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An Improved Upper Bound for the Hexagonal Lattice Site Percolation Critical Probability

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The hexagonal lattice site percolation critical probability is shown to be at most 0.79472, improving the best previous mathematically rigorous upper bound. The bound is derived by using the substitution method to compare the site model with the bond model, the latter of which is exactly solved. Shortcuts which eliminate a substantial amount of computation make the derivation of the bound possible.

1. Introduction

Percolation models are popular in the physical sciences as models exhibiting phase transitions and critical phenomena. Since their introduction by Broadbent and Hammersley [1], considerable progress has been made in both theory and applications. The monographs by Grimmett [4] and Kesten [7] describe the mathematical theory, while discussions of physical applications are available in books by Efros [3], Sahimi [10], Stauffer [12], and in the collection [2]. A major focus of interest in a percolation model is the critical probability, which is viewed as a phase transition point. The critical probability has been exactly determined for only a few percolation models. Finding exact solutions and deriving improved bounds for unsolved lattices are important and challenging problems. This paper improves the upper bound for the hexagonal lattice site percolation critical probability. Definitions of site and bond percolation models and the critical probability, and a summary of previous critical probability bounds for the hexagonal lattice, are provided in Section 2. The improved upper bound is derived by the substitution method. The substitution method was introduced by Wierman [15] to find mathematically rigorous bounds for critical probabilities in bond percolation models. The method allows us to derive information by comparing the percolative behaviour of two different lattices, typically comparing an unsolved model with a solved one to obtain bounds in the unsolved case. The method has been used to improve the best previous upper and lower bounds for the Kagomé lattice and square-octagon lattice bond models in Wierman [15]

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and to establish equality of critical exponents in the triangular and hexagonal lattice bond models in Wierman [16]. The method was adapted to site models in Wierman [17], improving the upper bound for the square lattice site model, although the two-phase approach used was quite cumbersome computationally. This paper introduces a simpler approach, which for the first time uses the substitution method to compare the site and bond models on the same lattice. Since the substitution method is described in [15], [16] and [17], its important features are only briefly reviewed in Section 3. The new upper bound for the hexagonal lattice site percolation model is derived and proved in Section 4, improving the value from 0.8079 to 0.79472. (Note that the best lower bound is 0.6527 and the value is estimated to be approximately 0.6962.) To accomplish this, a new technique for carrying out the computations is required. The previous relatively straightforward technique is impractical in this case, requiring the derivation and solution of an enormous set of polynomial equations. The new technique substantially reduces the number of equations to be solved to a manageable level, by identifying classes of equations that can be eliminated from consideration. Finally, concluding remarks are given in Section 5.

2. Preliminaries

2.1. Percolation models

A site percolation model consists of an infinite graph G, where each vertex is randomly labelled independently *open* with probability s, $0 < s < 1$, and *closed* otherwise. After the vertices are labelled, each edge is labelled *open* if and only if both its endpoint vertices are open. The *open cluster* containing the vertex $v \in G$, denoted C_v, is the set of all vertices that can be reached from v through a path of open edges and vertices. A bond percolation model is defined similarly, with the randomness associated with the edges rather than the vertices, which are all considered to be open. The *critical probability* of the site percolation model on G, denoted $p_c(G \text{ site})$, is defined by

$$p_c(G \text{ site}) = \inf\{s : P_s[|C_v| = \infty] > 0\},$$

where $|\cdot|$ denotes cardinality and P_s denotes the probability measure on site configurations on G corresponding to parameter value s. The bond percolation critical probability, defined similarly, is denoted $p_c(G \text{ bond})$. In this paper, we assume that G is connected, so $p_c(G \text{ site})$ and $p_c(G \text{ bond})$ are both independent of the choice of v.

2.2. Previous results

Percolation on the hexagonal lattice has been well studied over the past forty years. The exact critical probability value of the bond percolation model, $1 - 2\sin(\pi/18) \approx 0.6527$, was conjectured by Sykes and Essam [13] and proved by Wierman [14]. However, rigorous bounds for the site model critical probability are still quite loose. Since Hammersley [6] proved that $p_c(G \text{ bond}) \leqslant p_c(G \text{ site})$ for every G, the exact solution for the bond model gives a lower bound of 0.6527 for the site model, but there has been no improvement in this lower bound since 1981. An upper bound of 0.807901 was established by Łuczak and Wierman [8], who used a grouping method to show that the square root of the Kagomé lattice site model critical probability is an upper bound. In the physics literature,

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Stauffer [12] provided a Monte Carlo simulation estimate of 0.6962 and Shalitin [11] gave a heuristic method which derives a conjectured upper bound of 0.7072. This paper's upper bound of 0.79472 reduces the difference from the estimated value by nearly 12%, and the difference between the upper and lower bounds by more than 8%.

3. Application of the substitution method

To apply the substitution method, a graph G is decomposed into isomorphic copies of a subgraph, and the connectivity of a random graph on the subgraph is analysed. To have independent randomness in the various subgraphs, the decomposition must produce edge-disjoint subgraphs for a bond model, while the subgraphs must correspond to disjoint sets of vertices in the site model.

