# An Improved Upper Bound for the Bond Percolation Threshold of the Cubic Lattice

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**Abstract**

The bond percolation threshold of the cubic lattice is shown to be less than 0.447792 by applying the approach of Wierman and McCarthy (2015) based on the containment principle and substitution method, but employing a more efficient computational method. The bound is only a slight improvement of the their uppper bound of 0.452595, and the investigation suggests that substantial further improvements are unlikely using this approach.

**Key Words:** bond percolation, percolation threshold, substitution method, cubic lattice, stochastic ordering.

## 1. Introduction

Since the introduction of percolation models by Broadbent and Hammersley (1957), they have become widely adopted by physicists and engineers as simple models for phase transitions and critical phenomena. The quantity of most interest is the percolation threshold, which is viewed as a phase transition point, such as a freezing or melting temperature. The mathematical theory is surveyed in the research monographs by Kesten (1981), Hughes (1996), Grimmett (1999), and Bollobás and Riordan (2006). Physics and engineering perspectives, respectively, are presented in the books of Stauffer & Aharony (1991) and Sahimi (1994).

### 1.1 Definitions

To describe the bond percolation model, consider a graph $G$ which has a countably infinite vertex set, is connected, and is locally-finite (i.e., each vertex has finite degree). Each edge is randomly declared to be "open" with probability $p$, where $0 \leq p \leq 1$, and is "closed" otherwise. In an application, the vertices may represent atoms, and open edges may represent bonds between them. The corresponding probability measure on configurations of edges of $G$ is denoted by $P_p$. For a vertex $v \in G$, the connected component of open edges containing $v$ is denoted by $C_v$, and is called the open cluster containing $v$. Denote the number of vertices in $C_v$ by $|C_v|$. The *bond percolation threshold*, denoted $p_c(G)$, is the unique value of the parameter $p$ such that

$$p < p_c(G) \Longrightarrow P_p[\exists v \text{ such that } |C_v| = \infty] = 0$$

and

$$p > p_c(G) \Longrightarrow P_p[\exists v \text{ such that } |C_v| = \infty] = 1$$

The exact value of the bond percolation threshold is known for relatively few graphs, and is highly dependent on the detailed structure of the graph. It is exactly known

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only for certain infinite tree graphs and a class of two-dimensional translation-invariant lattice graphs which includes the square, triangular, and hexagonal tilings of the plane. Although three-dimensional lattices are of considerable interest for physics and engineering applications, the exact bond percolation threshold value is not known for any three-dimensional lattice graph. In addition, there are very few mathematically rigorous bounds, and they are not very accurate, so finding more accurate bounds is a challenge for the theory.

The most important and most-studied three-dimensional example is the bond percolation model on the cubic lattice. The standard representation is with vertex set $\mathbf{Z}^3$, the set of ordered triples of integers. Two vertices are connected by an edge if and only if their Euclidean distance is one, i.e. if their coordinates differ in only one coordinate, by a difference of one. Given its importance, it is surprising how few rigorous bounds have been obtained for the cubic lattice bond percolation threshold, and how poor they are, as described in the following subsection.

### 1.2 Estimates and Bounds

Since nearly all mathematically rigorous results about the values of percolation thresholds deal with two-dimensional lattice models, yet three dimensional lattices are important for real-world applications, there is a long history of estimates in the physics and engineering literature. For example, in the early years of percolation theory, a simulation by Domb and Sykes (1961) estimated its bond percolation threshold as $p_c(\text{ cubic }) \approx 0.24$. Chao (1982) proposed a theory of dual lattices in three dimensions and applied it to conjecture that $p_c(\text{ cubic }) = 1/4$. With improvements in algorithms and computing power, more precision has been obtained, with a recent estimate of Wang, Zhu, Zhang, Garoni, and Deng giving $p_c(\text{ cubic }) \approx 0.24881182(10)$. A mathematically rigourous 99.9999% confidence interval, $0.2485 \leq p_c(\text{ cubic }) \leq 0.2490$, was obtained by Ball (2014).

There are only a few previous mathematically rigorous bounds, pointed out in Wierman and McCarthy (2015): The lower bound $p_c(\text{ cubic }) \geq 0.213490$ is obtained by bounding the reciprocal of the connective constant of self-avoiding walks on the cubic lattice. Campanino and Russo (1985) proved that $p_c(\text{ cubic }) < 1/2$. Since the dice lattice is a subgraph of the cubic lattice, the containment principle proves that $p_c(\text{ cubic }) \leq p_c(\text{ dice }) \leq 0.477606$, where the numerical bound was determined by Wierman, Yu, and Huang (2015).

