

Home Search Collections Journals About Contact us My IOPscience

Correlated percolation: exact Bethe lattice analyses

This article has been downloaded from IOPscience. Please scroll down to see the full text article. 1987 J. Phys. A: Math. Gen. 20 6487 (http://iopscience.iop.org/0305-4470/20/18/045)

View the table of contents for this issue, or go to the journal homepage for more

Download details: IP Address: 129.252.86.83 The article was downloaded on 31/05/2010 at 12:12

Please note that terms and conditions apply.

Correlated percolation: exact Bethe lattice analyses

J W Evans

Ames Laboratory, Applied Mathematical Sciences, Iowa State University, Ames, Iowa 50011, USA

Received 13 April 1987, in final form 10 July 1987

Abstract. Certain classes of correlated site-percolation problems (or correlated spreading phenomena) on Bethe lattices are analysed exactly. Our analysis of percolation of, e.g., occupied sites, requires that spreading of clusters of occupied sites is determined by a finite number of conditional probabilities. A condition specifying the percolation threshold is provided, as well as expressions for the percolation probability and average cluster size. Previous results for random and nearest-neighbour Ising-model distributions are recovered as special cases. Results are illustrated with examples for equilibrium and non-equilibrium distributions, the latter obtained via irreversible cooperative filling. We also discuss 'two-phase percolation' for distributions with no occupied NN pairs of sites, correlated bond percolation and other problems.

1. Introduction

Any family of distributions of occupied sites on a lattice for various occupancy probabilities, p, between zero and unity generates a percolation problem [1]. Typically one defines clusters of occupied (\odot) and unnoccupied (\bigcirc) sites via a connectivity rule wherein nearest-neighbour (NN) sites of the same state are assigned to the same cluster. One then analyses the distribution of cluster sizes and the appearance or disappearance of infinite clusters as p varies. The latter 'percolation thresholds' will be denoted by $p = p_c$.

The simplest case of a random distributions, i.e. where the occupancies of different sites are independent, has been studied extensively [2]. However, in physical systems, correlations will typically exist between different sites and their effect on the percolation transition is of some interest. Such questions have been analysed for NN Ising-model distributions where the occupied sites or 'particles' interact via NN interactions and are in thermal equilibrium. Here one naturally varies the temperature to study the connection between percolative and thermal critical phenomena [1, 3]. Note that for any equilibrium distribution associated with pairwise interactions only, the percolation problems for occupied and unoccupied sites are not distinct because of 'particle-hole symmetry'. Such equilibrium distributions, however, represent only one class of correlated distributions, albeit the most familiar class, and do not describe physical systems out of equilibrium. Thus here we are motivated to also consider percolation problems for various classes of non-equilibrium correlated distributions. These could, for example, be generated from kinetic Ising models [4], via irreversible cooperative site filling [5] or restricted valence site filling [6], or specified directly as below. Here, in general, the percolation problems for occupied and unoccupied sites will be distinct. Such introduction of correlations, with finite correlation length, is not expected to change the critical exponents from their random percolation values [1].

0305-4470/87/186487 + 14\$02.50 © 1987 IOP Publishing Ltd

A variety of other modifications of the above percolation problems are possible. Some involve changing the definition of clusters, e.g., via longer range connectivity, multiple coordination, or even more drastic bootstrap models [1]. Here we only discuss one example of the former appropriate to the description of 'multiphase' distributions with no occupied NN pairs of sites. It is also common to consider bond rather than site percolation, so we will make a few comments on such problems.

Recently it has become popular to associate random percolation with various spreading phenomena [7]. Here percolation clusters can be grown as follows: start with a single occupied site surrounded by 'growth' sites; choose (in one of various ways) one of the 'allowed' growth sites at the cluster perimeter; either occupy it with probability p and create new adjacent growth sites, or make it permanently unoccupied with probability 1-p; repeat this process indefinitely. If correlations are present this procedure becomes more complicated. Now the probability of occupying (making permanently empty) the chosen growth site must be taken, not as p(1-p), but rather as the *conditional* probability that this site be occupied (unoccupied) given the state of all previously occupied cluster sites and those growth sites assigned permanently unoccupied[†].

Such conditional probabilities are implicitly prescribed by the choice of model, e.g., NN Ising model, irreversible cooperative filling model, etc, whose percolation properties are under consideration. The difficulty is that, for physical two- and threedimensional lattices, there are an infinite number of such distinct conditional probabilities. In the most general case, these depend on all previously assigned cluster sites. Even for Markov fields describing NN Ising-model distributions, these depend on suitably defined unoccupied or occupied perimeter sites of the previously assigned cluster, so there will still be infinitely many.

