Percolation threshold is not a decreasing function of the average coordination number

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It is commonly believed that the percolation critical probability is a monotonically decreasing function of the average coordination number for periodic lattice graphs in the same dimension. This paper provides counterexamples—a pair of planar lattices for which the bond percolation critical probabilities and average coordination numbers are in the same order, and a pair for which the site percolation critical probabilities and average coordination numbers are in the same order. These counterexamples confirm the existence of this counterintuitive phenomenon, which was observed in one case in numerical estimates by van der Marck.

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I. INTRODUCTION

Since the origins of percolation theory, determining the value of the critical probabilities of various lattices has been an important and challenging problem. Exact solutions are known for arbitrary trees [1] and a few periodic two-dimensional lattices: the bond percolation thresholds for the square [2], triangular and hexagonal [3], and bowtie lattice and its dual [4], the site percolation threshold for the triangular lattice [5], and various transformations of these solutions to related graphs, such as the Kagomé lattice site model and the $(3,12^2)$ lattice site model [6]. Rigorous bounds have been established in the mathematical literature. (See [7–11], and references therein.) Considerable work in the physics community has produced Monte Carlo simulation estimates (see [12] and references therein) and development of approximation formulas (see [13–16], and references therein).

A commonly accepted observation is that more richly connected lattice graphs have lower percolation thresholds. One rigorous result of this nature is Fisher's [17] containment principle: If G is a subgraph of H, then $p_c(G) \geqslant p_c(H)$, for both bond and site models. A result in the same spirit is the contraction principle [18]: If H is obtained from G by contracting edges, then $p_c(G) \geqslant p_c(H)$ for bond models. Such results, coupled with substantial numerical evidence from simulations, have led to a common belief that the critical probability is a monotonically decreasing function of the average coordination number of the lattice for lattices in the same dimension, that is, if two lattices have average coordination numbers in one order, $d(G) \leqslant d(H)$, then the percolation thresholds have the opposite order, $p_c(G) \geqslant p_c(H)$. This belief has been built in to several "universal" approximation formulas for critical probabilities in the physics literature, where the formulas based on dimension and coordination number or average coordination number all imply that the critical probability is a decreasing function of the average coordination number if the dimension is fixed (see, for example, Refs. [19–22,13]).

However, recently van der Marck [23] noted "one exception to this rule: the site percolation threshold of the pentagonal lattice (0.6471) is lower than that of the Kagomé lattice (0.6527...), although its average coordination number is lower ($3\frac{1}{3}$ vs 4)." (Note that in the mathematical literature in graph theory, the term "degree" is used, rather than "coordination number.")

II. RESULTS

This paper proves that critical probabilities and average coordination numbers of lattices in the same dimension can have the same order, for both site models and bond models.

Unfortunately, current mathematical bounds are not sufficiently accurate to verify the ordering of the pentagonal lattice and Kagomé lattice site percolation thresholds observed numerically by van der Marck.

For bond percolation, we prove that a modification of the $(3,12^2)$ lattice has critical probability between 0.69523 and 0.69825 and average coordination number $3\frac{3}{4}$, which may be compared to the hexagonal lattice, with exact percolation threshold 0.6527... and uniform degree 3. The proof, using the substitution method [24,25,9–11], is given in Sec. III.

The site percolation example is based on the bond model example. We use the result of Sec. III to show that a planar subgraph of the line graph of the modification of the $(3,12^2)$ lattice has site percolation critical probability greater than 0.69523, while its average degree is 5. This contrasts with the Kagomé lattice, which has percolation threshold equal to 0.6527... and average degree 4. The lower bound for the critical probability of the first graph is obtained by elementary reasoning involving the bond-to-site transformation and the containment principle. The proofs are given in Sec. IV.