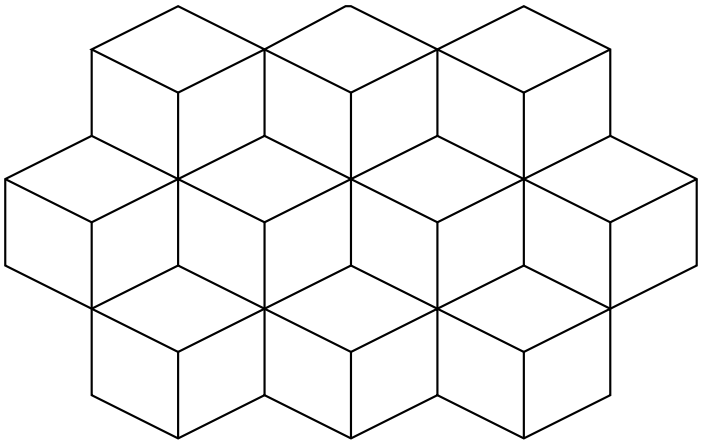

**Figure 1**: A subgraph of the dice lattice.

Wierman and McCarthy (2015) lowered the upper bound to

$$p_c(\text{ cubic }) < 0.452595.$$

The reason for concentrating on improving the upper bound is that it is much further from the estimated value than the lower bound is.

### 1.3 Result and Outline

This article improves the computational efficiency of the Wierman and McCarthy (2015) approach, using the containment principle and the substitution method, to find the slightly improved upper bound

$$p_c(\text{ cubic }) \leq 0.447792.$$

The approach, and modifications from the Wierman and McCarthy approach, are described in Section 2. The limitations of the approach are discussed in Section 3, and a possible growth process approach is mentioned.

## 2. The Improved Upper Bound

### 2.1 The Substitution Method

The substitution method has been used to derive many of the most precise rigorous bounds for percolation thresholds. It was introduced in Wierman(1990), and further developed and applied by May and Wierman (2005, 2007), Wierman (1995, 2001, 2002, 2002a), and Wierman, Yu, and Huang (2015). The method is described in Chapter 6 of Bollobás and Riordan (2006).

The substitution method compares probabilities of connections on a finite "substitution region" of a lattice for which the percolation threshold is unknown with those on a substitution region of a lattice for which the percolation threshold is exactly known, and computes mathematically rigorous bounds for the percolation threshold of the unsolved lattice. The substitution regions of the two lattices must have the same number of boundary vertices, i.e. vertices through which a path could enter or leave the region from the rest of the lattice. Each lattice must be an edge-disjoint union of isomorphic copies of its substitution region. The validity of the method relies on the equivalence of stochastic ordering and coupling in probability theory. Here we will describe the method as necessary to discuss its application to our problem.

#### *2.1.1 Substitution Regions*

We have considered several different subgraphs of the cubic lattice and compared them with different exactly-solved bond percolation models using the substitution method. In this section, we describe only the application which provided the smallest upper bound for the cubic lattice bond percolation threshold.

For our smallest upper bound, we consider a subgraph constructed from "flattened" cubes. We represent a stack of two cubes in the cubic lattice as planar "flattened cubes" as shown in Figure 2. We compute bond percolation threshold bounds for a subgraph of the cubic lattice which is isomorphic to the lattice $L$ represented in Figure 3, corresponding to sets of cubes from four levels of the cubic lattice. Neighboring cubes are in different levels so that the cubes are edge-disjoint, and thus the events of their edges being open are stochastically independent.