Here we consider Bethe lattices and more general branching media where exact solution of the random percolation problem is straightforward [8]. Such analysis can be naturally interpreted in terms of spreading phenomena, or as branching or cascade processes [9]. In this paper, we focus on their extension to classes of correlated distributions, where only a finite number of conditional probabilities of the type described above are required to prescribe spreading. To this end, we first introduce the concept of *n*th-order spatially Markovian distributions for Bethe lattices with coordination number z. Here a string of n sites with any prescribed state, adjacent to some particular site, shields this site from the influence of sites in the branch of the lattice attached to the other end of the string (see figure 1). These distributions are a completely determined prescription of 2^{n^*} conditional probabilities for finding an occupied (or unoccupied) site given various configurations of the $n^* = \sum_{i=0}^{n-1} (z-1)^i$ sites within n lattice vectors and within a single branch of the lattice attached to this site (see figure 2). These quantities, some of which may be equivalent from symmetry considerations, automatically generate probabilities for all smaller configurations (see [10]) and, in fact, for all configurations (exploiting the *n*th-order Markovian property). One can also show that spatial correlations exhibit asymptotic exponential decay for large separations. It is important to note that there is a correspondence between these distributions and the equilibrium distributions obtained from Ising models with various choices of general (i.e. not just pairwise) range-n interactions and of temperature.

⁺ Clearly the probability of finite portions of the percolation cluster, at any stage of growth, can be written as products of these conditional probabilities. In fact, each order of creating the cluster generates such a product, and equality of these implies consistency relations between conditional probabilities [5].



Figure 1. Sixth-order Markovian condition on a z = 3 Bethe lattice. The specified string of six sites in the full box shields the leftmost empty site from the influence of those in the branch enclosed in the broken box.



Figure 2. Conditional probabilities required to specify (a) first-order, (b) second-order Markovian distributions on z = 3 Bethe lattices. Sites inside boxes have specified state influencing the site outside.

To broaden the scope of our Bethe lattice analysis beyond such equilibrium distributions, we shall consider broader classes of *n*th-order \bullet - (\bigcirc -) Markovian distributions where *only* occupied (unoccupied) strings of *n* sites are assumed to shield in the way described above. We further note that analysis of such distributions is natural since they retain precisely those features of the above *n*th-order Markovian distributions sufficient for an exact analysis of the percolation characteristics of occupied (unoccupied) sites. This is reflected by the property that the probability of any occupied (unoccupied) cluster can still be calculated here from a finite number of conditional probabilities.

Finally we note that distributions generated by irreversible cooperative filling or adsorption (emptying or desorption) exhibit finite-order \bigcirc - (\bigcirc -) Markovian properties. However such distributions do *not* exhibit a finite-order Markovian property, and spatial correlations do not exhibit large-separation asymptotic exponential decay [5, 11].

In § 2, we analyse percolation of occupied sites for zeroth-, first- and second-order •-Markovian distributions on Bethe lattices, and in § 3 we extend this treatment to third- and higher-order distributions. We focus on determining a condition specifying the percolation threshold and on calculating the average size, S, of the cluster containing some occupied site and the percolation probability, P, that some unoccupied site is in an infinite cluster. By interchanging occupied and unoccupied site designations, these results can be applied to percolation of unoccupied sites for the corresponding order \bigcirc -Markovian distributions. In § 4, we extend these considerations to decorated Bethe lattices and to bond percolation and, in § 5, to polychromatic and a new class of multiphase percolation problems. Some explicit examples are treated in § 6. Concluding remarks are given in § 7, together with some comments on treatment of correlated percolation for physical lattices.

2. Zeroth-(random), first- and second-order O-Markovian distributions

Previously developed techniques for the analysis of percolation for random-[2] and first-order Markovian NN Ising-model distributions [12] are straightforwardly extended here to treat up to second-order spatially Markovian distributions. Specifically, we consider percolation of occupied sites for second-order \oplus -Markovian distributions on a Bethe lattice of coordination number z.

Consider the z-1 sites neighbouring one end of an NN pair of sites specified occupied. Let g(i) (f(i)) denote the conditional probability of finding a specific subset of *i* of these occupied, and the other z-1-i unoccupied (unspecified), so $g(z-j) = \sum_{i=1}^{j} (-1)^{j-1} {j-1 \choose i-1} f(z-i)$, for $0 \le j \le z$. Thus f(1) is the conditional probability of finding an occupied site given an adjacent occupied NN pair. Now since on average (z-1) f(1) of these z-1 neighbouring sites are occupied, for an occupied cluster to 'spread' indefinitely or percolate from the occupied NN pair, one must have (z-1) $f(1) \ge 1$. Therefore at the percolation threshold, $p = p_c$, one has

$$1 = (z - 1)f(1).$$
(2.1)

We thus recover previous first-order results (here $f(1) = \tilde{f}(1)$, the probability that a site is occupied given that a neighbour is occupied) and random results (here f(1) = p).

It is also instructive to consider the conditional probability, Q, that one end of an occupied NN pair is *not* connected to an infinite cluster. Enumerating all possible states of the z-1 sites neighbouring one end, and exploiting the second-order \bigoplus -Markovian property yields the recursive formula (see [2])

$$Q = \sum_{i=0}^{z-1} {\binom{z-1}{i}} g(i) Q^{i}$$
(2.2)

i.e. Q consists of a contribution of g(0) from where all z - 1 neighbours are unoccupied, z - 1 contributions of g(1)Q from where one is occupied but not connected to an infinite cluster, etc. The continuous physical solution to (2.2) satisfies $Q \equiv 1$, for $p \leq p_c$, and

$$\sum_{i=1}^{z-1} {\binom{z-1}{i}} f(i)(Q-1)^{i-1} = 1$$
(2.3)

for $p \ge p_c$. The latter Q depends on all the f(i) and vanishes as f(1) or p approach unity.