3.1. The substitution region

To compare the site and bond models on the hexagonal lattice, denoted by $\mathscr{H}$, it is useful to subdivide certain edges of $\mathscr{H}$ to provide a subgraph that satisfies both requirements. Given a hexagonal cycle in $\mathscr{H}$, subdivide each of the six edges which are incident to exactly one vertex of the cycle, replacing each such edge by two 'half-edges' in series, with the new vertex considered to be open with probability one in the site model. (See Figure 1.) In the bond model with parameter p, let each half-edge be open with probability $b = \sqrt{p}$, producing a model equivalent to the original bond model (in terms of probabilities of open connections between the original vertices). The desired subgraph comprises the central hexagon together with the six incident half-edges, providing both edge-disjointness and random vertex-disjointness of the regions in the decomposition. This graph has six vertices – those inserted in the subdivision – through which paths in the lattice may enter or exit the subgraph, and thus are called 'boundary vertices'.

3.2. Partitions

Consider a fixed subgraph H in this decomposition. Denote its six boundary vertices by A, B, C, D, E, F, listed clockwise around the hexagon. (See Figure 1.) Any configuration (*i.e.*, designation of edges or vertices as open or closed) on H determines a partition of the boundary vertices into clusters of vertices that are connected by open edges. Each such 'boundary partition' may be denoted by a sequence of vertices and vertical bars, where vertices are in distinct open clusters if and only if they are separated by a vertical bar. For example, $ABDF|C|E$ indicates that, within H, the vertices A, B, D and F are in the same open cluster, but C and E are each in separate clusters. Note that this partition has positive probability in the bond model, but zero probability in the site model.

The bond percolation and site percolation models on $\mathscr{H}$ each assign probability to each configuration on H. The probability, $P_b^B(\pi)$ or $P_s^S(\pi)$ respectively, for the partition π is determined by summing the probabilities of all configurations that produce the partition π of the boundary vertices. The set of boundary partitions is a partially ordered set (poset). A partition π is a *refinement* of σ, denoted $\pi \leqslant \sigma$, if every cluster in π is contained entirely in a cluster of σ. Equivalently, π is a refinement of σ if every cluster in σ is a union of

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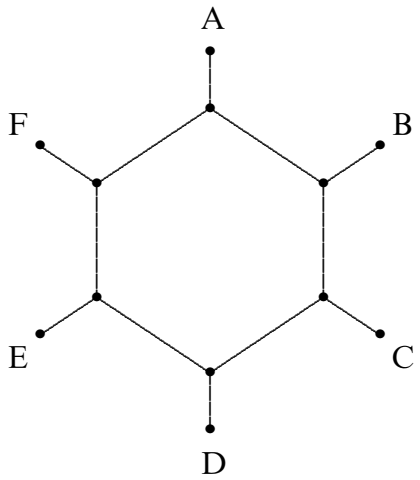


Figure 1 The subgraph H of the subdivided hexagonal lattice. Unlabelled vertices are vertices of the original hexagonal lattice. Labelled vertices were inserted when subdividing the edges. The edges between labelled and unlabelled vertices are the 'half-edges' created by subdividing original edges

clusters in π. The set of boundary partitions ordered by refinement is called the *partition lattice*.

3.3. Comparison by stochastic ordering

The substitution method compares percolation models through a comparison by stochastic ordering of probability measures on the partition lattice. An *upset* in a poset S is a subset $U \subset S$ such that if $g \geqslant f$ and $f \in U$, then $g \in U$. If P and Q are two probability measures on S, then P is *stochastically smaller than* Q, denoted $P \leq_{st} Q$, if $P(U) \leqslant Q(U)$ for every upset U. To compare the hexagonal lattice bond and site models, we compare $P^B_{b_0}$ and P^S_s, with the parameter for the bond model set at criticality, *i.e.*, $b_c = \sqrt{1 - 2\sin(\pi/18)}$. Then any value of s satisfying $P^B_{b_c} \leq_{st} P^S_s$ is an upper bound for p_c(Hexagonal site), so we seek the smallest such value s. For justification of this procedure by standard results relating stochastic ordering and coupling, see Section 2 of Wierman [17].

4. Derivation and proof

In this section, we derive and prove the following upper bound for the site percolation critical probability of the hexagonal lattice.

Theorem 4.1. $p_c(\textit{Hexagonal site}) < 0.79472$.

The result is proved by checking that the stochastic ordering $P^B_{b_c} \leq_{st} P^S_s$ holds when $s = 0.79472$. To establish this, we verify that $P^B_{b_c}(U) < P^S_s(U)$ for all nontrivial upsets U when $s = 0.79472$. Since all upset probability functions are polynomials, and thus

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continuous, the inequalities are also satisfied for slightly smaller values of s, which establishes the strict inequality in Theorem 4.1.

4.1. Computational approach

A convenience in the derivation of the bound is an alternate characterization of the solution of the upset inequalities.