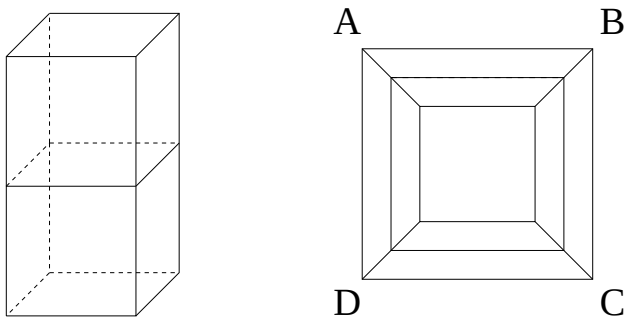


**Figure 2**: A planar representation of two cubes, for comparison to planar bond percolation models.

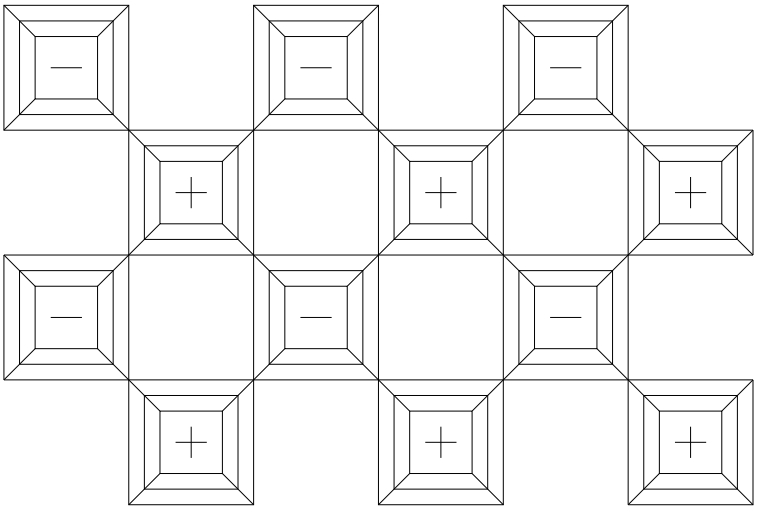

**Figure 3**: A subgraph $G$ of the cubic lattice containing some flattened cubes from four layers. Cubes marked "+" are above the $(x, y)$-plane, and cubes marked "−" are below the plane, so the cubes are edge-disjoint.

We compare the lattice $L$ with the square lattice shown in Figure 4, with the substitution region being a 4-cycle. The square lattice is also an edge-disjoint union of isomorphic copies of its substitution region graph. A celebrated result of Kesten (1981) proved that the bond percolation threshold of the square lattice is exactly $\frac{1}{2}$.

In Figures 2 and 4, the boundary vertices of the substitution regions are labelled $A$, $B$, $C$, and $D$ counterclockwise starting with the upper left corner.

### *2.1.2 Partition Probability Functions*

A *configuration* is a designation of every edge of a substitution region as open or closed. Each configuration determines a partition of the set of boundary vertices into blocks which are connected by open edges within the substitution region. A partition is denoted by listing the boundary vertices in blocks, with blocks separated by vertical bars. For example, $AB|CD$ denotes the partition in which $A$ and $B$ are in the same connected component and $C$ and $D$ are in a different connected component. The probability of a configuration is $p^m(1-p)^n$, where $m$ is the number of open edges and $n$ is the number of closed edges. The probability of a partition is the sum

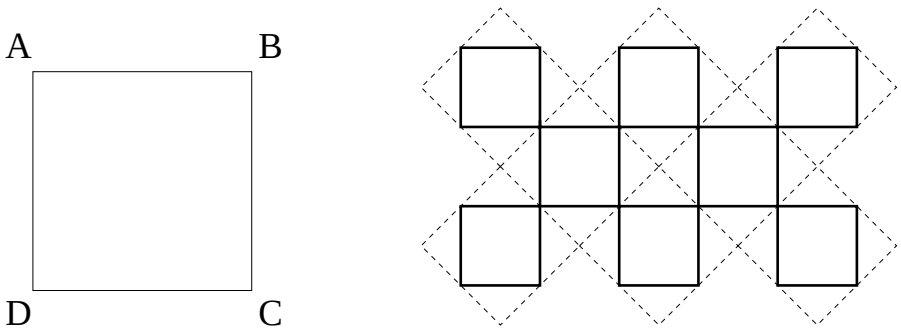


**Figure 4**: The substitution region for the square lattice (left) and the square lattice shown to be the edge-disjoint union of isomorphic copies of the substitution region (right). The dashed lines show that the entire plane may be tiled with edge-disjoint copies of the region.

of the probabilities of the configurations in it, and thus is a polynomial function of $p$.