We now determine the percolation probability, P, that some occupied site is in an infinite cluster. Let $\tilde{g}(i)$ $(\tilde{f}(i))$ denote the conditional probability at a specific set of i of its neighbours are occupied, and that the other z - i are unoccupied (unspecified).

Enumerating all ways that this site can be in a finite cluster and exploiting the second-order \bullet -Markovian property yields (see [2])

$$1 - P = \sum_{i=0}^{z} {\binom{z}{i}} \tilde{g}(i)Q^{i} \quad \text{or} \quad P = \sum_{i=1}^{z} {(-1)^{i-1} {\binom{z}{i}}} \tilde{f}(i)(1-Q)^{i} \quad (2.4)$$

for $p \ge p_c$, i.e. 1-P consists of a contribution $\tilde{g}(0)$ from where all z neighbours are unoccupied, z contributions of $\tilde{g}(1)Q$ from where just one neighbour is occupied but not connected to an infinite cluster, etc. Thus, using (2.3), one concludes that

$$P \sim z\tilde{f}(1)(1-Q) \sim 2z(z-1)^{-1}(z-2)^{-1}\tilde{f}(1)f(2)^{-1}[(z-1)f(1)-1]$$
(2.5)

as p approaches p_c from above. The average cluster size, S, can be calculated from the average number, T, of occupied sites connected to one end of an occupied NN pair using (see [2])

$$S = \sum_{i=0}^{z} {\binom{z}{i}} \tilde{g}(i) \ (1+i+iT) = 1 + z\tilde{f}(i)(1+T) \qquad \text{for } p < p_{\text{c}}$$
(2.6)

i.e. S includes a contribution of $\tilde{g}(i)$ (1+i+iT) from each of the $\binom{z}{i}$ configurations where exactly *i* neighbours of the chosen cluster site are occupied. T is determined from the recursive formula (see [2])

$$T = \sum_{i=0}^{z-1} {\binom{z-1}{i}} g(i)(i+iT) = (z-1)f(1)[1-(z-1)f(1)]^{-1} \qquad \text{for } p < p_c$$
(2.7)

i.e. T includes a contribution of g(i)i(1+T) from each of the $\binom{z-1}{i}$ configurations where exactly *i* neighbours of the occupied NN pair are also occupied.

For first-order \bullet -Markovian distributions, one has $f(i) = \tilde{f}(i) = \lambda^i$, where $\lambda = \tilde{f}(1)$ is the conditional probability of a occupied site given an occupied neighbour, and (see [10])

$$Q = 1 - \lambda + \lambda Q^{z-1} \qquad 1 - P = (1 - \lambda + \lambda Q)^z \qquad S = (1 + \lambda) [1 - (z - 1)\lambda]^{-1}.$$
(2.8)

Random percolation results follow immediately after setting $\lambda = p$.

3. Third- and higher-order O-Markovian distributions

First we consider percolation of occupied sites for third-order \bullet -Markovian distributions on a Bethe lattice of coordination number z. Unlike the above examples, here one cannot trivially obtain a condition for the percolation threshold.

Let c_k denote an occupied NN pair of sites together with k occupied and z-1-kunoccupied sites neighbouring the right end (see figure 3). Let $g_k(i)(f_k(i))$ denote the conditional probability that, given c_k , a specific subset of i sites of the z-1 sites



Figure 3. Configurations, c_k , associated with percolation quantities for third-order Markovian distributions on a z = 3 Bethe lattice.

neighbouring the left end of c_k are occupied, and that the other z - 1 - i are unoccupied (unspecified). Here one has

$$g_k(z-j) = \sum_{i=1}^{j} (-1)^{j-1} {j-1 \choose i-1} f_k(z-i).$$

Finally let Q_k denote the probability that the left end of c_k is not connected to an infinite cluster. Enumerating all ways that this can occur, and exploiting the third-order \bullet -Markovian property, yields for Q_k the coupled non-linear equations (cf (2.2))

$$Q_k = \sum_{i=0}^{z-1} {\binom{z-1}{i}} g_k(i) Q_i^i \quad \text{for } k = 0 \text{ to } z - 1$$
(3.1)

whose solutions satisfy $Q_k = 1$ for $p \le p_c$, $Q_k < 1$ for $p > p_c$ and $Q_k \to 0$ as $p \to 1$ (for all k). The percolation probability, P, satisfies

$$1 - P = \sum_{i=0}^{z} {\binom{z}{i}} \tilde{g}(i) Q_{i-1}^{i}$$
(3.2)

with \tilde{g} defined as previously.