Proposition 4.2. *The minimum s for which P_s^S is stochastically larger than $P_{b_c}^B$ is equal to the maximum solution for s among all upset equations $P_{b_c}^B(U) = P_s^S(U)$.*

Proof. Let U be an upset. $P_s^S(U)$ is a nondecreasing function of s. (This follows from a standard coupling argument.) Thus, there is a unique parameter value s_U, for which

$$P_{b_c}^B(U) = P_{s_U}^S(U)$$

and

$$P_{b_c}^B(U) \leqslant P_s^S(U) \text{ for } s > s_U.$$

If s is the maximal solution of the upset equations, all upset inequalities hold. For any smaller s, at least one of the inequalities will not be satisfied. □

To implement this straightforward computational approach, one must compute the probability (which is a polynomial function of the parameter) for each partition in each model, determine the structure of the partition lattice and collection of all upsets, and then solve all the upset equations to find the maximum solution. However, this approach is quite impractical for our problem. To see this, consider the fact that 90 of the 203 partitions have exactly 3 clusters, and thus are mutually incomparable in the partition lattice. Each subset of these partitions generates a distinct upset (consisting of the maximal element and all partitions above any partition in the subset). Thus, there are at least $2^{90} > 10^{27}$ upset equations to solve. The method of this paper eliminates the need to solve such a large number of upset equations.

4.2. Computing partition probability functions

Computation of the partition probability functions is straightforward and tedious. Owing to the symmetry of the hexagonal substitution region, there is a substantial reduction in the number of different partition probability functions. While there are 203 distinct partitions, 129 of them form 21 classes, $\mathscr{C}_i, i = 1, 2, 3, \ldots, 21$, such that, within each class, all partitions have identical nonzero probability functions in the bond percolation model P_b^B. (The other 74 partitions have probability zero under P_b^B, but they may be ignored in our calculation.) Notice that class $\mathscr{C}_{16}$ is split into two subclasses, labelled $\mathscr{C}_{16a}$ and $\mathscr{C}_{16b}$, for technical reasons explained in the following subsection. The common probability function for partitions in $\mathscr{C}_i$ will be denoted by $B_i(b)$, for $i = 1, 2, 3, \ldots, 21$. As for the bond model, many partitions have probability zero under P_s^S, while the others may be classified into 7 classes. Each of these seven classes is one of the 21 classes under P_b^B. The common site percolation probability function will be denoted by $S_i(s)$ for class $\mathscr{C}_i$. A complete list of partitions in the 21 classes, and their probability functions, is given in the Appendix.

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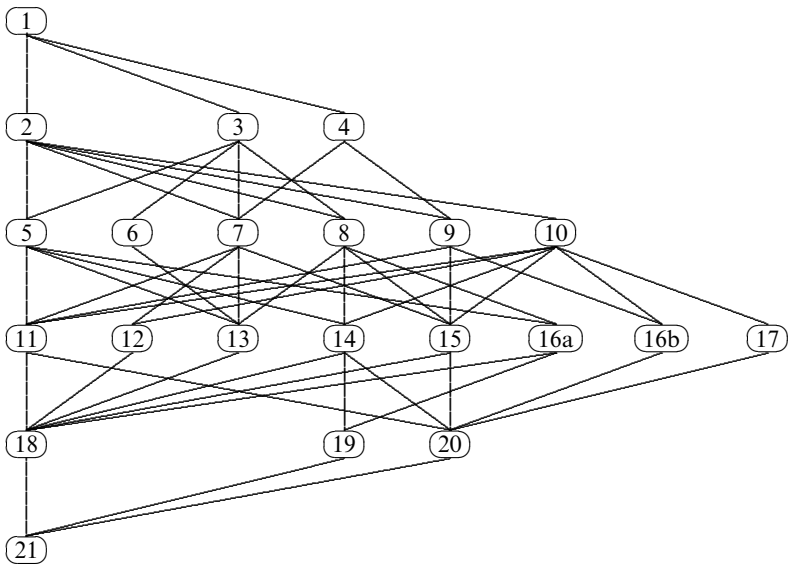


Figure 2 The Hasse diagram of the poset of classes $\mathscr{C}_i$, $1 \leqslant i \leqslant 21$, with each class represented by an oval containing its index

4.3. The class poset

The set of partition classes $\{\mathscr{C}_i : 1 \leqslant i \leqslant 21\}$ may be viewed as a partially ordered set $(\mathscr{C}, <)$, where $\mathscr{C}_i < \mathscr{C}_j$ if and only if there exist partitions $\pi_i \in \mathscr{C}_i$ and $\pi_j \in \mathscr{C}_j$ with $\pi_i < \pi_j$. We must treat the subclasses $\mathscr{C}_{16a}$ and $\mathscr{C}_{16b}$ as separate elements of the class poset, in order to satisfy the transitivity property of a partially ordered set. The Hasse diagram of the poset $(\mathscr{C}, <)$ is shown in Figure 2. This poset will be the object of study of our first calculation, which gives an initial candidate for the upper bound.

4.4. Effect of including partitions

For convenience, we simplify notation for the probability measures on the partition lattice. Define

$$\beta(A) = P^B_{\sqrt{1-2\sin(\pi/18)}}(A)$$

for any set A of boundary partitions, for the probability measure corresponding to the bond model at criticality. Corresponding to the parametrized family of site models, define

$$\sigma(A, s) = P^S_s(A).$$

With this notation, for each upset U, s_U is the solution of the upset equation

$$\sigma(U, s) = \beta(U).$$

We begin by investigating the effect on the solution of the upset equation due to including additional partitions in an upset.