III. BOND MODEL EXAMPLE

The exact value of the bond percolation critical probability for the hexagonal lattice, $1-2\sin(\pi/18)=0.6527...$, was conjectured by Sykes and Essam [26] and proved by Wierman [3]. We will compare the hexagonal lattice with a modification of the $(3,12^2)$ lattice, denoted L, in which we add a central vertex in each triangle, connected by an edge to each vertex of the triangle, which corresponds to replacing the triangle by a K_4 (complete graph on 4 vertices). See Figs. 1 and 2.

The lattice L contains the $(3,12^2)$ lattice, which satisfies

$$0.7385 \leqslant p_c((3,12^2) \text{ bond}) \leqslant 0.7449,$$

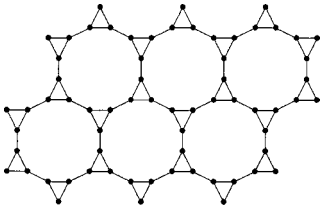

FIG. 1. An induced subgraph of the $(3,12^2)$ lattice.

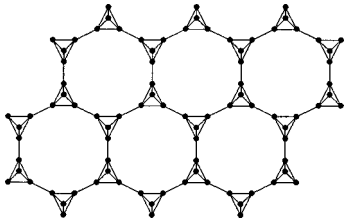

FIG. 2. An induced subgraph of the lattice L.

so it has a lower critical probability. The purpose of adding the central vertices and edges is to increase the average degree, while lowering the critical probability relatively little, keeping it above that of the hexagonal lattice.

We apply the substitution method to compute accurate bounds for the bond percolation critical probability of L. To apply the substitution method, we decompose the $(3,12^2)$ lattice into isomorphic edge-disjoint subgraphs, and substitute alternative subgraphs in order to obtain another lattice (which, in this case, is exactly solved). To facilitate this, we first subdivide each edge which connects two triangles in the $(3,12^2)$ lattice, i.e., replace it by two ''half-edges'' in series. The vertices inserted between the half-edges are called *boundary vertices*. To maintain equivalence with the bond percolation model with parameter p, each of the half-edges is open with probability $\sqrt{p}$. The lattice may then be decomposed into isomorphic subgraphs, each consisting of a K_4 with three incident half-edges. Substituting three-stars for these subgraphs produces a subdivided hexagonal lattice. See Fig. 3.

Consider subgraphs in the decompositions of L and the hexagonal lattice, with the boundary vertices of both labeled A, B, and C. To compare probabilities of open connections on the two subgraphs, we compute probabilities of partitions of the boundary vertices. A partition is denoted by a sequence of vertices and vertical bars, where vertices not separated by a vertical bar are in the same cluster.

The bond percolation model on each lattice assigns a probability to each configuration on the corresponding subgraph. We denote the probability measure corresponding to the bond percolation model on L by $P_p(\cdot)$, and the probability measure corresponding to the hexagonal lattice bond model by $Q_q(\cdot)$. A probability is determined for each partition π by summing the probabilities of all configurations which produce the partition π.

The set of partitions, ordered by refinement, form a partially ordered set: α is a refinement of β if every cluster of α is contained in a cluster of β. ABC is the maximum element and $A|B|C$ is the minimum element, and, for example, $AB|C$ is a refinement of ABC. An upset U is a set of partitions such that if α is a refinement of β and $\alpha \in U$ then $\beta \in U$. The probability of an upset is the sum of the probabilities of the partitions in the upset.

We now calculate the partition probability measures corresponding to the two bond percolation models.

