Tight Lower Bound for Percolation Threshold on an Infinite Graph

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We construct a tight lower bound for the site percolation threshold on an infinite graph, which becomes exact for an infinite tree. The bound is given by the inverse of the maximal eigenvalue of the Hashimoto matrix used to count nonbacktracking walks on the original graph. Our bound always exceeds the inverse spectral radius of the graph's adjacency matrix, and it is also generally tighter than the existing bound in terms of the maximum degree. We give a constructive proof for existence of such an eigenvalue in the case of a connected infinite quasitransitive graph, a graph-theoretic analog of a translationally invariant system.

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Percolation theory is well established in physics as an effective approach for dealing with strong disorder. Examples include problems like quantum or classical transport [1], bulk properties of composite materials [2], and diluted magnetic transitions [3]. Percolation is also an important phase transition in its own right [4–6].

An ability to process and store large amounts of information led to an emergence of big data in many areas of research and applications. This caused a renewed interest in graph theory as a tool for describing complex connections in various kinds of networks: social, biological, technological, etc. [7–11]. In particular, percolation on graphs has been used to describe Internet stability [12,13], spread of contagious diseases [14–16], and computer viruses [17]; related models describe market crashes [18] and viral spread in social networks [19–21]. Percolation has also been linked to decoding thresholds in certain classes of quantum error-correcting codes [22,23].

In a graph, a *degree* of a vertex is the number of its neighbors. Degree distribution is a characteristic easy to extract empirically. A simple approach to network modeling is to study random graphs with the given degree distribution [12,13,24–26]. In the absence of correlations, the site percolation threshold on such a random graph is [12,13,24,25]

$$p_c = \frac{\langle d\rangle}{\langle d^2\rangle - \langle d\rangle}, \tag{1}$$

where $\langle d^m\rangle \equiv \sum_i d_i^m/n$ is the mth moment of the vertex degree distribution and n is the number of vertices in the graph. While this result is very appealing in its simplicity, Eq. (1) has no predictive power for any actual network where correlations between degrees or enhanced connectivity ("clustering") of nearby vertices may be present. Substantial effort has been spent on attempts to account for such correlations [27–30] in random graphs. However, such approaches can only account for local correlations and are flawed when applied to artificial networks like the power grid, which may have a carefully designed robust backbone (e.g., as in Example 1). Such strong correlations make Eq. (1) or its versions accounting for local correlations seemingly irrelevant.

There are only a handful of results on percolation for general graphs [31,32]. These include the exact lower bound for the site percolation threshold for any graph with the maximum vertex degree $d_{\max}$ [33],

$$p_c \geq (d_{\max} - 1)^{-1}, \tag{2}$$

which coincides with that for the bond percolation [32]. Both bounds are achieved on d-regular tree $\mathcal{T}_d$. Unfortunately, for graphs with wide degree distributions, Eq. (2) may underestimate the percolation threshold by far.

An estimate of the percolation threshold for dense graphs (with some conditions) as the inverse *spectral radius* of the graph, $\rho(\mathcal{G}) \equiv \rho(A_{\mathcal{G}})$, defined as the maximum magnitude of an eigenvalue of its adjacency matrix, $A_{\mathcal{G}}$, has been suggested in Ref. [34]. Unfortunately, the conditions are rather restrictive, and the estimate is clearly not very accurate for sparse degree-regular graphs where the spectral radius $\rho(\mathcal{G}) = d$, as this estimate never reaches the lower bound in Eq. (2).

Example 1.—Consider a tree graph $\mathcal{T} \equiv \mathcal{T}_{d;r,L}$ constructed by attaching r chains of length L to each vertex of a d-regular tree $\mathcal{T}_d$; see Fig. 1. The percolation threshold coincides with that of $\mathcal{T}_d$, $p_c = p_c(\mathcal{T}_d) = (d-1)^{-1}$. On the other hand, Eq. (1) gives $p_c \to 0$ if we take $L = 1$,

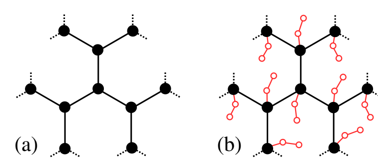

FIG. 1 (color online). (a) A d-regular tree used for the backbone of the graph in Example 1. (b) The tree $\mathcal{T}_{d;r,L}$ is grown from the backbone by placing r chains of fixed length L (shown: $d = 3$, $r = 1$, $L = 2$) at each vertex of the backbone.

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r large, and $p_c \to 1$ if we take $r = 1$, L large. Similarly, the spectral radius is $\rho(\mathcal{T}_{d;r,1}) = d/2 + [(d/2)^2 + r]^{1/2}$ (we took $L = 1$); the corresponding estimated threshold varies in the range $0 < [\rho(\mathcal{G})]^{-1} \le 1/d$, while the lower bound (2) varies in the range $0 < p_c^{\min} \le (d-1)^{-1}$.

Thus, Eq. (1), the lower bound (2), and the inverse spectral radius $[\rho(\mathcal{G})]^{-1}$ do not give accurate estimates of the percolation threshold for this graph family.