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Lemma 4.3. *Let $U \neq \mathscr{P}$ be an upset and A be a set of partitions disjoint from U.*
(a) *If $\sigma(A, s_U) < \beta(A)$, then $s_{U \cup A} > s_U$.*
(b) *If $\sigma(A, s_U) > \beta(A)$, then $s_{U \cup A} < s_U$.*

Proof. By the definition of s_U, we have $\sigma(U, s_U) = \beta(U)$. For part (a),

$$\begin{aligned} &\sigma(U \cup A, s_U) \\ &= \sigma(U, s_U) + \sigma(A, s_U) \\ &< \beta(U) + \beta(A) \\ &= \beta(U \cup A). \end{aligned}$$

Since σ is an increasing function of the parameter s, the solution $s_{U \cup A}$ must be larger than s_U. Part (b) follows similarly. □

The goal of our computations is to find the largest solution s_U over all nontrivial upsets U. Owing to the large number of upsets, we prefer to work with partitions, rather than upsets, as much as possible.

4.5. Completion of upsets

Lemma 4.3 provides a basis for deciding whether we prefer to include or exclude certain partitions from our upset. We first apply Lemma 4.3 with the fact that many classes of partitions have zero probability in all probability measures P_s^S corresponding to the site model. We can always increase s_U by increasing U to include partitions with zero probability under all site models. As long as the resulting set of partitions remains an upset, this generates valid solutions s_U for determining an upper bound for the site percolation critical probability. For a fixed upset U, define the completion of U, denoted by U^C, by

$$U^C = U \cup \{\pi \in \mathscr{P} : \sigma(\pi, s) = 0 \ \forall s, \sigma(\gamma, s) = 0 \ \forall s \ \forall \gamma \geqslant \pi, \gamma \notin U\}.$$

Then U^C is an upset, and by application of Lemma 4.3, $s_{U^C} \geq s_U$ for every upset U. Thus, in computing the upper bound, we need only find the maximum solution over all completions of upsets. This fact substantially reduces the number of upsets that need to be considered.

4.6. Constructing a candidate upset

In order to construct the optimal upset, we will first construct an upset that is intended to approximate the upset corresponding to the maximum solution. This 'candidate' upset is the solution to a restricted problem where we consider maximizing s_U over all upsets that are unions of equivalence classes $\mathscr{C}_i$. This restricted problem is relatively easy because of the simple structure of the subposet of equivalence classes with nonzero site model probabilities, with a small number of upsets. This structure is illustrated in Figure 3.

To find our candidate upset, we calculate s_{U^C} for all upsets U generated by the classes $\mathscr{C}_i$, $i = 1, 2, 5, 11, 12, 18$ which have nonzero probability functions for the site model: see Table 1.

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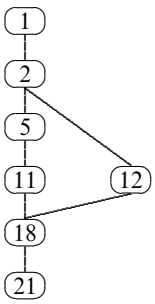


Figure 3 The subposet of classes of partitions that have positive probability in the site model. Each class is represented by an oval containing its index

Table 1

Upset classes	Classes in completion	Solution
1	1, 3, 4, 6	0.73006
1, 2	1, …, 4, 6, …, 10, 15, 17	0.75125
1, 2, 5	1, …, 10, 13, …, 17, 19	0.79472
1, 2, 5, 12	1, …, 10, 12, …, 17, 19	0.77955
1, 2, 5, 11	1, …, 11, 13, …, 17, 19, 20	0.78305
1, 2, 5, 11, 12	1, …, 17, 19, 20	0.75716
1, 2, 5, 11, 12, 18	1, …, 20	0.76990

The maximum solution $s^* = 0.79472$ occurs for the upset $U^* = (\mathscr{C}_1 \cup \mathscr{C}_2 \cup \mathscr{C}_5)^C$. The remainder of the proof demonstrates that s^* is actually the maximum solution for any upset in the partition lattice $\mathscr{P}$, not just the maximum solution for upsets that are unions of classes $\mathscr{C}_i$.

4.7. Modifying the candidate upset

We continue by using Lemma 4.3 in a slightly different manner. For any set A of partitions, we may solve the inequality $\sigma(A, s) \geqslant \beta(A)$ to find an interval or union of intervals that we denote by I_A. Then, if we have an upset U and a set A of partitions disjoint from U with $s_U \in I_A$, the solution is decreased by including A, *i.e.*, $s_{U \cup A} \leqslant s_U$. Similarly, for $s_U \notin I_A$, the solution is increased by including A. Thus, we prefer to exclude A if $s_U \in I_A$ and prefer to include A if $s_U \notin I_A$. First, let us revisit the previous argument involving completions. For the classes $\mathscr{C}_i : 1 = 3, 4, 6, \ldots, 10, 13, \ldots, 17, 19, 20$, we have $\sigma(A, s) = 0 < \beta(A)\ \forall s \in [0, 1]$, so $I_{\mathscr{C}_i} = [0, 1]$. Thus, we always prefer to include these classes, which we did through the concept of completion. Secondly, we consider the classes with positive site percolation probabilities, and numerically determine the corresponding intervals, as shown in Table 2.