To calculate the probability of the maximum partition, ABC, notice that all half-edges must be open, and then decompose the event according to the number of edges in the original triangle that are open, to obtain

$$\begin{aligned} P_p(ABC) &= p^{3/2}\{p^3+3p^2(1-p)+3p^2(1-p)^2 \\ &\quad \times[p^2+2p(1-p)]+p^3(1-p)^3\} \\ &= 3p^{7/2}+5p^{9/2}-18p^{11/2}+15p^{13/2}-4p^{15/2}. \end{aligned}$$

A similar (somewhat more complicated) decomposition into cases and simplification yields

$$P_p(AB|C)=P_p(AC|B)=P_p(BC|A)=p^2-p^{5/2}+2p^3+p^{7/2}+5p^{9/2}-7p^5-11p^{11/2}+7p^6+8p^{13/2}-2p^7-2p^{15/2}.$$

To calculate $P_p(A|B|C)$, decompose the event according to the number of half-edges that are open, to obtain

$$\begin{aligned} P_p &= (A|B|C) \\ &= p^{3/2}[3p(1-p)^5+(1-p)^6]+3p(1-p^{1/2}) \\ &\quad \times[2p(1-p)^3(1+2p-2p^2) \\ &\quad +3p(1-p)^5+(1-p)^6]+3p^{1/2}(1-p^{1/2})^2+(1-p^{1/2})^3 \\ &= 1-3p^2-6p^3+6p^{7/2}+10p^{9/2}+21p^5-36p^{11/2} \\ &\quad -21p^6+30p^{13/2}+6p^7-8p^{15/2}. \end{aligned}$$

We compare this distribution with that determined by the bond model on the subdivided hexagonal lattice, denoted Q_q:

$$Q_q(ABC)=q^3,$$

$$Q_q(AB|C)=Q_q(AC|B)=Q_q(BC|A)=q^2(1-q),$$

$$Q_q(A|B|C)=(1-q)^3+3q(1-q)^2.$$

The probability measures P_p and Q_q are compared by stochastic ordering: If P and Q are two probability measures on the same partially ordered set S, then P is stochastically

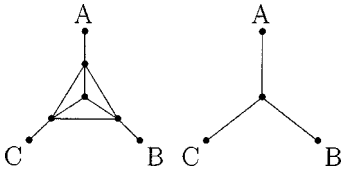

FIG. 3. The substitution used in deriving the bound for the bond percolation critical probability of L. L is decomposed into copies of the subgraph shown on the left, while the subdivided hexagonal lattice is decomposed into copies of the subgraph shown on the right. The boundary vertices are labeled A, B, and C.

smaller than Q, denoted $P \leqslant_{st} Q$, if $P[U] \leqslant Q[U]$ for every upset U of S. The set of probability measures on S are partially ordered by stochastic ordering.

Set q equal to the critical probability of the subdivided hexagonal lattice, i.e.,

$$q_0 = \sqrt{1-2\sin(\pi/18)} = 0.8079\ldots .$$

By standard arguments relating coupling and stochastic ordering, if $P_p \leqslant_{st} Q_{q_0}$, then p is less than or equal to the critical probability of L, and if $P_p \geqslant_{st} Q_{q_0}$ then p is greater than or equal to the critical probability of L. Thus, our lower and upper bounds are the maximum value of p for which $P_p[U] \leqslant Q_{q_0}[U]$ for all nontrivial upsets U, and the minimum value of p for which $P_p[U] \geqslant Q_{q_0}[U]$ for all nontrivial upsets U, respectively. Equivalently, the lower and upper bounds are the smallest and largest (respectively) solutions for p of the equations

$$P_p[U] = Q_{q_0}[U]$$

for nontrivial upsets U.

The nontrivial upsets consist of the partition ABC and 0, 1, 2, or 3 of the partitions $AB|C$, $AC|B$, and $BC|A$. Thus, there are only four different upset equations, with the form

$$P_p(ABC) + iP_p(AB|C) = Q_{q_0}(ABC) + iQ_{q_0}(AB|C),$$

for $i = 0, 1, 2, 3$.

Using the bounds

$$0.807900764 \leqslant \sqrt{1-2\sin(\pi/18)} \leqslant 0.807900765,$$

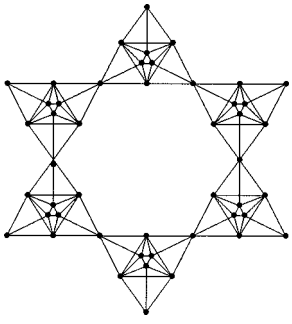

FIG. 4. An induced subgraph of the line graph of L.