Consideration of partitions instead of configurations considerably reduces the amount of computation required. Since there are 20 edges in the substitution region of flattened cubes, there are $2^{20} = 1{,}048{,}576$ configurations, while there are only $2^4 = 16$ configurations for the square lattice substitution region. However, there are only $Bell(4) = 15$ partitions of the boundary vertices for our substitution regions. The substitution method compares the probabilities of these 15 partitions, but must compute the partition probabilities from the configurations.

### *2.1.3 Stochastic Ordering*

The boundary partitions form a partially ordered set, ordered by refinement: $\pi \leq \nu$ if each block of $\pi$ is contained in a block of $\nu$. The resulting partially ordered set on $n$ boundary vertices is the *partition lattice* $\mathcal{P}_n$.

Stochastic ordering is used to compare the two probability measures defined on the partition lattice $\mathcal{P}_n$. A subset $U$ of $\mathcal{P}_n$ is an *upset* if $\forall f, g \in \mathcal{P}_n$, if $f \in U$ and $f \leq g$, then $g \in U$. If $P$ and $Q$ are two probability measures on a set $\mathcal{P}_n$, we say $P$ is *stochastically smaller* than $Q$, denoted $P \leq_{st} Q$, if $P(U) \leq Q(U)$ for all upsets $U$ of $\mathcal{P}_n$.

We compute probability measures on the partition lattice $\mathcal{P}_n$. A family of probabilty measures parameterized by $p$, denoted $P_p^L$, describes the connection probabilities for the substitution region for the unsolved lattice $L$. The probability measure $P^S$ describes the connection probabilities for the substitution region for the solved square lattice at its percolation threshold value $\frac{1}{2}$. Any value of $p$ for which $P^S \leq_{st} P_p^L$ is an upper bound for the percolation threshold of $G$, so we find the smallest such $p$. Similarly, the largest $p$ for which $P_p^L \leq_{st} P^S$ provides a lower bound for the percolation threshold of $L$.

Note that, although the definition of stochastic ordering involves upset probability inequalities, we may convert the problem into one of checking upset probability equations. For each non-trivial upset $U$, the partition probability function $P_p^L(U)$ is a strictly increasing function of $p$ which increases from 0 to 1, so there exists a unique solution $p_U$ to the equation $P_p^L(U) = P^S(U)$. If $p$ is greater than or equal to all the upset equation solutions, then $P_p^L \geq_{st} P^S$, while if $p$ is less than or equal

to all the upset equation solutions, $P_p^L \leq_{st} P^S$. Therefore, the upper and lower bounds for the percolation threshold of $L$ are the maximum and minimum of the upset equation solutions, respectively.

#### *2.1.4 Reduction of Computations for Checking Stochastic Ordering*

There are a couple computational reductions that make checking of stochastic ordering more efficient.

The first is restriction to partitions which are called "non-crossing," which only slightly reduces the computations. Note that, because both substitution regions are planar graphs, the partition $AC|BD$ cannot occur. This is because if A is connected to C by an open path, and C is connected to D by an open path, the paths must cross, making A, B, C, and D all connected to each other, producing the partition $ABCD$. Such a partition is called a "crossing partition." Since it has zero probability for both substitution regions, it does not play a role in any of the upset inequalities that are involved in checking stochastic ordering. Note also that, due to the form of the square lattice model's substitution region, the partitions $AC|B|D$ and $A|BD|C$ also have probability zero, but must be considered because they have non-zero probability in the two flattended cube substitution region.

The second reduction is by grouping the non-crossing partitions into classes. Within each class, each partition may be transformed into any other partition by reflection and rotation, and thus share the same partition probability function. We consider the "class lattice," a partially ordered set ordered by refinement, in which class A is a refinement of class B if there exists a partition in class A which is a refinement of a partition in class B. The Hasse diagram of the class lattice is shown in Figure 5. May and Wierman (2005) proved that the upsets in the original partition lattice which produce the smallest upper bound and the largest lower bound must correspond to upsets in the class lattice, that is, must contain either all or no partitions of each class. Reducing to seven equivalence classes decreases the number of relevant upset probability inequalities from over 400 to 8. The following provides the upset probability description for each of the 8 non-trivial upsets in the class lattice, using one representative from each class for brevity:

$P[ABCD]$
$P[ABCD] + 4P[ABC|D]$
$P[ABCD] + 2P[AB|CD]$
$P[ABCD] + 4P[ABC|D] + 2P[AB|CD]$
$P[ABCD] + 4P[ABC|D] + 2P[AB|CD] + 4P[AB|C|D]$
$P[ABCD] + 4P[ABC|D] + 2P[AC|B|D]$
$P[ABCD] + 4P[ABC|D] + 2P[AB|CD] + 2P[AC|B|D]$
$P[ABCD] + 4P[ABC|D] + 2P[AB|CD] + 4P[AB|C|D] + 2P[AC|B|D]$

### 2.2 Computing the Improved Bound

#### *2.2.1 Class Probabilities for the Square Lattice*

The partition probabilities for the square lattice bond percolation model at criticality ($p_c = \frac{1}{2}$) are easily computed by hand. Grouped into the seven classes, they are given by:

Class 1: $P^S[ABCD] = 5/16$,
Class 2: $P^S[ABC|D] = P^S[A|BCD] = P^S[ACD|B] = P^S[ABD|C] = 1/16$,
Class 3: $P^S[AB|CD] = P^S[AD|BC] = 1/16$,

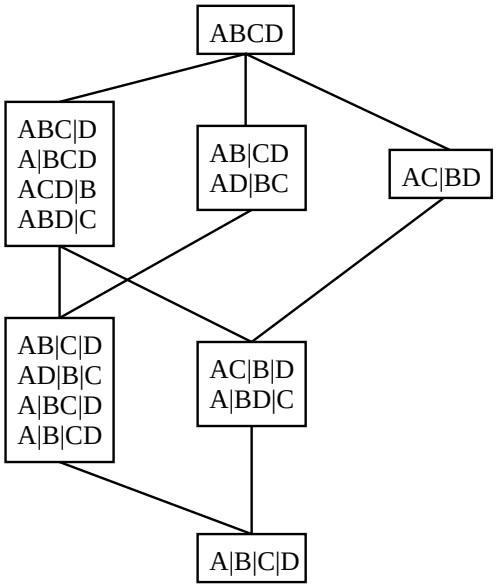


**Figure 5**: The Hasse diagram of the class lattice.

Class 4: $P^S[AC|BD] = 0$,
Class 5: $P^S[AB|C|D] = P^S[AD|B|C] = P^S[A|BC|D] = P^S[A|B|CD] = 1/16$,
Class 6: $P^S[AC|B|D] = P^S[A|BD|C] = 0$,
Class 7: $P^S[A|B|C|D] = 1/16$.

### *2.2.2 Class Probability Functions for L*

The partition probability functions for the unsolved lattice $L$ were computed using MATLAB on a Windows-based personal computer. The computational burden of doing this increases with the number of configurations, which is exponential in the number of edges in the substitution region. Using the standard approach that was employed by Wierman and McCarthy for the single flattened cube substitution region, the calculation would take approximately 10 days. The advance that allowed the improved bound to be obtained is the following conditioning approach, which performs 5 separate calculations and combines them, taking a total of approximately 13 hours.

We now describe the conditioning argument in more detail.

Suppose that three or four of the edges in the top level of the two stacked cubes are open, an event that occurs with probability $p^4 + 4p^3(1-p)$. In this event, all four vertices on the top level are connected, so we can consider them to be identified as a single vertex, as illustrated by the graph in Figure 5 at the upper left. A partition probability measure $P_4$ on partitions of the boundary vertices may be computed using this graph. Since the graph has only 16 edges instead of 20, the computational time required is much less than that for computing partition probabilities for the full substitution region.

Similarly, condition on the top level containing two adjacent open edges, two opposite open edges, one open edge, and no open edges, illustrated by the other four graphs in Figure 5. Using subscripts to denote the sizes of sets of connected vertices on the top level, we obtain partition probability measures $P_3$, $P_{2,2}$, $P_2$, and $P_0$.