Next we determine the condition specifying the percolation threshold. Set $\delta Q_k = Q_k - 1$ and let δQ denote the vector with (z-1) components, δQ_k , for $1 \le k \le z-1$. Let $\mathbf{M}(\mathbf{I})$ denote a $(z-1) \times (z-1)$ matrix with components $M_{ki} = (z-1) \binom{z-2}{i-1} g_k(i)$ $(I_{ki} = \delta_{ki})$ for $1 \le k$, $i \le z-1$, and let \mathbf{M}_m denote a submatrix obtained from \mathbf{M} by restricting k, i to a subset of m labels. Set $R = \sum_{m \ge 2} (-1)^m \det(\mathbf{M}_m)$, where det() denotes the determinant. Linearising (3.1) about $Q_k = 1$ (or $\delta Q = 0$) yields

$$(\mathbf{M} - \mathbf{I})\delta \boldsymbol{Q} \approx \mathbf{0}$$
 for $p \approx p_c$. (3.3)

Thus for (3.3) to be consistent, at $p = p_c$ we must have $0 = (-1)^z \det(\mathbf{M} - \mathbf{I})$

$$= -1 + (z-1) \sum_{i=1}^{z-1} {\binom{z-2}{i-1}} g_i(i) - R$$

$$= -1 + (z-1)f_1(1) + (z-1) \sum_{i=2}^{z-1} {\binom{z-2}{i-1}} \left[\sum_{j=1}^{i} (-1)^{i-j} {\binom{i-1}{j-1}} f_j(i) \right] - R$$

$$= -1 + (z-1)f_1(1) + R'.$$
(3.4)

The terms R' vanish at p = 0 or 1, or for second-order \bullet -Markovian distributions. Provided the $f_j(i)$ vary continuously from zero to unity with p, $(-1)^2 \det(M-I)$ varies continuously from -1 to z - 1, so indeed (3.4) can be solved for $p = p_c$. Its reduction to the results of § 2 is immediate.

When z = 3, the quadratic Q_1 and Q_2 equations can be solved exactly. Here we just note that (3.4) assumes the explicit form (see figure 4)

$$1 = 2f_1(1) + 2[f_2(2) - f_1(2)] - 4[f_1(1)f_2(2) - f_2(1)f_1(2)]$$
(3.5)



Figure 4. Diagrammatic representation of condition (3.5) for the percolation thresholds for third-order Markovian distributions on z = 3 Bethe lattices. Sites inside boxes have specified state.

at $p = p_c$. Typically the quadratic f term should be smaller than the linear f difference term. Note that here $g_k(1) = f_k(1) - f_k(2)$ and $g_k(2) = f_k(2)$.

We calculate the average cluster size, S, via the auxiliary quantities, T_k , which denote the average number of occupied sites attached to the left end of c_k , using

$$S = \sum_{i=0}^{z} {\binom{z}{i}} \tilde{g}(i)(1+i+iT_{i-1}) = 1 + z \sum_{i=1}^{z} {\binom{z-1}{i-1}} \tilde{g}(i)T_{i-1} \qquad \text{for } p < p_{\text{c}}.$$
 (3.6)

If T[f] denotes the vector with (z-1) components $T_k[f_k(1)]$ for $1 \le k \le z-1$, then standard enumeration arguments yield the T_k equations

$$(\mathbf{I} - \mathbf{M})\mathbf{T} = (z - 1)\mathbf{f} \qquad \text{for } p < p_c \tag{3.7}$$

so, as required, T, and thus S, diverges as $p \rightarrow p_c$, where det $(I - M) \rightarrow 0$.

The treatment of fourth- and higher-order \bullet -Markovian distributions is somewhat more complicated than the above, but proceeds in an analogous fashion, and analogous structure is manifested. A few sample results are given in the appendix for the case z = 3.

4. Decorated Bethe lattices and bond percolation

It is well known that exact treatment of random site (or bond) percolation can be extended from Bethe lattices to more general branching media (decorated Bethe lattices) [8]. The same is clearly true for the correlated distributions considered above. This observation also demonstrates that exact treatment is possible for correlated *n*th-order Markovian bond percolation on Bethe lattices, since this corresponds to site percolation on suitably decorated Bethe lattices (e.g., bond percolation on a z = 3 Bethe lattice corresponds to site percolation on a triangular cactus [8]).

Bond-percolation problems can, of course, be treated directly and involve consideration of essentially the same configurations as the site problems. A mapping between s site and s-1 bond configurations has been elucidated by Fisher and Essam [8]. This result suggests that there should be a correspondence between *n*th-order Markovian site percolation and (n-1)th-order Markovian bond percolation. This is readily verified, e.g., by deriving closing equations for the probabilities that certain sets of configurations are *not* connected to infinite clusters. Examples of these sets for second- and third-order Markovian bond percolation are shown in figure 5, and the corresponding percolation thresholds are given by expressions analogous to the site-percolation expressions. Expressions for *n*th-order Markovian bond-percolation



Figure 5. Configurations for z = 3 Bethe lattice bond percolation or triangular cactus site percolation for (a) second-order, (b) third order Markovian distributions. Full (broken) lines represent filled (empty) bonds.

probabilities map into (n+1)th-order site-percolation probabilities for *adjacent pairs* of occupied sites to be in an infinite cluster.

