Applying Percolation Techniques to Two-Dimensional Ferromagnets

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The Fortuin-Kasteleyn transformation is employed to relate two-dimensional classical ferromagnets to correlated site-bond percolation problems. Modulo some technical assumptions, this approach is used to produce an alternative rigorous proof for the existence of a phase characterized by algebraic decay of correlations in the O(2) model. Certain rigorous results are also derived for some discrete spin models [Z(N), cube, dodecahedron].

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A few years back Brower and Tamayo [1] and Patrascioiu [2] proposed a new way of updating Monte Carlo studies of the nonlinear O(N) sigma models. The crucial observation was that one can introduce an Ising variable $\sigma = \pm 1$ and parametrize the spin as

$$\mathbf{s}_i = |\mathbf{s}_i \cdot \mathbf{u}| \sigma_i \mathbf{u} + \mathbf{s}_{ip} \,. \tag{1}$$

Here **u** is an arbitrary unit vector and $\mathbf{u} \cdot \mathbf{s}_{ip} = 0$. In terms of these variables the partition function of the O(N) model with the usual standard nearest-neighbor action (SNNA) becomes

$$Z = \sum_{\{\sigma\}} \left(\prod_{i \in \Lambda} \int ds_{i\parallel} d\mathbf{s}_{ip} \right) \\ \times \exp \left[\beta \sum_{\langle i,j \rangle} (s_{i\parallel} s_{j\parallel} \sigma_i \sigma_j + \mathbf{s}_{ip} \cdot \mathbf{s}_{jp}) \right],$$
(2)

where $s_{i\parallel} = |\mathbf{s} \cdot \mathbf{u}|$. With respect to the σ variables, this is the partition function of an Ising ferromagnet, for which the Swendsen-Wang [3] Monte Carlo procedure can be applied.

It is well known [3] that at the basis of the Swendsen-Wang procedure lies the exact mapping of the Ising model into a correlated site-bond percolation problem established by Fortuin and Kasteleyn [4]. In a separate paper [5] we use this mapping to obtain certain analytical results concerning the phase structure of some spin models. We believe that this percolation approach to classical spin models is very powerful and provides an intuitive understanding of the phenomena responsible for the phase transitions and we would like to bring it to the attention of the community. The present Letter contains only a brief description of the techniques employed and of the results obtained. Among the latter (we note that modulo three conjectures are needed for technical reasons), we give an independent rigorous proof for the existence of the Kosterlitz-Thouless phase transition in the O(2) model (original proof by Froehlich and Spencer [6]). We also obtain rigorous results for certain discrete spin models such as Z(N) (Abelian) and the cube and the dodecahedron (non-Abelian).

We consider the following modification of the SNNA O(N) models—to be called "cut action": The Gibbs factor in Eq. (2) remains unchanged provided $|\mathbf{s}(i) - \mathbf{s}(j)| < \epsilon$ for some $0 < \epsilon < 2$ and vanishes otherwise (we forbid angular deviations between any two spins at adjacent sites larger than a certain value). At small temperatures $1/\beta$, several rigorous results [7,8] guarantee that for the SNNA the probability for big angular deviations between nearest-neighboring spins is exponentially suppressed (in β). We introduce the "cut" model to avoid estimates of the entropy of defects—bonds with large angular deviations—but in view of the above, we expect the cut and the SNNA models to exhibit similar behavior for large β and $\epsilon > O(1/\sqrt{\beta})$.

Next we would like to state our three conjectures, which, as will be seen, are needed only for technical purposes. It is well known that in two dimensions (2D) a continuous symmetry is not broken (Mermin-Wagner theorem [9]). The rigorous proof [10] requires a twice differentiable Hamiltonian and thus does not apply to the cut action. However, we will assume the following.

Conjecture 1.— Every invariant Gibbs state of the cut action model is O(N) symmetric.

A crucial property used in our approach regards the ergodic properties of the Gibbs state. In the case of a continuous symmetry model, in view of conjecture 1, it is reasonable to expect that there is a unique translational invariant Gibbs state-independent of the boundary conditions. In a case where the symmetry is discrete, we would expect that at least for given boundary conditions, the Gibbs state is unique. If that is the case, by Birkoff's ergodic theorem, ensemble averages equal spatial averages. To be specific, imagine a Monte Carlo study of one of these models. After a certain number of "thermalization" sweeps, one starts the measurements by computing time averages over successive configurations. By ergodicity, an alternative procedure would be to use only one "thermalized" configuration and to measure on it the spatial average of the observable. In the infinite volume limit, the two procedures would yield the same result. Let us call any such well-thermalized, infinite-volume configuration for which the spatial average equals the ensemble average, a "typical" configuration. Our second conjecture is as follows.