Thus, at the largest solution s_U found in the exploratory step, $s* = 0.79472$, we would prefer to exclude $\mathscr{C}_1$, $\mathscr{C}_2$, $\mathscr{C}_{11}$ and $\mathscr{C}_{12}$ but include $\mathscr{C}_5$ and $\mathscr{C}_{18}$. However, to preserve the

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Table 2

A	I_A
$\mathscr{C}_1$	[0.66961, 1.00000]
$\mathscr{C}_2$	[0.58805, 0.96547]
$\mathscr{C}_5$	[0.52058, 0.79382]
$\mathscr{C}_{11}$	[0.31884, 0.84099]
$\mathscr{C}_{12}$	[0.37682, 0.88771]
$\mathscr{C}_{18}$	[0.14648, 0.75063]

upset structure, partitions in $\mathscr{C}_1$ or $\mathscr{C}_2$ cannot be excluded without also excluding some partitions with site probability zero. Similarly, partitions in $\mathscr{C}_5$ cannot be included without including some partitions from $\mathscr{C}_2$, and partitions in $\mathscr{C}_{18}$ cannot be included without including some partitions from $\mathscr{C}_{11}$ and $\mathscr{C}_{12}$. We examine the effects of such exclusions and inclusions in the following two subsections.

4.8. Excluding partitions from U*

Lemma 4.4. *If upset* $U \subset U^*$, *then* $s_U < s*$.

Proof. Recall that at $s = s^*$ we would prefer to exclude partitions in $\mathscr{C}_1$ and $\mathscr{C}_2$. However, if we exclude any of them, we must also exclude some partitions that we would prefer to include. By considering sets of partitions that must be excluded together, we will see that there is no upset $U \subset U^*$ with $s_U > s^*$. Clearly, we may not exclude the partition $ABCDEF \in \mathscr{C}_1$, since it is the maximal element. The refinement relationship establishes a one-to-one correspondence between partitions in $\mathscr{C}_{13}$ and $\mathscr{C}_5$, so excluding k partitions in $\mathscr{C}_5$ requires excluding their k refinements in $\mathscr{C}_{13}$. If $\pi \in \mathscr{C}_5$ and $\pi' \in \mathscr{C}_{13}$ is the refinement of π, then for $A = \{\pi, \pi'\}$ we have numerically determined that $\sigma(A, s) < \beta(A)$ for all $s, 0 \leqslant s \leqslant 1$. Thus, excluding that set decreases the solution s_U for every upset U, and excluding k such sets, $1 \leqslant k \leqslant 6$, one at a time, decreases the solution each time. It also requires excluding partitions in $\mathscr{C}_{14}$ and $\mathscr{C}_{16}$, which would lower the solution even more. Therefore, excluding only partitions in $\mathscr{C}_5$ and their refinements produces upsets with solutions less than s^*. For each partition in $\mathscr{C}_2$ that is excluded, we must also exclude one refinement from $\mathscr{C}_5$, two from $\mathscr{C}_7$, two from $\mathscr{C}_8$, one from $\mathscr{C}_9$, one from $\mathscr{C}_{13}$, two from $\mathscr{C}_{14}$, and two from $\mathscr{C}_{15}$. We have determined numerically that such a subset A has $\sigma(A, s) < \beta(A)$ for all $s \in [0, 1]$, so repeatedly excluding such sets reduces the solution. Note that the refinement relation is not a one-to-one correspondence between $\mathscr{C}_2$ and $\mathscr{C}_5$, but at least one partition from $\mathscr{C}_5$ must be excluded for each one excluded from $\mathscr{C}_2$. If the subset of $\mathscr{C}_2$ excluded requires a larger number from $\mathscr{C}_5$ to be excluded, excluding additional partitions from $\mathscr{C}_5$ and $\mathscr{C}_{13}$ (disjoint from any already excluded) decreases the solution even further, by the same reasoning as in the earlier paragraph. Finally, excluding partitions from $\mathscr{C}_2$ also requires excluding partitions from $\mathscr{C}_{10}$, $\mathscr{C}_{16}$, $\mathscr{C}_{17}$, and $\mathscr{C}_{19}$ from U^*, but this decreases the solution further since these all have site model probability zero. Therefore, we conclude that all upsets $U \subseteq U^*$ have $s_U < s^*$. □

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Table 3

		j			
		0	1	2	3
	0	0	0	0	0
	1	0	0	0	0
	2	0	1	1	1
i	3	0	1	2	2
	4	0	2	2	3
	5	0	2	3	4
	6	0	2	4	6

4.9. Including partitions in U^*

Lemma 4.5. *If upset* $U \supseteq U^*$, *then* $s_U < s^*$.

