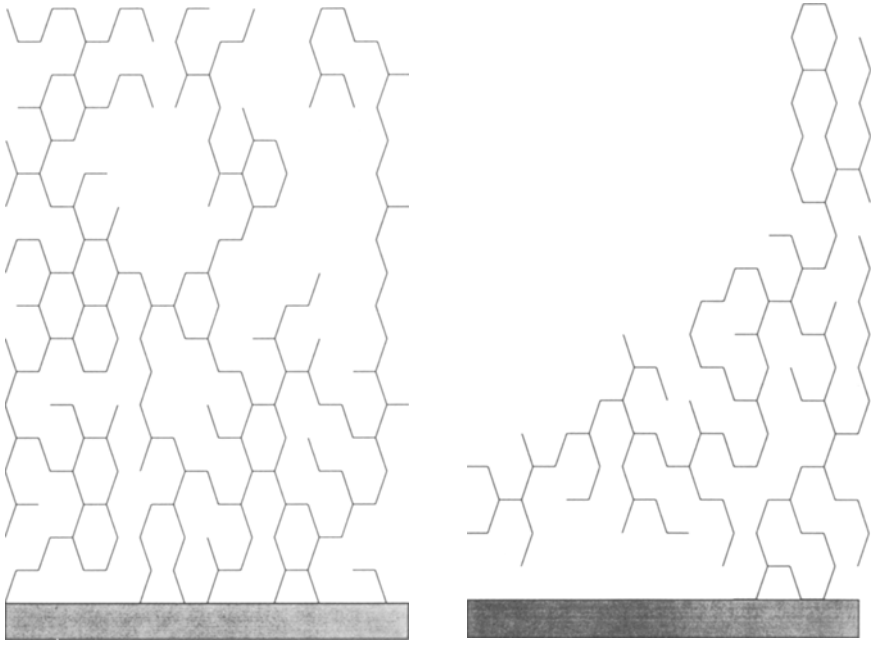
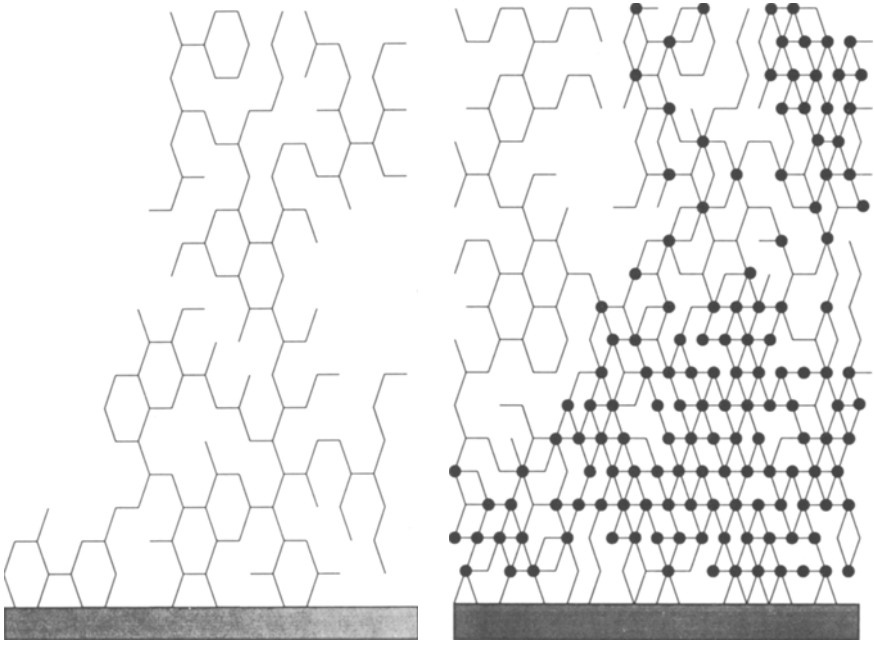


Fig. 2. An ordered state along the bottom edge of the network imposed in the linear 3PAFT model. This is marked by a bar. Shown are the connected clusters of the three honeycomb sublattices corresponding to the (a) AB, (b) AC, and (c) BC bonds. (d) The sites, marked by (●), that belong to the intersection of two of the three sublattices. These sites are ordered in the *linear* model.



(c) (d)

FIGURE 2 *(continued)*

where β_1^j is the first component of the perturbed vector in j. There are also three neighbors k whose reference state is C. Thus the total energy of the bonds originating in i is

$$E = E_{AB} + E_{AC}$$
$$= J\left[\sum \varepsilon_j(\beta_1^j + \alpha_2)^2 + \sum \varepsilon_k(\beta_1^k + \alpha_3)^2\right] \tag{5}$$

We see that this energy is naturally the sum of two independent contributions: one coming from AB-type bonding and another from AC bonding. For the complete lattice, there are three types of terms in the expression of the energy, reflecting AB, BC, and CA interactions. Each of these terms is summed over an independent honeycomb lattice (see Fig. 2). We have therefore merely reduced the original problem three percolation problems as follows.