Conjecture 2.— There exist typical configurations in the O(N) spin models.

We cannot prove this fact but let us stress that this assumption is made tacitly in numerical studies, where one uses spatial averaging to improve the statistics. Conjecture 2 really implies conjecture 1 because if the Gibbs state is unique it will automatically be O(N) invariant. But for the sake of clarity we state the two conjectures separately. For discrete models the symmetry may be spontaneously broken; in that case there will still be typical configurations for each pure phase (ergodic component).

Any typical configuration must reflect the properties of the ensemble. Suppose that we asked the following question: In a typical configuration of O(N), do the sites where the associate Ising spin σ is positive [defining a hemisphere of S(N-1)] percolate? By percolation we mean the existence of an infinite chain of adjacent sites where $\sigma = +1$. On a square lattice S one can define * percolation by also allowing connections across the diagonal. It is easy to see that on S, the boundary of any ordinarily connected cluster is a *-connected cluster. On a triangular lattice T, there is no distinction between ordinary and * percolation and this is the reason for our discussing T lattices. Returning now to the question asked by the Mermin-Wagner theorem, if a cluster with $\sigma = +1$ percolated, so should one with $\sigma = -1$. The problem is that because the measure which has produced this typical configuration enjoys the symmetries of the lattice -translations and discrete rotations-in 2D two clusters cannot percolate at the same time. Indeed, if there is one site having an infinite chain attached to it, by translational invariance, there will be many others, and by rotational invariance, they will be running in arbitrary directions. In 2D, these chains, along which $\sigma = +1$, will inevitably cross and produce a circuit surrounding the origin. A cluster of $\sigma = -1$ could no longer escape to infinity. This property has been proved rigorously for the ordinary Ising model [11] and we state it as a conjecture for the O(N)or discrete spin models. Namely, let E be some set (such as $\sigma = +1$) and E its complement.

Conjecture 3.—In 2D, for the O(N) or discrete spin models, one cannot have simultaneous percolation of E and \overline{E} on the T lattice.

Having stated our three conjectures, let us briefly sketch the way they are being employed. We will address here the case of O(2) and refer the reader to Ref. [5] for the discrete spin models. We would like to consider the magnetic susceptibility of the Ising variable σ :

$$\chi_{\rm ls} \equiv \frac{1}{|\Lambda|} \sum_{x_i r \in \Lambda} \langle \sigma_x \sigma_y \rangle.$$
(3)

Here $\langle \cdots \rangle$ means expectation value with respect to the original Gibbs measure. In view of conjecture 2, we can replace this expectation value by the one obtained for an ordinary Ising spin in which the coupling constants $\beta_{ij} = \beta_{Si\parallel S_{j\parallel}}$, with s taking the values of a typical configuration. According to the Fortuin-Kasteleyn result [4], χ_{1s} equals the expected mean cluster size of clusters constructed as follows: A bond is placed only between clusters of like σ 's and then only with probability $1 - \exp(2\beta_{ij})$. We will call clusters of like σ 's H clusters and those of Fortuin and Kasteleyn, FK clusters. Each FK cluster can be flipped randomly with probability $\frac{1}{2}$. Consequently for the cut model, the bond occupation probability must be modified slightly, namely, a bond must also be placed between like σ 's if

$$-s_{i\parallel}s_{j\parallel} + \mathbf{s}_{ip} \cdot \mathbf{s}_{jp} < 1 - \epsilon^2/2.$$
(4)

In particular, these inequalities require placing a bond between like σ 's if

$$s_{i\parallel} > \epsilon/2 \,. \tag{5}$$

Therefore in the case of the cut action model, the FK clusters must contain clusters of sites defined by Eq. (5). As we shall argue next, the mean cluster size of the latter has to be divergent and that will complete the proof.