5. Polychromatic and multiphase percolation

The problems considered above could be described as two-colour percolation, i.e. occupied (unoccupied) sites are described as black (white). One can readily generalise our treatment to handle polychromatic percolation on Bethe lattices where the sites are assigned one of a finite number of colours, according to *n*th-order Markovian statistics.

We now focus on a special type of correlated polychromatic percolation which we describe as two-phase percolation. Here we consider occupied site distributions on Bethe lattices containing no neighbouring pairs of occupied sites (so $p \leq \frac{1}{2}$), and define 'occupied 2NN clusters' via the natural second-nearest-neighbour (2NN) connectivity requirement. These have one of two phases, and 'abutting' clusters of different phase are separated by an unoccupied pair 'domain boundary' (see figure 6). In addition to occupied 2NN cluster percolation, one can consider percolation of clusters of unoccupied sites which have all nearest neighbours unoccupied (using a NN connectivity requirement). Describing the latter sites as white and occupied 2NN cluster sites of different phases as green and yellow, say, we can then have a correlated trichromatic percolation problem. Such problems have been considered on a square lattice to model $c(2 \times 2)$ ordering on surfaces [13]. In the analysis below, we assume that the statistical characteristics of both occupied phases are identical.



Figure 6. Out-of-phase 'filled 2NN clusters' separated by an empty pair domain boundary on a z = 3 Bethe lattice.

We first consider two-phase percolation for up to third-order Markovian distributions. Let F(1) be the conditional probability that a site is occupied given that a 2NN site is occupied. For percolation, it is necessary for the cluster to spread to one of the $(z-1)^2$ other unspecified 2NN sites, so one must have $(z-1)^2F(1) \ge 1$. At the percolation threshold for occupied 2NN clusters, one thus has

$$1 = (z - 1)^2 F(1).$$
(5.1)

The special case of first-order Markovian distributions corresponds to the equilibrium

Ising models with *infinitely repulsive* NN interactions. Here F(1) becomes the conditional probability of a occupied site given an unoccupied NN, which equals $p(1-p)^{-1}$. Thus, from (5.1), here one has $p_c = (z^2 - 2z + 2)^{-1}$ (which is less than $\frac{1}{2}$ for $z \ge 3$).

To calculate the corresponding percolation probability, P, start by considering the z-1 sites neighbouring the unoccupied end of an (adjacent) unoccupied-occupied pair. Let G(i) (F(i)) denote the conditional probability that a specific subset of i of these will be occupied, and that the rest will be unoccupied (unspecified). The F(j) generalise F(1) above. The probability, Q, that the occupied site in the unoccupied-occupied occupied pair is *not* connected to an infinite 2NN occupied cluster through one of these z-1 sites satisfies (see (2.2))

$$Q = \sum_{i=0}^{z-1} {\binom{z-1}{i}} G(i) Q^{(z-1)i}$$
(5.2)

consistent with (5.1). *P* can be readily calculated from the *Q*. One could also readily calculate average occupied 2NN cluster sizes.

Next we sketch some results for fourth-order Markovian distributions. Define configuration C_k as follows. Start with an adjacent unoccupied-occupied pair; assign the other z-1 neighbours of the occupied site (E_k) to be unoccupied; of the z-1 other neighbours of the unoccupied site, assign a specific k to be occupied and the rest to be unoccupied. Let Q_k denote the probability that C_k is not connected to an infinite occupied zNN cluster through E_k . A coupled closed set of non-linear equations can be obtained for the Q_k which we linearise about $Q_k = 1$ to obtain a condition for the percolation threshold. Pick one site in E_k and let $G_k(i)$ be the conditional probability that, of its z-1 neighbours not in C_k , a specific subset of i are occupied, and the rest are unoccupied. If **M** is the matrix with components $M_{ki} = (z-1)^2 {\binom{z-2}{i}} G_k(i)$, then the condition for p_c becomes det($\mathbf{M}-\mathbf{I}$) = 0 (see figure 7, for z = 3, which should be compared with figure 4).

Finally we comment on the analysis of the percolation characteristics of white sites (unoccupied sites with all NN unoccupied). A condition for the percolation threshold is easily determined by considering the probabilities that certain configurations are *not* connected to infinite white clusters. Results for third- and 4th-order Markovian distributions are represented diagrammatically in figure 8 for z = 3. For the fifth-order



Figure 7. Diagrammatic representation of the percolation threshold condition for filled 2NN clusters for fourth-order Markovian distributions. Sites inside boxes have specified state.



Figure 8. Diagrammatic representation of the percolation threshold conditions for white sites for (a) third-order, (b) fourth-order Markovian distributions. Sites inside boxes have specified state.

case with z = 3, let $H_k(i)$ be the conditional probability that *i* specific neighbours of the top left site in configuration e_k (shown in figure 9) are unoccupied, that the other z - i are occupied and that both neighbours of the bottom left site are unoccupied. If **M** denotes the 3×3 matrix with components $M_{ki} = 2\binom{2}{i}H_k(i)$ for $0 \le k$, $i \le 2$, then at $p = p_c$ one has det(**M**-**I**) = 0. Calculation of associated *P* and *S*, and extension to more complicated distributions, is straightforward.