The continuous version of the site-diluted 3-state Potts antiferromagnetic model on a triangular lattice at zero temperature, once linearized, has a threshold for the propagation of order p_{lin}^* which amounts

to the site-percolation threshold on a honeycomb lattice, i.e., $p^*_{\text{lin}} = 0.6962$.[1] The bond-diluted problem similarly has a threshold $p^*_{\text{lin}} = p_c = 1 - 2\sin(\pi/18) = 0.65271$.[1] At threshold, on each of these honeycomb lattices we have a problem identical to the random resistor network percolation problem. Let us consider a potential V equal to the second component of $\mathbf{s}$ on A-type sites and to minus the first component of $\mathbf{s}$ on B-type sites. Then, in terms of this potential, the AB contribution of the energy is

$$E_{AB} = J \sum \varepsilon_i \varepsilon_j (V_i - V_j)^2 \tag{6}$$

Thus, this may be interpreted as the energy dissipated in a site-diluted percolation problem on a honeycomb lattice with conductances $2J$. Finally, we know that the conductance of the lattice will go to zero critically at threshold as $(p - p_c)^t$, where t is the conductivity critical exponent $t = 1.30 \pm 0.01$.[1] Therefore, we deduce that the "rigidity" modulus of the linearized 3PAFT vanishes at threshold as $(p - p^*)^t$. By rigidity, we mean the second-order tensor which defines the quadratic energy with respect to the perturbation angles.

All properties of this model can thus be deduced from those of usual percolation. However, we note that nonlocality is still present in the linearized model, though now being rather trivial, in the form of having to gather different partial information from two lattices at each site: for a site with spin $(1, \alpha_2, \alpha_3)$, we need to know that it belongs to the infinite cluster of the AB sublattice and the infinite cluster of the AC sublattice. The first of these two requirements determines α_2 to be zero, while the second one forces α_3 to be zero. Therefore, nonlocality has an observable consequence, namely that there exists a set S_{order} of ordered sites (completely determined state) whose structure can be directly understood from the previous observation: it is the union of three (one for each state A, B, and C) intersections of two infinite clusters (two sublattices per site),

$$\begin{aligned} S_{\text{order}} &= S_A \cup S_B \cup S_C \\ &= (S_{AB} \cap S_{AC}) \cup (S_{AB} \cap S_{BC}) \cup (S_{AC} \cap S_{BC}) \end{aligned} \tag{7}$$

where S_{AB} is the infinite cluster of the AB network (see Fig. 2d). The fractal codimension of S_A is obtained as the sum of the codimensions of two independent percolation clusters S_{AB} and S_{AC}. Since the three sets S_A, S_B, and S_C are on different sites, their union has the same statistical properties as each, and thus we deduce that the fractal dimension of the set S_{order} is $d_{\text{order}} = d - 2\beta/\nu$, where d is the space dimension, β and ν are the critical exponent for percolation,[1] $\beta = 5/36$ and $\nu = 4/3$, thus $d_{\text{order}} = 43/24 = 1.79$.

We also note that this set is not necessarily connected. On the other hand, sites with partial order form a connected cluster whose fractal dimension at threshold is identical to that of percolation, i.e., $d-\beta/\nu = 91/48 = 1.89$.

Unfortunately, the linearization we have performed is not innocent. The linearized model may be ordered even though the continuous one is not, for the same initial geometry. An example of this is given in Fig. 3. If a single path from one honeycomb lattice exists (*MNP...*), suppose that M is of type A; then N is not A, and P can be anything. In the linearized model, if the vector in M is $(1, 0, 0)$ and in N is $(\beta_1, 1, \beta_3)$, then in the ground state, $\beta_1 = 0$. Up to this point, the two models agree. Now if the state in P is $(1, \alpha_2, \alpha_3)$, then a zero energy requires $\alpha_2 = -\beta_1 = 0$. The information propagates (as an electric potential) all along the path *MNP...* in the linearized model, although it stops after one step in the continuous model. The site marked by an arrow in Fig. 3 shows a typical example of this.

The difference between the full and the linear 3PAFT occurs because of a lower bound for the threshold: $p^* \geqslant p^*_{\text{lin}} = 0.6962$. This bound is well inside the interval given in ref. 4 for the problem of site dilution ($0.635 < p^* < 0.782$).

The reason underlying the possible difference thresholds for the two models is fundamental. In the linearized model, we consider infinitesimal changes in the orientation of the spin **s** and we compute the energy with respect to the "*undeformed*" geometry, i.e., changing only one spin at a time and leaving all the other, as in their reference state. We will come back to this point below in connection with the CFP problem.