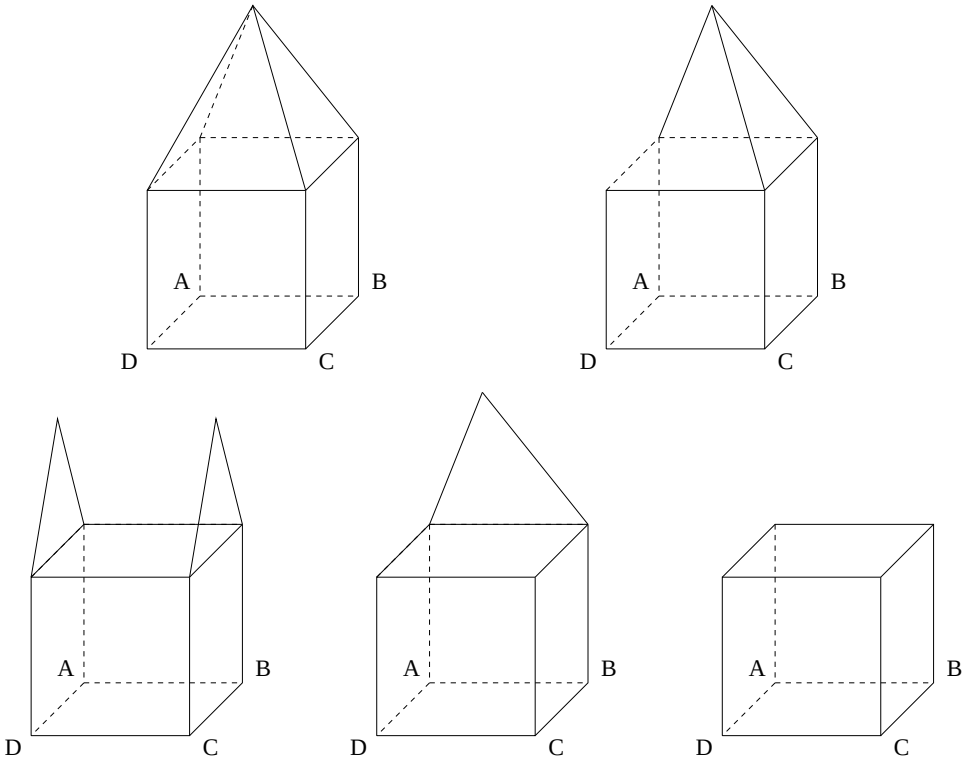


**Figure 6**: The computations are substantially reduced by conditioning on the configuration of open edges on the top level of the two cubes, with the boundary vertices being on the bottom level. There are five cases, which correspond to generators with fewer edges. Upper left: The generator equivalent to three or four of the edges open on the top level. Upper right: A generator equivalent to two adjacent open edges on the top level. Lower left: A generator equivalent to two non-adjacent open edges on the top level. Lower middle: A generator equivalent to only one open edge on the top level. Lower right: The generator equivalent to no open edges on the top level.

We desire to combine the conditional probability measures, weighted by the probabilities of their conditioning events, to obtain the probability measure for the substitution region for two flattened cubes. However, this is not completely straightforward, because rotations of the conditioning events and rotations of the partitions both need to be taken into consideration.

Two of the conditioned substitution regions – that corresponding to three or four open edges on the top level, and that corresponding to no open edges on the top level – have four-fold rotational symmetry. Therefore, within each of the the seven classes, the partitions have equal probabilities.

For the other conditioned substitution regions, which are not symmetric, partitions in a class may have unequal probabilities. For example, for the probability measure $P_3$,

$$P[ABC|D] = P[ACD|B] = 32p^{15} - 262p^{14} + 915p^{13} - 1752p^{12} + 1946p^{11} - 1179p^{10} + 264p^9 + 66p^8 - 21p^7 - 9p^6 - 2p^5 + 3p^4 - 2p^3 + p^2,$$

$$P[ABD|C] = 32p^{15} - 260p^{14} + 896p^{13} - 1671p^{12} + 1746p^{11} - 871p^{10} - 32p^9 + 231p^8 - 61p^7 - 13p^6 + p^5 + 3p^4 - 2p^3 + p^2,$$

and

$$P[A|BCD] = 32p^{15} - 260p^{14} + 896p^{13} - 1675p^{12} + 1772p^{11} - 940p^{10} + 62p^9 + 165p^8$$
$$-43p^7 - 10p^6 - p^5 + 3p^4 - 2p^3 + p^2.$$

We must consider four rotations of the measure $P_3$. Let $P_3^A$ denote the measure for the substitution region when the vertex above $A$ is not connected to the top vertex, and define $P_3^B$, $P_3^C$, and $P_3^D$ $(=P_3)$ similarly. By considering rotations of the partitions, notice that

$$P_3^A[ABC|D] = P_3^B[A|BCD],$$
$$P_3^A[ABD|C] = P_3^B[ABC|D],$$
$$P_3^A[ACD|B] = P_3^B[ABD|C],$$

and

$$P_3^A[A|BCD] = P_3^B[ACD|B].$$

Thus, the sum of the four partition probabilities in the class is the same under $P^A$ and $P^B$, and by similar reasoning, also the same as under $P^C$ and $P^D$. Similar reasoning also applies to each class, and to the probability measures $P_{2,2}$ and $P_2$.