Figure 9. Configurations, e_k , associated with white site percolation for fifth-order distributions on a z = 3 Bethe lattice.

To conclude this section, we note that the above treatment can be generalised to multiphase, or specifically *m*-phase, percolation by considering occupied site distributions on Bethe lattices where no occupied site has any first, second, ..., (m-1)th NN sites occupied. In addition, we can allow the various occupied phases to have different statistical characteristics without any real complication.

6. Some examples

The ideas discussed above are illustrated here with several examples of correlated percolation on Bethe lattices.

6.1. First-order Markovian NN Ising-model equilibrium distributions

Occupied sites here correspond to an equilibrated lattice gas with NN interactions ε at temperature T. We set $\beta^{-1} = kT$ where k is Boltzmann's constant. We can calculate the conditional probability, $\tilde{f}(1)$, of a occupied site given a neighbouring occupied site, from the probability of an unoccupied-occupied pair, $p(1-\tilde{f}(1))$. The latter equals $2p(1-p) \{[1+4p(1-p)(e^{-\beta\varepsilon}-1)]^{1/2}+1\}^{-1}$ expect in an 'antiferromagnetic' ordered region for repulsive $\varepsilon > 0$, or in the coexistence region for attractive $\varepsilon < 0$ [12, 14]. Thus the occupied site-percolation threshold, p_c^{\bullet} , can be obtained, from (2.1), as

$$p_{c}^{\bullet} = \frac{(z-1) e^{\beta \epsilon}}{(z-2)^{2} + (2z-3) e^{\beta \epsilon}}$$
(6.1)

recovering previous results [12]. Since these distributions are invariant under the replacements $p \leftrightarrow 1 - p$, unoccupied sites \leftrightarrow occupied sites, it follows that the threshold for unoccupied site percolation is given by $p_c = 1 - p_c^{\bullet}$.

6.2. Second-order \bigcirc -Markovian distributions from irreversible cooperative filling

Here the rates, k_i , for irreversible filling of the lattice sites depend on the number, i, of occupied neighbouring sites. We choose $k_i \propto \alpha'$, and make the identification $\alpha \leftrightarrow e^{-\beta \epsilon}$

for comparison with the above equilibrium results. Note that $\alpha > 1$ corresponds to clustering distributions, and ferromagnetic or attractive interactions. The second-order \bigcirc -Markovian property allows us to obtain a closed set of equations for the probability of an unoccupied site, an unoccupied pair, and the quantities corresponding to the f(i) of § 2 for unoccupied sites [11]. These quantities determine the probabilities of all connected unoccupied configurations. The f(1) quantity for unoccupied sites determines the unoccupied site-percolation threshold, p_c^{\bigcirc} , which we have shown in figure 10 for z = 3 as a function of α . The corresponding equilibrium values are also shown for comparison. We note that, for the equilibrium case, $(1 - p_c^{\bigcirc}) e^{-\beta \epsilon} \rightarrow 2$ as $-\beta \epsilon \rightarrow \infty$, in contrast to irreversible cooperative filling where $(1 - p_c^{\bigcirc}) \alpha = 0.689, 0.690, 0.751, 0.788, 0.840$ for $\alpha = 5, 10, 50, 100, 300$. The percolation probability and average cluster size for unoccupied sites can also be evaluated.



Figure 10. Variation of the empty site-percolation threshold, p_c^{\odot} , with NN cooperativity parameter α , for irreversible filling (full curve), and with NN interaction ε , for equilibrium distributions (broken curve), on a z = 3 Bethe lattice. Some second-order Markovian approximations to filled site-percolation thresholds (×) for irreversible cooperative filling are also shown, as well as the equilibrium ferromagnetic and antiferromagnetic ordered phase boundaries (dotted curves).

These distributions are not invariant under the replacements $p \leftrightarrow 1 - p$, unoccupied \leftrightarrow occupied, and are not \bullet -Markovian to any order, except when $\alpha = 1$. Thus exact determination of the occupied site-percolation threshold, p_c^{\bullet} , is not possible. One can however evaluate exactly, e.g., the conditional probabilities, q_s , of an occupied site given an adjacent string of s occupied sites ($q_0 = q, q_1 = \tilde{f}(1), q_2 = f(1)$), after determining the probabilities of suitable sets of disconnected unoccupied configurations (see [15] for z = 2). Here we forego a detailed description of these extensive calculations, and mention only that evaluation of q_s requires determination of 0, 6, 12, 24, 39 such additional independent quantities for s = 1, 2, 3, 4, 5, respectively. In table 1, we have displayed q_s behaviour for p presumably close to the occupied site-percolation threshold ($(z-1)q_2 \approx 1$ in the second-order Markov approximation) for z = 3. If α is not too far from unity, i.e. if the cooperativity is not too strong, the occupied site distribution