Proof. Recall that, for $s = s^*$, we would prefer to include $\mathscr{C}_{18}$ but not $\mathscr{C}_{11}$ or $\mathscr{C}_{12}$. There are six partitions in $\mathscr{C}_{11}$ and three in $\mathscr{C}_{12}$. The brute force approach would consider each of the 2^9 subsets of these 9 partitions, determine their completions, and find the solution s_U for each completion. Since the probabilities of partitions within each class are identical, we need only consider completions of subsets of i partitions from $\mathscr{C}_{11}$ and j partitions from $\mathscr{C}_{12}$, where $0 \leqslant i \leqslant 6$ and $0 \leqslant j \leqslant 3$. Given such a subset, we determine the completion by including as many partitions from $\mathscr{C}_{18}$ and $\mathscr{C}_{20}$ as possible while still preserving upset structure. Note that refinement provides a one-to-one correspondence between partitions in $\mathscr{C}_{11}$ and $\mathscr{C}_{20}$, and a two-to-one correspondence between the six partitions in $\mathscr{C}_{18}$ and the three partitions in $\mathscr{C}_{12}$. The relationship between $\mathscr{C}_{11}$ and $\mathscr{C}_{18}$ is somewhat more complex, with each partition in $\mathscr{C}_{11}$ having two refinements in $\mathscr{C}_{18}$ and each partition in $\mathscr{C}_{18}$ having two covering partitions in $\mathscr{C}_{11}$. Note that partitions in $\mathscr{C}_{20}$ are not refinements of any partitions in $\mathscr{C}_{12}$, because blocks in $\mathscr{C}_{12}$ are pairs of neighbouring vertices. Table 3 provides the maximum number of partitions from $\mathscr{C}_{18}$ that can be included in an upset for any set of i partitions from $\mathscr{C}_{11}$ and j partitions from $\mathscr{C}_{12}$.

The entries in the table are determined mostly by a case-by-case analysis, aided by some general bounds. Clearly no partition from $\mathscr{C}_{18}$ can be included unless there are partitions from both $\mathscr{C}_{11}$ and $\mathscr{C}_{12}$ included, so the first row and first column entries are all zero. Including any $\mathscr{C}_{18}$ partition requires at least two $\mathscr{C}_{11}$ partitions, so row $i = 1$ has all zero entries. The relationship between $\mathscr{C}_{11}$ and $\mathscr{C}_{18}$ requires row i entries to be at most $i - 1$, for $i = 1, 2, \ldots, 5$. Similarly, column j entries must be at most $2j$ for $j = 0, 1, 2, 3$. The entries in each row and each column of the table must be nondecreasing. For a fixed integer value appearing in the body of the table, the largest s_U for U containing U^* will be obtained with the smallest i and j values. Thus, we need to check the following cases for (i, j): $(2, 1)$ for 1, $(4, 1)$ and $(3, 2)$ for 2, $(5, 2)$ and $(4, 3)$ for 3, $(6, 2)$ and $(5, 3)$ for 4, and $(6, 3)$ for 6: a total of eight cases. Owing to the one-to-one correspondence between $\mathscr{C}_{11}$ and $\mathscr{C}_{20}$, and incomparability of partitions in $\mathscr{C}_{12}$ and $\mathscr{C}_{20}$, we can include one partition from $\mathscr{C}_{20}$ for each partition included from $\mathscr{C}_{11}$. The numbers of partitions from each class, and the interval for which the site probability is larger, for the eight cases given in Table 4.

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Table 4

$\mathscr{C}_{11}$	$\mathscr{C}_{12}$	$\mathscr{C}_{18}$	$\mathscr{C}_{20}$	Interval
2	1	1	2	[0.27205, 0.81331]
4	1	2	4	[0.26479, 0.80423]
3	2	2	3	[0.25918, 0.81326]
5	2	3	5	[0.25837, 0.80677]
4	3	3	4	[0.25406, 0.81324]
6	2	4	6	[0.25015, 0.80246]
5	3	4	5	[0.24635, 0.80765]
6	3	6	6	[0.23070, 0.79986]

The intersection of these intervals is $[0.27205, 0.79986]$. Since s^* lies in this interval, none of the possible sets will produce a larger value if included in the upset U^*. Thus, there is no upset $U \supseteq U^*$ such that $s_U > s^*$. □

4.10. General upsets

The following proposition completes the proof of Theorem 4.1.

Proposition 4.6. *If upset* $U \neq U^*$, *then* $s_U < s^*$.

Proof. In Lemmas 4.4 and 4.5 we have treated the cases of $U \subseteq U^*$ and $U \supseteq U^*$, and we will employ those arguments to obtain the general proof. Suppose we are given an upset $U \neq U^*$ which necessarily satisfies $U \cap U^* \neq \emptyset$. Note that the intersection of two upsets is an upset, so $U \cap U^*$ is an upset contained in U^*, for which we know that $s_{U \cap U^*} < s^*$. We will now show that including any partitions from $(U^*)^c$ in $U \cap U^*$ will decrease the value of the solution, so, in particular, $s_U < s_{U \cap U^*} < s^*$. Recall that we numerically determined that the only partitions from $(U^*)^c$ that will increase the solution are included in $\mathscr{C}_{18}$ and $\mathscr{C}_{20}$. In order to include any such partitions, it is necessary to include partitions in $\mathscr{C}_{11}$ and $\mathscr{C}_{12}$ also. For any set of i partitions from $\mathscr{C}_{11}$ and j partitions from $\mathscr{C}_{12}$ we previously determined the maximum number of partitions from $\mathscr{C}_{18}$ and $\mathscr{C}_{20}$ that could be included and preserve upset structure. However, in each of the eight cases, including the additional partitions from $\mathscr{C}_{11}$, $\mathscr{C}_{12}$, $\mathscr{C}_{18}$, and $\mathscr{C}_{20}$, decreased the solution. This reasoning remains valid when considering including partitions into $U \cap U^*$ to obtain U. Preserving upset structure may reduce the maximum number of partitions from $\mathscr{C}_{18}$ and $\mathscr{C}_{20}$ that may be included for a particular i and j, but this only decreases the solution further. Therefore, for all upsets $U \neq U^*$ we have $s_U < s^*$. □

