Hamiltonian formulation of bond percolation: an alternative derivation

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Abstract. An alternative derivation of the relationship between bond percolation and the Ashkin–Teller–Potts model, discovered by Kastelyn and Fourtuin, is presented. The derivation is in terms of a correlated bond expansion of standard form. A class of percolation models related to the general p-state model is defined, and a relationship between bond density and internal energy is derived. The nature of the $p = 1$ percolation limit and its correlation function are also discussed.

1. Introduction

Kastelyn and Fortuin (Kastelyn and Fortuin 1969, Fortuin and Kastelyn 1972) have shown that bond percolation can be described in terms of the $p = 1$ limit of the p-state Ashkin–Teller–Potts (ATP) (Ashkin and Teller 1943; Potts 1953) model. The result is frequently quoted because it established a Hamiltonian formalism for the percolation problem. The formalism used by Kastelyn and Fortuin was developed in their paper. In an appendix to a recent paper, Stephen (1977) has presented a different derivation. The purpose of the present paper is to present an alternative derivation which, we believe, brings out more clearly the relationship between percolation and standard ideas and series expansion techniques for the Ising and ATP models.

While we derive no essentially new results, and our discussion is of course formally equivalent to that of Kastelyn and Fortuin (1969) and Stephen (1977), the role of percolation in phase transitions seems to come out more clearly. In particular we show that a generalised percolation model can be related to the ATP model for general p. The Kastelyn and Fortuin bond probability shows up as an expansion parameter but the actual density of bonds is related to the internal energy. The bond distribution becomes free in the $p = 1$ percolation limit because the energy vanishes identically in this limit.

The site correlation functions discussed by Stephen (1977) are seen to be the $p = 1$ limit of the p-state spin correlation function.

2. The correlated bond expansion

We shall use a formalism previously developed for the three-state Potts model

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(Alexander and Yuval 1974). The Hamiltonian for the general p-state ATP model can be written:

$$H = -\tfrac{1}{2} \sum_{i,j} J\boldsymbol{\sigma}_i \tau \boldsymbol{\sigma}_j \tag{1}$$

where J is the nearest-neighbour interaction and $\boldsymbol{\sigma}_i$ is a p-dimensional vector describing the spin state at site i. Thus $\boldsymbol{\sigma}_i$ has one component which is unity and all its other $(p-1)$ components vanish. Finally the p-dimensional interaction matrix τ can be written:

$$\tau = \mathbf{1} - \Pi \tag{2}$$

where $\mathbf{1}$ is the p-dimensional unit matrix and all elements of the (p-dimensional) projection operator Π are equal to $1/p$. The partition function is:

$$Z = \mathrm{Tr}_{\sigma_i} \exp(-\beta H). \tag{3}$$

In analogy with standard expansions for the Ising model this can be written as a product over bonds

$$Z = \mathrm{Tr}_{\sigma_i} \prod_{\substack{\text{bonds} \\ i,j}} \langle \sigma_i | \exp[(p-1)\beta J/p]\mathbf{1} + \exp(-\beta J/p)(p\Pi - 1)|\sigma_j\rangle \tag{4}$$

where the operators in brackets are defined as in equation (2), and the brackets indicate matrix elements with respect to the vectors $\boldsymbol{\sigma}_i$, $\boldsymbol{\sigma}_j$. Equation (4) can be written as a matrix product only for a one-dimensional chain, i.e. when each $\boldsymbol{\sigma}_i$ appears only twice. It is convenient to use the somewhat more compact notation of Alexander and Yuval (1974) and write equation (4) in the form

$$Z_\mathrm{p} = \mathrm{Tr}_{\sigma_i} \prod_{\text{bonds}} * [\exp[(p-1)\beta J/p]\mathbf{1} + \exp(-\beta J/p)(p\Pi - 1)]_{ij} \tag{5}$$

where the $*$ product is defined by equation (4).

As written, equation (5) leads to an expansion in equal spin ($\mathbf{1}$) bonds (or in broken ($p\Pi - 1$) bonds). It thus relates a weighted site percolation problem to the partition function. This does not seem to lead to any useful results. Equation (5) can be rewritten in the form

$$Z_\mathrm{p} = \mathrm{Tr}_{\sigma_i} v^{N_\mathrm{b}/p} \prod_{\text{bonds}} * (t\mathbf{1} + p\Pi)_{ij} \tag{6}$$

where N_b is the number of bonds and

$$v = \exp(-\beta J) \tag{7}$$

$$t = (1-v)/v = \exp(\beta J) - 1; \tag{8}$$

clearly v is the *a priori* probability that a given bond is uncorrelated, i.e. of type $p\Pi$.