First, we would like to point out that from conjectures 1 and 3 it follows that on a T lattice H clusters cannot percolate. However, one could wonder if a larger subset of the circle \overline{A} percolates. We shall prove that provided A is sufficiently large so that the constraint prevents jumps across it,

$$A = \{\varphi \in S^{\perp} | \cos\varphi > 1 - \epsilon\}, \tag{6}$$

neither \overline{A} nor A can percolate. Indeed, suppose the opposite, namely, that \overline{A} percolates and A does not. Let A_R be the set obtained from A by a 180° rotation and decompose \overline{A} as $\overline{A} = A_1 \cup A_R \cup A_2$, where A_1 and A_2 are adjacent to A and A_R , but not to each other. By conjecture 1, if A does not percolate, neither does A_R . In the cut model, this implies that the supposed percolating cluster of \overline{A} is contained entirely in either A_1 or A_2 . That means A_1 or A_2 , which are subclusters of H clusters, percolate, which is impossible. QED. Russo [12] has proved the following theorem: If in a percolation process produced by a translationally invariant measure on a T lattice neither the clusters of E (set) nor \overline{E} (its complement) percolate, then the mean cluster size of both E and Ediverges. This is intuitively clear since if neither E nor \overline{E} percolate, the origin must be surrounded by an infinite sequence of alternating circuits of E, respectively, \overline{E} . Since in view of the above proven property, the subsets of the FK clusters defined by Eq. (5) fulfill the conditions of Russo's theorem, we conclude that the mean size of the FK clusters diverges and so does χ_{1s} . QED.

How does our result relate to the usual Kosterlitz-Thouless picture that links the existence of the soft phase to the suppression of free vortices? Our proof requires $\epsilon < \sqrt{2}$, which forbids vortices. Numerical simulations reveal, however, that the system is in the soft phase for $\epsilon < 1.57$, $\beta = 0$, i.e., also in a range where vortices are allowed, but have small entropy. For $\epsilon > 1.57$, $\beta = 0$ the system is in a disordered phase with exponential decay of correlations. So ϵ can be taken as the parameter driving the Kosterlitz-Thouless transition, a role usually played by β .

In the case of the discrete spin models we consider a modified action in which jumps (in spin space) farther than one of the nearest neighbors are forbidden. For models with discrete symmetries, symmetry breaking can occur: Conjecture 1 need not be true. On a T lattice we prove that with this modified action such models are either in a phase with long-range order or with algebraic decay for any $\beta \ge 0$. The percolation approach is not sufficiently powerful to shed light on a long-lasting dilemma [13]: Does the constraint Z(4) model on a T lattice possess a massless intermediate phase at $\beta = 0$? Modulo two technical assumptions (conjectures 2 and 3), we prove rigorously that it cannot have a phase with exponential decay. The same conclusion applies to the constraint discrete Gaussian model. We conducted Monte Carlo studies of some of these discrete spin models and the results are reported in a separate paper [14].

In closing we would like to state that the percolation approach can be applied to all O(N) models, as well as to many discrete models containing a Z(2) symmetry. The cases addressed here and in Ref. [5] are facilitated by the special topological properties present in some models on the *T* lattice. An attempt to extend these proofs to more complicated problems such as O(N), $N \ge 3$, is presented by one of us in a separate paper [15].

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- [1] R. C. Brower and P. Tamayo, Phys. Rev. Lett. 62, 1087 (1989).
- [2] A. Patrascioiu, Nuovo Cimento B 105, 91 (1989).
- [3] R. H. Swendsen and J. S. Wang, Phys. Rev. Lett. 58, 86 (1987).
- [4] C. M. Fortuin and P. W. Kasteleyn, J. Phys. Soc. Jpn. Suppl. 26, 86 (1969).
- [5] A. Patrascioiu and E. Seiler, "Phase Transitions in Classical Two Dimensional Ferromagnets," Max Planck Institut für Physik report, 1991 (to be published).
- [6] J. Froehlich and T. Spencer, Commun. Math. Phys. 81, 527 (1981).
- [7] H. O. Georgii, Commun. Math. Phys. 81, 455 (1981).
- [8] J. Bricmont and J. R. Fontain, J. Stat. Phys. 26, 745 (1981).
- [9] N. D. Mermin and H. Wagner, Phys. Rev. Lett. 17, 1133 (1966).
- [10] R. L. Dobrushin and S. B. Shlosman, Commun. Math. Phys. 42, 31 (1975).
- [11] A. Coniglio, C. R. Nappi, F. Perugi, and L. Russo, Commun. Math. Phys. 51, 315 (1976).
- [12] L. Russo, Z. Wahrshc. Verw. Gebiete 42, 39 (1978).
- [13] Y. Stavans and E. Domany, Phys. Rev. B 27, 3043 (1983).
- [14] A. Patrascioiu and E. Seiler, "Monte Carlo Investigation of Some 2D Ferromagnets with Discrete Spin Symmetries," Max Planck Institute für Physik report, 1991 (to be published).
- [15] A. Patrascioiu, "Existence of a Massless Phase in the Non-Abelian Sigma Models in 2D," University of Arizona report 1991 (to be published).