5. Conclusion

This paper shows that it is possible to greatly reduce the computations needed to determine a critical probability bound via the substitution method. The main innovation of this paper is using comparison of partition probabilities, rather than upset probabilities. This approach, which allows us to see which partitions will increase or decrease the solution, considerably improves the analysis needed to apply the substitution method, since there

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are far fewer partitions than upsets. For the hexagonal lattice site percolation model, the improved bound of 0.79472 could be computed by solving only a few polynomial equations, while the straightforward approach requires solution of at least 2^{90} upset equations. This progress suggests that the substitution method can be applied using larger regions of lattices and thus determine sharper bounds. The second innovation in this paper is comparing the site and bond percolation models on the same lattice. This comparison avoided use of a two-step procedure to find a bound for the site model. Since more bond models are exactly solved than site models, this approach has potential to improve bounds for other site models. A disadvantage of this approach is that the substitution region is enlarged to include 'half-bonds', which affect the lower bound substantially: this application did not improve the long-standing lower bound for the hexagonal lattice site model.

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Appendix

This appendix provides a listing of the partitions in each of the 21 classes of partitions considered in this paper. In class $\mathscr{C}_i$, the partitions have identical site percolation probability functions $S_i(s)$ and identical bond percolation probability functions $B_i(b)$. See Section 4.2 for a discussion of the classes and probability functions.

$\mathscr{C}_1 = \{\text{ABCDEF}\}$

$$S_1(s) = s^6$$
$$B_1(b) = 6b^{16} - 5b^{18}$$

$\mathscr{C}_2 = \{\text{ABCDE|F, ABCDF|E, ABCEF|D, ABDEF|C, ACDEF|B, BCDEF|A}\}$

$$S_2(s) = s^5 - s^6$$
$$B_2(b) = b^{13} + 4b^{15} - 6b^{16} - 4b^{17} + 5b^{18}$$

$\mathscr{C}_3 = \{\text{ABCD|EF, BCDE|FA, CDEF|AB, DEFA|BC, EFAB|CD, FABC|DE}\}$

$$S_3(s) = 0$$
$$B_3(b) = b^{14} - 2b^{16} + b^{18}$$

$\mathscr{C}_4 = \{\text{ABC|DEF, BCD|EFA, CDE|FAB}\}$

$$S_4(s) = 0$$
$$B_4(b) = b^{14} - 2b^{16} + b^{18}$$

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$\mathscr{C}_5 =$ {ABCD|E|F, BCDE|F|A, CDEF|A|B, DEFA|B|C, EFAB|C|D, FABC|D|E}

$$S_5(s) = s^4 - 2s^5 + s^6$$
$$B_5(b) = b^{10} - 2b^{13} + 2b^{14} - 8b^{15} + 5b^{16} + 8b^{17} - 6b^{18}$$

$\mathscr{C}_6 =$ {AB|CD|EF, BC|DE|FA}

$$S_6(s) = 0$$
$$B_6(b) = b^{12} - 3b^{14} + 3b^{16} - b^{18}$$

$\mathscr{C}_7 =$ {ABC|DE|F, BCD|EF|A, CDE|FA|B, DEF|AB|C, EFA|BC|D, FAB|CD|E, A|BC|DEF, B|CD|EFA, C|DE|FAB, D|EF|ABC, E|FA|BCD, F|AB|CDE}

$$S_7(s) = 0$$
$$B_7(b) = b^{11} - b^{13} - 2b^{14} - b^{15} + 4b^{16} + b^{17} - 2b^{18}$$

$\mathscr{C}_8 =$ {ACD|B|EF, BDE|C|AF, CEF|D|AB, ADF|E|BC, ABE|F|CD, BCF|A|DE, ADE|BC|F, BEF|CD|A, ACF|DE|B, ABD|EF|C, BCE|AF|D, CDF|AB|E}

$$S_8(s) = 0$$
$$B_8(b) = b^{13} - b^{14} - 2b^{15} + 2b^{16} + b^{17} - b^{18}$$

$\mathscr{C}_9 =$ {ABC|DF|E, BCD|AE|F, CDE|BF|A, DEF|AC|B, AEF|BD|C, ABF|CE|D}

$$S_9(s) = 0$$
$$B_9(b) = b^{13} - b^{14} - 2b^{15} + 2b^{16} + b^{17} - b^{18}$$

$\mathscr{C}_{10} =$ {ABCE|D|F, BCDF|E|A, ACDE|F|B, BCDF|A|C, ACEF|B|D, ABDF|C|E, ABDE|C|F, BCEF|D|A, ACDF|E|B}

$$S_{10}(s) = 0$$
$$B_{10}(b) = 2b^{12} - 2b^{13} + 2b^{14} - 8b^{15} + 3b^{16} + 8b^{17} - 5b^{18}$$