α	p	q_1	<i>q</i> ₂	<i>q</i> ₃	 q_4	95
10	0.156	0.519 83	0.500 93	0.492 89	0.491 06	0.491 28
5	0.222	0.511 19	0.500 38	0.496 71	0.496 26	0.496 38
2	0.361	0.502 012	0.500 431	0.500 060	0.5000 041	0.500 045
1	0.5	0.5	0.5	0.5	0.5	0.5
ł	0.645	0.500 191	0.500 127	0.500 652	0.500 583	0.500 582
1 5	0.651	0.498 70	0.499 80	0.504 12	0.502 24	0.502 53
$\frac{1}{10}$	0.661	0.498 52	0.500 11	0.506 33	0.502 67	0.503 64

Table 1. Conditional probabilities, q_s , of a filled site given an adjacent string of s filled sites, and p values, when $q_2 \approx \frac{1}{2}$. Results are shown for distributions obtained by irreversible cooperative filling for various values of α .

is quite accurately represented by a second-order \bullet -Markovian distribution, and thus p_c^{\bullet} is readily estimated.

6.3. First-order O-Markovian distributions from random dimer filling

The distribution obtained from irreversible (dimer) filling of adjacent sites on a Bethe lattice is first-order \bigcirc -Markovian. At coverage p, the conditional probability of an unoccupied site given an adjacent unoccupied site equals $(z-2)^{-1}[(z-1)(1-p)^{(z-2)/2}-1]$, for z > 2 [11]. We thus obtain the unoccupied site-percolation threshold

$$p_{c}^{\circ} = 1 - \left[(2z - 3)(z - 1)^{-2} \right]^{z/(z-2)}$$
(6.2)

which should be compared with the saturation coverage $p^* = (z-1)^{-z/(z-2)}$ [11]. We note that unoccupied site percolation for random dimer filling on physical twodimensional lattices has been proposed as a model for the geometry of solid ionic conduction [16].

6.4. Two-phase percolation for filling with NN blocking

For filling with NN blocking, we set the filling rates, k_i , of § 6.2 to zero when $i \ge 1$. Distributions with no occupied NN pairs are generated for a range of coverages up to saturation $(<\frac{1}{2})$. These are distinct from the "corresponding" equilibrium distributions obtained from the NN Ising model with infinitely repulsive NN interactions. Exact treatment of occupied 2NN cluster percolation for the former is not possible because of the lack of a finite-order Markov property. However, a percolation transition is expected to occur for all $z \ge 3$. Consider the case z = 3, where percolation is most difficult to achieve. For the 'corresponding' equilibrium distributions, we know, from § 5, that this transition occurs at coverage $\frac{1}{5}$. Presumably, for irreversible filling, the transition will still occur in this vicinity, which is well below the saturation coverage of 0.375 [11]. To support this assertion, we note that the second-order Markov approximation to the threshold is p = 0.212. At this point the conditional probability of a occupied site given an adjacent unoccupied-occupied pair, i.e. F(1), equals $\frac{1}{4}$, and given an adjacent unoccupied-occupied-unoccupied-occupied string it equals 0.25038. (These results were obtained by the methods described in § 6.2.) The percolation threshold for white clusters (of unoccupied sites with all NN unoccupied) can be calculated exactly as p = 0.219 (compare with $p = (\sqrt{2} - 1) (2\sqrt{2} - 1)^{-1} \approx 0.227$ for the 'corresponding' equilibrium distributions).

7. Conclusions

Our treatment of correlated percolation on Bethe lattices has extended previous exact results for random and NN Ising-model distributions to longer range Ising-model and certain non-equilibrium distributions. Unoccupied site percolation for irreversible cooperative filling provides explicit examples of the latter. Our examples have the same critical exponents as for random percolation (see (2.5)). The key to exact analysis was a finite-order \bullet - or \bigcirc -Markovian property. However, even for distributions with no such property, the corresponding finite-order Markovian approximations, together with our results, would provide, for example, a convergent sequence of approximations to $p_{\rm c}$. We have also introduced an interesting new class of multiphase percolation problems, which are necessarily correlated. Our work naturally suggests the development of approximate spreading or cluster growth algorithms for correlated percolation on physical (and most easily two-dimensional) lattices, using ideas described in the introduction. Here we would retain only a finite number of conditional probabilities to determine spreading, by neglecting the influence of more distant sites. We have already undertaken a finite-size scaling analysis of correlated percolation for irreversible cooperative filling on a square lattice [17].

Acknowledgments

Ames Laboratory is operated for the US Department of Energy by Iowa State University under Contract no W-7405-ENG-82. This work was supported by the Applied Mathematical Sciences subprogram of the Office of Basic Energy Sciences.

Appendix. Higher-order •-Markovian distributions

Consider first fourth-order \bullet -Markovian distributions on Bethe lattices with z = 3. Let Q_{γ} denote the probability that the left end of configuration $\gamma = 1k$, k' with k = 0, 1, 2 (see figure 11) is *not* connected to an infinite occupied cluster. Let $g_{1k}(i)$ denote the conditional probability that *i* specific sites neighbouring the left end of 1k are occupied, and that the rest are unoccupied. Set det $g_{1k}(i) = g_{11}(1)g_{12}(2) - g_{11}(2)g_{12}(1)$. Here Q_{11} and Q_{12} are obtained as linear combinations of Q_{11} and $Q_{1'}$, and Q_{11} can be eliminated to obtain $1 - Q_{12} = h_{12}(2)(1 - 2g_{11}(1))(1 - Q_{1'})$, where $h_{12}(2) = g_{12}(2) - 2 \det g_{1k}(i)$. The $Q_{k'}$ are obtained as second-order polynomials in Q_{12} and $Q_{2'}$, and thus in $Q_{1'}$, and



Figure 11. Configurations, γ , associated with percolation quantities for fourth-order Markovian distributions on a z = 3 Bethe lattice.