Adler *et al.*[4] suggested that some connection might exist between the

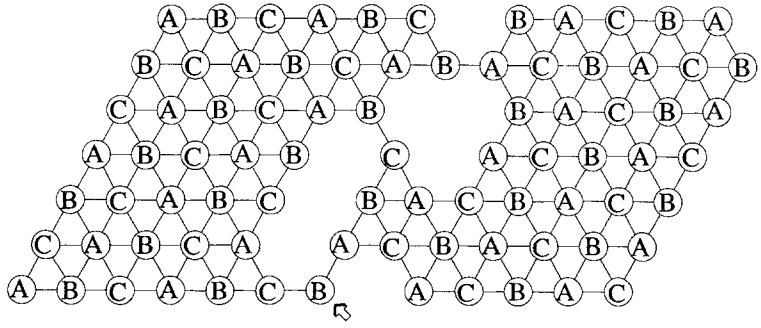


Fig. 3. The network of Fig. 1 where one site has been removed. This network is no longer ordered, as is exemplified by the spin distribution shown, which is different from the one of Fig. 1. However, in the *linear* 3PAFT, this network is still ordered, since all the three honeycomb sublattices still percolate through the entire network.

3PAFT problem and the CFP problem.[5–7] Let us briefly recall the definition of the latter: linear Hookean springs are distributed on the bonds of a triangular lattice in such a way that the springs are free to rotate at their endpoints. A fraction p (chosen at random) of the bonds is present, while $1-p$ are missing. The elastic modulus of the lattice goes to zero at the CFP threshold $p = p_{\text{cen}}$. The Hamiltonian of the lattice reads

$$H_{\text{cen}} = J \sum \varepsilon_{ij} [(\mathbf{u}_i - \mathbf{u}_j) \cdot \mathbf{n}_{ij}]^2 \tag{8}$$

where ε_{ij} is 1 if the bond $i-j$ is present and zero otherwise, $\mathbf{u}_i$ is the displacement of the site i, $\mathbf{n}_{ij}$ is a unit vector aligned along the bond $i-j$, and J is an elastic constant. In this problem, too, the propagation of information through a single bond is only partial: only the displacement along the axis of the bond counts. This renders the determination of the threshold very difficult.

In most studies (refs. 5–7 and following works), only the linearized model of CFP is considered. The full Hamiltonian, where $\mathbf{n}_{ij}$ is a function of $\mathbf{u}_i$ and $\mathbf{u}_j$, is necessary to account for buckling or large deformation; however, it quickly becomes numerically intractable. Although some recent attempts have been made[9] in this nonlinear description, the simultaneous occurrence of nonlinearity at the basic level and of criticality is a prohibiting factor. In the linearized version, $\mathbf{n}_{ij}$ is the direction of the bond in the "*undeformed*" geometry. (This is the usual procedure followed to linearize continuous medium elasticity.[10] In this way, the Hamiltonian H_{cen} turns out to be quadratic in $\mathbf{u}$. Indeed, the continuous 3PAFT and the CFP are very close to one another, even in their nonlinear characteristics, and some understanding may be gained in comparing both problems. If CFP and the 3PAFT models were identical, this would also hold for their linearized versions. We note that these differ at least in one important (and intrinsic) respect: the linear 3PAFT model is decoupled, whereas this is not true for the CFP. In other words, it can be shown that in one case it is possible to diagonalize simultaneously all interaction matrices for all bonds originating from one site, and not in the other. (Only an extreme situation exists where the CFP problem can be partially decoupled,[11] and thus can give rise to a usual percolation problem.) A numerical result also shows a difference in the thresholds estimated to be $p_{\text{cen}} = 0.642 \pm 0.002$[7] and $p_{\text{lin}}^* = 0.65271$ for bond dilution in both cases.

Although these two models are not equivalent one to the other, we can compare some of their properties:

1. Both models are nonlinear and nonlocal in their original (continuous) formulation.

2. Both can be linearized, under similar assumptions, and still have a nonlocal character.

3. The linear 3PAFT model has been shown here to belong to the universality class of percolation; this has also been suggested to be true for the CFP problem on the basis of numerical simulations.[7]

4. We have also seen for the 3PAFT that the partially ordered sites have a fractal codimension equal to that of percolation, whereas that of the totally ordered sites was twice as large. A recent investigation of the surface properties of the CFP model[12] revealed that the sites that have at least one degree of freedom frozen had the same scaling exponent as in usual percolation, and totally rigid sites had a larger codimension, close to, but smaller than, the double (0.55 compared to 2/3). The reason why this second codimension is somewhat smaller might come from the fact that since no decoupling occurs in the component of the displacement vectors, correlations exist in the lattices where partial information is transmitted.

Pursuing the correspondence between both problems, it would be of interest to find the equivalent discrete model of CFP (in the spirit of the original 3PAFT).[4] Let us finally stress the interest in solving linearized versions of more complex problems in order to gain some insight on whether the properties are related to the nonlinear aspects or are intrinsically part of the problem. Such an approach has been carried out fruitfully, for instance, for the Kauffman cellular automaton.[13] In parallel, it would be very helpful to have a better understanding of some simple nonlinear problems, such as bootstrap percolation.

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