$\mathscr{C}_{11} =$ {ABC|D|E|F, BCD|E|F|A, CDE|F|A|B, DEF|A|B|C, EFA|B|C|D, FAB|C|D|E}

$$S_{11}(s) = s^3 - 2s^4 + s^5$$
$$B_{11}(b) = b^7 - 2b^{10} - 2b^{11} - 2b^{12} + 6b^{13} - 4b^{14} + 14b^{15} - 5b^{16} - 15b^{17} + 9b^{18}$$

$\mathscr{C}_{12} =$ {AB|C|DE|F, BC|D|EF|A, CD|E|FA|B}

$$S_{12}(s) = s^4 - 2s^5 + s^6$$
$$B_{12}(b) = b^8 - 4b^{11} - 2b^{12} + 4b^{13} + 4b^{14} + 4b^{15} - 7b^{16} - 4b^{17} + 4b^{18}$$

$\mathscr{C}_{13} =$ {AB|CD|E|F, BC|DE|F|A, CD|EF|A|B, DE|FA|B|C, EF|AB|C|D, FA|BC|D|E}

$$S_{13}(s) = 0$$
$$B_{13}(b) = b^8 - b^{10} - 2b^{11} - b^{12} + 5b^{14} + 6b^{15} - 8b^{16} - 4b^{17} + 4b^{18}$$

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$\mathscr{C}_{14} =$ {ACD|B|E|F, BDE|C|F|A, CEF|D|A|B, ADF|E|B|C, ABE|F|C|D, BCF|A|D|E, ADE|B|C|F, BEF|C|D|A, ACF|D|E|B, ABD|E|F|C, BCE|F|A|D, CDF|A|B|E}

$$S_{14}(s) = 0$$
$$B_{14}(b) = b^9 - b^{10} + b^{11} - 4b^{12} + 3b^{13} - 6b^{14} + 12b^{15} + b^{16} - 13b^{17} + 6b^{18}$$

$\mathscr{C}_{15} =$ {AE|BC|D|F, BF|CD|E|A, AC|DE|F|B, BD|EF|A|C, CE|AF|B|D, DF|AB|C|E, AC|EF|B|D, BD|AF|C|E, CE|AB|D|F, DF|BC|E|A, AE|CD|F|B, BF|DE|A|C}

$$S_{15}(s) = 0$$
$$B_{15}(b) = b^{10} - b^{11} - b^{12} - b^{13} + b^{14} + 5b^{15} - 3b^{16} - 3b^{17} + 2b^{18}$$

$\mathscr{C}_{16a} =$ {AD|BC|E|F, BE|CD|F|A, CF|DE|A|B, AD|EF|B|C, BE|AF|C|D, CF|AB|D|E}

$\mathscr{C}_{16b} =$ {AE|BD|C|F, BF|CE|D|A, AC|DF|E|B}

$$S_{16}(s) = 0$$
$$B_{16}(b) = b^{12} - 2b^{13} - b^{14} + 4b^{15} - b^{16} - 2b^{17} + b^{18}$$

$\mathscr{C}_{17} =$ {ACE|B|D|F, BDF|A|C|E}

$$S_{17}(s) = 0$$
$$B_{17}(b) = 3b^{11} - 6b^{12} + 3b^{13} - 6b^{14} + 10b^{15} + 3b^{16} - 12b^{17} + 5b^{18}$$

$\mathscr{C}_{18} =$ {AB|C|D|E|F, BC|D|E|F|A, CD|E|F|A|B, DE|F|A|B|C, EF|A|B|C|D, FA|B|C|D|E}

$$S_{18}(s) = s^2 - 2s^3 + 2s^5 - s^6$$
$$B_{18}(b) = b^4 - 2b^7 - 3b^8 - 2b^9 + 3b^{10} + 6b^{11} + 11b^{12} - 10b^{13} + 7b^{14} - 32b^{15} + 5b^{16} + 32b^{17} - 16b^{18}$$

$\mathscr{C}_{19} =$ {AD|B|C|E|F, BE|A|C|D|F, CF|A|B|D|E}

$$S_{19}(s) = 0$$
$$B_{19}(b) = 2b^8 - 4b^9 + 2b^{10} - 4b^{11} + 6b^{12} - 4b^{13} + 15b^{14} - 16b^{15} - 10b^{16} + 20b^{17} - 7b^{18}$$

$\mathscr{C}_{20} =$ {AC|B|D|E|F, BD|A|C|E|F, CE|A|B|D|F, DF|A|B|C|E, AE|B|C|D|F, BF|A|C|D|E}

$$S_{20}(s) = 0$$
$$B_{20}(b) = b^6 - b^7 - 2b^9 + b^{10} - 3b^{11} + 9b^{12} - 5b^{13} + 13b^{14} - 20b^{15} - 7b^{16} + 23b^{17} - 9b^{18}$$

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$$\mathscr{C}_{21} = \{\mathrm{A}|\mathrm{B}|\mathrm{C}|\mathrm{D}|\mathrm{E}|\mathrm{F}\}$$

$$S_{21}(s) = 1 - 6s^2 + 6s^3 + 3s^4 - 6s^5 + 2s^6$$

$$B_{21}(b) = 1 - 6b^4 - 6b^6 + 12b^7 + 3b^8 + 24b^9 - 18b^{10} + 12b^{11} - 71b^{12} + 60b^{13} - 93b^{14} + 112b^{15} + 69b^{16} - 156b^{17} + 57b^{18}$$

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