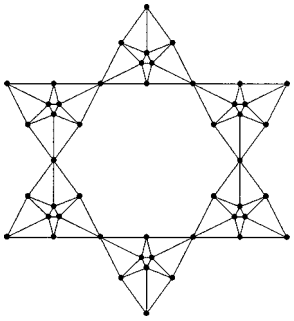

FIG. 5. A planar subgraph of the line graph of L.

we obtain the following bounds for the solutions of the upset equations, with s_i, $i = 0, 1, 2, 3$, denoting the solutions:

$$0.69523 \leqslant s_0 \leqslant 0.69524,$$

$$0.69582 \leqslant s_1 \leqslant 0.69583,$$

$$0.69671 \leqslant s_2 \leqslant 0.69672,$$

$$0.69824 \leqslant s_3 \leqslant 0.69825.$$

Thus, taking the lower bound for s_0 and the upper bound for s_3, we obtain

$$0.69523 \leqslant p_c(L_1) \leqslant 0.69825.$$

IV. SITE MODEL EXAMPLE

We first note that the lattice L and the hexagonal lattice are a pair of graphs with site percolation critical probabilities and average degrees in the same order: Wierman [10] showed that the site percolation critical probability of the hexagonal lattice is less than 0.79472. L has site percolation threshold equal to that of the $(3,12^2)$ lattice, because the vertex at the center of each triangle of the $(3,12^2)$ lattice is not essential to the creation of an infinite open cluster, i.e., if there is an infinite open cluster, there is an infinite open cluster using only the vertices of the $(3,12^2)$ lattice. Thus the addition of the central vertices in the triangles merely serves to raise the average degree, without contributing to percolative behavior. For this reason, this example is unsatisfying, and we provide a more substantive example.

The bond-to-site transformation converts the bond percolation model on a graph G into an equivalent site percolation model on a different graph G^*, called the *line graph* (in the mathematical literature) or the *covering graph* (in the physics literature). Applying the bond-to-site transformation to the graphs in Sec. III, we obtain the Kagomé lattice as the line graph of the hexagonal lattice, and the graph shown in Fig. 4 as the line graph of L. By the equivalence, the Kagomé lattice site percolation critical probability is 0.6527... and the site percolation critical probability of the line graph of L is greater than 0.69523. Since the Kagomé lattice has uniform degree 4 and the line graph of L has average degree equal to 5.6 (since 60% of the vertices have degree 6, while 40% have degree 5), the site percolation critical probabilities and average degrees are in the same order.

Note that the line graph of L is not planar, however, since there are three pairs of crossing edges in each subgraph cor-

responding to the substitution region in Fig. 3. For an example involving only planar graphs, delete the three crossing edges that form a triangle (see Fig. 5). The resulting graph has site percolation critical probability larger than that of the line graph of L (by the containment principle), so it is larger than that of the Kagomé lattice. Its average degree is 4.8 (40% of vertices have degree 4, 40% have 5, and 20% have 6), which is also larger than that of the Kagomé lattice.

V. CONCLUDING REMARKS

For more than four decades, intuition has suggested that more richly connected lattices have lower percolation thresholds. One specific interpretation of this statement is that the percolation threshold is a decreasing function of the average coordination number. However, while the statement is true in most cases, this paper shows that it is not always true. Thus, some refinement of the (usually correct) intuition is called for.

Toward this end, one may view the counterexample as an indication that variability in bond density may increase the percolation threshold. In the counterexample, one lattice has relatively uniform density, while the other has regions of high density linked across sparse regions. The sparse regions may act as bottlenecks which tend to impede the formation of large clusters, while the dense regions increase the average coordination number without greatly affecting connectivity.

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