 $Q_{2'}$, using the above relation. Linearisation about $\delta Q_{k'} \equiv Q_{k'} - 1$ implies that, at $p = p_c$, one has

$$0 = 1 - 2[g_{11}(1) + g_{22}(2)] + 4[g_{11}(1)g_{22}(2) + g_{21}(1)g_{12}(2)] + 8g_{21}(1) \det g_{1_{k}}(i) + 8g_{12}(2) \det g_{2_{k}}(i) - 16 \det g_{1_{k}}(i) \det g_{2_{k}}(i)$$

with $g_{2_k}(i)$ and det $g_{2_k}(i)$ defined in an analogous way to $g_{1_k}(i)$ and det $g_{1_k}(i)$ but for configurations 2k (see figure 11). For third-order \bullet -Markovian distributions $g_{jk}(i) \rightarrow g_j(i)$, so reduction of this result to (3.5) is immediate.

The percolation probability, P, can be determined from the Q_{1_k} and $Q_{k'}$ with k = 0, 1, 2. To determine the average cluster size, S, we must first evaluate the auxiliary quantities, T_{γ} , denoting the average number of occupied sites attached to the left end of $\gamma = 1k$, k' with k = 0, 1, 2. Here we just note that one can extract a pair of linear inhomogeneous equations for the $T_{k'}$ involving the same matrix as the linearised $\delta Q_{k'}$ equations, and thus incorporating the requisite divergent behaviour.

In continuing to fifth-, sixth-order, etc, \bullet -Markovian distributions, the primary quantities of interest are still calculated via auxiliary quantities (Q_{γ} giving the probability that configuration γ is *not* connected to an infinite cluster in a certain way, etc). The main complication is in the greater variety of γ that must be considered to obtain closed sets of equations for these quantities.

References

- [1] Stauffer D, Coniglio A and Adam M 1982 Advances in Polymer Science vol 44 (Berlin: Springer) pp 103-58
- [2] Stauffer D 1979 Phys. Rep. 54C 1-74; 1985 Introduction to Percolation Theory (London: Taylor and Francis)
- Müller-Krumbhaar H 1974 Phys. Lett. 50A 27-9
 Coniglio A, Nappi C, Peruggi F and Russo L 1977 J. Phys. A: Math. Gen. 10 205-28
 Heermann D W and Stauffer D 1981 Z. Phys. B 44 339-44
- [4] Kawasaki K 1971 Phase Transitions and Critical Phenomena vol 2, ed C Domb and M S Green (New York: Academic) p 443
- [5] Evans J W, Burgess D R and Hoffman D K 1983 J. Chem. Phys. 79 5011-22; 1984 J. Math. Phys. 25 3051-63
 - Evans J W, Bartz J A and Sanders D E 1986 Phys. Rev. A 34 1434-48
- [6] Kertész J, Chakrabarti B K and Duarte J A M S 1982 J. Phys. A: Math. Gen. 15 L13-8
- Bunde A, Herrmann H J, Margolina A and Stanley H E 1985 Phys. Rev. Lett. 55 653-6
 Grassberger P 1985 J. Phys. A: Math. Gen. 18 L215-9; 1986 J. Phys. A: Math. Gen. 19 L241-6
- [8] Fisher M E and Essam J W 1961 J. Math. Phys. 2 609-19
- [9] Harris T E 1948 Ann. Math. Stat. 19 474-94
- [10] Gonzalez J J and Hemmer P C 1977 J. Chem. Phys. 67 2496-508
- [11] Evans J W 1948 J. Math. Phys. 25 2527-32
- [12] Kikuchi R 1970 J. Chem. Phys. 53 2713-8
 Coniglio A 1975 J. Phys. A: Math. Gen. 8 1773-9; 1976 Phys. Rev. B 13 2194-207
 Murata K K 1979 J. Phys. A: Math. Gen. 12 81-9
- [13] Evans J W 1987 J. Chem. Phys. 87 3038-48
 Evans J W and Nord R S 1987 J. Vac. Sci Technol. A 5 1040-4
- [14] Fowler R and Guggenheim E A 1965 Statistical Thermodynamics (Cambridge: Cambridge University Press)
- [15] Plate N A and Noah O V 1979 Adv. Polym. Sci. 31 133-73
 Nord R S, Hoffman D K and Evans J W 1985 Phys. Rev. A 31 3820-30
- [16] Harder H, Bunde A and Dieterich W 1986 J. Chem. Phys. 85 4123-8
- [17] Evans J W and Sanders D E 1988 J. Vac. Sci. Technol. A 6 to be published; 1988 in preparation