We can now expand the product in equation (6). A general term in the expansion will have l equal spin ($\mathbf{1}$) bonds and $N_\mathrm{b} - l$ uncorrelated ($p\Pi$) bonds. By construction a term in this expansion vanishes unless all sites in each cluster connected by $\mathbf{1}$ bonds are in the same spin state. Different clusters are connected by $p\Pi$ bonds and are therefore uncorrelated. We can therefore perform the spin trace in terms of the clusters of connected sites. Each cluster gives a factor p. Thus:

$$Z_\mathrm{p} = v^{N_\mathrm{b}/p} \sum_l t^l Q_{lp} \propto \sum_l v^{N_\mathrm{b}-l}(1-v)^l Q_{lp} \tag{9}$$

where

$$Q_{lp} = \sum_{\gamma} p^{\gamma} q_{l\gamma} \tag{10}$$

$q_{l\gamma}$ is the number of ways one can form γ connected clusters with l bonds on the lattice. Thus $q_{l\gamma}$ is a purely combinatorial factor, determined uniquely by the geometry of the lattice.

In the percolation limit ($p = 1$) there is only a single spin configuration. Thus one does not have to perform a trace in equation (6). The probability that two sites are connected by a **1** bond is thus $(1 - v)$ and the probability that they are uncorrelated is v. The bond densities are then given directly by the *a priori* probabilities.

We can, however, also calculate the correlated (**1**) bond density from equation (9):

$$\rho_{cb}^{p} = \langle l \rangle_p / N_b = (1/N_b)\, d(\ln Z_p)/d(\ln t). \tag{11}$$

This leads to a relation with the internal energy (U_p):

$$\frac{d(\ln Z_p)}{d(\ln t)} = \frac{d(\ln Z_p - \beta J N_b / p)}{d\beta} \frac{d\beta}{d(\ln t)} \tag{12}$$

so that

$$\rho_{cb}^{p} = [(1/p) - (U_p/N_b J)](1 - v). \tag{13}$$

This is the density of connected bonds for any p. Since we have seen that ρ_{cb} must go to $1 - v$ as $p \to 1$, it follows that

$$\lim_{p \to 1} U_p / N_b J = 0 \tag{14}$$

for all temperatures.

While this seems odd, it actually follows directly from the behaviour of the Hamiltonian (equation (1)) in this limit. It simply reflects the fact that the interaction between parallel spins ($J_{\parallel}^{p}$)

$$J_{\parallel}^{p} = J(1 - 1/p) \tag{15}$$

vanishes in this limit. It is important to note that the temperatures (β^{-1}) and the *a priori* bond probabilities v (equation (7)) are related to the p-independent parameter J and not to the ground state energy ($J_{\parallel}^{p}$) for given p.

The number of clusters can be obtained directly from equation (9):

$$\langle \gamma \rangle_p = \frac{d(\ln Z_p + \beta N_b J / p)}{d(\ln p)} \tag{16}$$

which reduces to the Kastelyn and Fortuin expression (Kastelyn and Fortuin 1969) in the limit $p \to 1$.

Adding a magnetic field to H (equation (1)):

$$H_1 = -\sum_i \boldsymbol{h}_i \tau \boldsymbol{\sigma}_i \tag{17}$$

and taking the proper derivatives one obtains the relationships (Kastelyn and Fortuin 1969):

$$P_{ic} = [p/(p - 1)\beta]M \tag{18}$$

$$\langle n^2 \rangle = [p^2/(p - 1)\beta^2]\chi \tag{19}$$

where P_{ic} is the probability that a site belongs to the infinite cluster, $\langle n^2 \rangle$ is the mean square size of a cluster and M and χ are the magnetisation and susceptibility, respectively. One also notes that the spin correlation function, when calculated from this expansion (equation (6)) is simply the probability that the sites belong to the same connected cluster. This demonstrates the relationship between the ATP model correlation functions and those relevant to percolation (Stephen 1977) in a very straightforward way.

3. Discussions

The derivation we have presented seems to have several intuitive advantages, which seem attractive because of the pathological and rather formal nature of the $p = 1$ percolation limit. Mainly these result from the fact that bond percolation is obtained as a limit of well defined p-state percolation problems related to the p-state magnetic models. In particular it becomes obvious that the temperature (β^{-1}) is related to the *a priori* bond probabilities (or to the parameter J) and not to the ground state energy at fixed p.

The relationship between the bond density and the internal energy is apparently new. It should be useful in the interpretation of continuum model results (Harris *et al* 1975, Priest and Lubensky 1976, Amit 1976, Stephen 1976, 1977, Nutterman 1976) where there is no direct way to define this density.

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