Therefore, the desired class probability measure for the two flattened cube substitution region is given for a class $\mathcal{C}$ by

$$(4p^3-3p^4)P_4(\mathcal{C})+p^2(1-p)^2P_3(\mathcal{C})+p^2(1-p)^2P_{2,2}(\mathcal{C})+p(1-p)^3P_1(\mathcal{C})+(1-p)^4P_0(\mathcal{C}).$$

### *2.2.3 Upset Equation Solutions*

The eight class upset expressions and the solutions to the corresponding upset equations, rounded to ten decimal places, are:

$P[ABCD]$
0.4301434872

$P[ABCD] + 4P[ABC|D]$
0.4235413264

$P[ABCD] + 2P[AB|CD]$
0.4392933631

$P[ABCD] + 4P[ABC|D] + 2P[AB|CD]$
0.4320340643

$P[ABCD] + 4P[ABC|D] + 2P[AB|CD] + 4P[AB|C|D]$
0.4477916601

$P[ABCD] + 4P[ABC|D] + 2P[AC|B|D]$
0.4203424277

$P[ABCD] + 4P[ABC|D] + 2P[AB|CD] + 2P[AC|B|D]$
0.4287124239

$P[ABCD] + 4P[ABC|D] + 2P[AB|CD] + 4P[AB|C|D] + 2P[AC|B|D]$
0.4374769592

### 2.3 The Improved Bound

As mentioned previously, the smallest and largest upset probability equation solutions provide lower and upper bounds, respectively, for the percolation threshold of $L$, so (rounded down and up to six decimal place accuracy, respectively) the bounds obtained are

$$0.420334 < p_c(L) < 0.447792.$$

Since $L$ is a subgraph of the cubic lattice, by the containment principle the upper bound for $p_c(L)$ is an upper bound for the cubic lattice bond percolation threshold. The lower bound for $p_c(L)$ does not provide any information regarding $p_c($ cubic $)$, since it is a lower bound for an upper bound.

Thus, using a substitution region corresponding to two flattened cubes did improve the result of Wierman and McCarthy (2015), but only slightly, from 0.452595 to 0.447791. To extend this approach to flattening a stack of three cubes would take an estimated 5 to 6 months of computation time, with prospects of improvement of much less than 0.01.

## 3. Prospects for Future Improvement

### 3.1 Limitations of the Current Approach

Wierman and McCarthy considered future research comparing the "double-dice" lattice to other lattices to be promising. The smallest substitution region that is appropriate corresponds to one cube in the cubic lattice, and has six boundary vertices instead of four, and requires substantially more computations. MATLAB programs that were developed for the Wierman, Yu, and Huang (2015) research were applied to use the substitution method to compare the double-dice lattice to the dice lattice, hexagonal lattice, and triangular lattices. The smallest upper bound obtained was 0.459327, using a comparison to the solved hexagonal lattice bond model as the reference lattice.

It is somewhat surprising that none of these results produced a better upper bound for the cubic lattice than the smaller and simpler substitution region used in Wierman and McCarthy (2015), and that the resulting bounds remain a substantial distance from the estimated value for the threshold. For these reasons, the approach of this paper, extending the "flattened cube" substitution region to flattening two cubes was investigated.

More efficient algorithms for computing the partition probability functions and class lattices need to be developed in order to do the calculations for larger substitution regions, so substantial improvements in the upper bound for the cubic lattice are unlikely unless a new approach is found.

### 3.2 A Possible Growth Prcoess Approach

While the approach of confining comparison processes to thin slabs of the cubic lattice which are essentially two-dimensional seems unlikely to produce improvements, it suggests trying an approach that does not have such a limitation. Yu and Wierman are just beginning to examine a possible approach of this type, which lets a stochastic growth process expand through a random number of levels of the cubic lattice. The growth process will be related to the bond percolation model on the two-dimensional square lattice. Preliminary indications suggest that the approach may produce an upper bound less than 0.40.

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