In this Letter we suggest a tight lower bound for the site percolation threshold p_c on an infinite graph. It is given by the inverse maximum eigenvalue of the linearized mean-field (MF) equations, $p_c \ge p_c^{(\min)} = 1/\lambda_{\max}$. These equations relate probabilities that neighboring bonds lead to infinite clusters; they are exact for tree graphs which do not have cycles. The matrix H corresponding to the MF equations was first introduced by Hashimoto [35] to generate nonbacktracking walks on graphs. The infinite-dimensional matrix H is not symmetric; it is nontrivial that the maximum eigenvalue $\lambda_{\max} \equiv \lambda_{\max}(H)$ be real or nonzero. We show that the eigenvalue $\lambda_{\max}(H)$ gives a physically meaningful bound $0 < p_c^{(\min)} \le 1$ and can be obtained as a solution of a finite eigensystem for any connected infinite *quasitransitive graph* $\mathcal{G}$, a graph-theoretic analog of a translationally invariant system with a finite number of inequivalent vertices. For such graphs we also give a constructive proof that our threshold is indeed a lower bound by building a tree $\mathcal{T}$ locally equivalent to the original graph $\mathcal{G}$, except that a cycle on $\mathcal{G}$ is mapped to an open path connecting two equivalent vertices on $\mathcal{T}$. We also show that the inverse spectral radius $\rho(\mathcal{G})$ of the original graph gives a smaller (inexact) lower bound for the percolation threshold,

$$p_c \ge p_c^{(\min)} \equiv 1/\lambda_{\max}(H) > 1/\rho(\mathcal{G}). \tag{3}$$

Definitions.—A graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ with vertex set $\mathcal{V} \equiv \mathcal{V}(\mathcal{G})$ and edge set $\mathcal{E} \equiv \mathcal{E}(\mathcal{G})$ is called *transitive* if and only if for any two vertices i, j in $\mathcal{V}$ there is an automorphism (symmetry) of $\mathcal{G}$ mapping i onto j. Graph $\mathcal{G}$ is called *quasitransitive* if there is a finite set of vertices $\mathcal{V}_0 \subset \mathcal{V}$ such that any $i \in \mathcal{V}$ is taken into $\mathcal{V}_0$ by some automorphism of $\mathcal{G}$. We say that any vertex which can be mapped onto a vertex $i_0 \in \mathcal{V}_0$ is in the equivalence class of i_0. The regular tree in Fig. 1(a) is an example of a transitive graph; Fig. 1(b) shows a quasitransitive graph with three inequivalent vertex classes.

Let Γ be a group of automorphisms of a graph $\mathcal{G}$. The *quotient graph* $\mathcal{G}/\Gamma$ is the graph whose vertices are equivalence classes $\mathcal{V}(\mathcal{G})/\Gamma = \{\Gamma i : i \in \mathcal{V}(\mathcal{G})\}$, and an edge $(\Gamma i, \Gamma j)$ appears in $\mathcal{G}/\Gamma$ if there are representatives $i_0 \in \Gamma i$ and $j_0 \in \Gamma j$ that are neighbors in $\mathcal{G}$, $(i_0, j_0) \in \mathcal{E}(\mathcal{G})$. The same definition also applies in the case of a digraph $\mathcal{D}$, except that we need to consider directed edges, e.g., $(i_0 \to j_0) \in \mathcal{E}(\mathcal{D})$.

In *site percolation* on a graph $\mathcal{G}$, each vertex is open with probability p and closed with probability $1-p$; two neighboring open vertices belong to the same cluster. Percolation happens if there is an infinite cluster on $\mathcal{G}$. When the graph is not connected, percolation happens independently on different connected components. In the following, we will consider only connected graphs.

Mean field equations: Let us first consider an infinite *tree* $\mathcal{T}$, a graph with no cycles. We will assume that the vertex degrees are bounded, so that according to Eq. (2), the corresponding percolation threshold be strictly nonzero, $p_c \equiv p_c(\mathcal{T}) > 0$. The percolation threshold can be found exactly by constructing a set of recursive equations starting with some arbitrarily chosen root [36]. For a given pair of neighboring open vertices i and j (denoted $i \sim j$), let us introduce the probability Q_{ij} that i is connected to a finite cluster through j. The corresponding recursive equations have the form

$$Q_{ij} = \prod_{l \sim j : l \neq i} (1 - p + pQ_{jl}), \tag{4}$$

where the product is taken over all neighbors l of j such that $l \neq i$, so that only hitherto uncovered independent branches be included. The growth of a branch into an infinite custer is impeded by the site l being closed (probability $1-p$), or being open but connecting to a finite branch (probability pQ_{jl}).

Below the percolation threshold, $p < p_c$, Eq. (4) is satisfied identically with $Q_{ij} = 1$. Right at the percolation threshold, we expect the probability of an infinite cluster to be vanishingly small, and the probabilities Q_{ij} can be expanded:

$$Q_{ij} = 1 - \epsilon_{ij}, \qquad i \sim j, \tag{5}$$

where ϵ_{ij} is infinitesimal. Expanding Eq. (4) to linear order in ϵ_{ij}, we obtain the following eigenvalue problem at the threshold, $p = p_c$,

$$\lambda \epsilon_{ij} = \sum_{l \sim j : l \neq i} \epsilon_{jl}, \qquad \lambda \equiv 1/p_c. \tag{6}$$

The percolation threshold corresponds to the largest real eigenvalue $\lambda = \lambda_{\max}$ corresponding to a non-negative eigenvector, $\epsilon_{ij} \ge 0$. To ensure the probability $p_c \le 1$, the eigenvalue needs to be sufficiently large, $\lambda_{\max} \ge 1$.

Extending Eq. (4) to an arbitrary connected graph $\mathcal{G}$, we obtain a mean-field approximation to percolation, a generalization of the MF approach by Bethe [37]. The probabilities Q_{ij} correspond to directed edges in $\mathcal{G}$, meaning that generally $Q_{ij} \neq Q_{ji}$, and this pair of variables is defined if and only if the corresponding component of the adjacency matrix is nonzero, $A_{ij} \neq 0$. Let us introduce a *symmetric digraph* $\tilde{\mathcal{G}}$ with the same adjacency matrix A.

Namely, $\tilde{\mathcal{G}}$ has the same vertex set $\mathcal{V}(\tilde{\mathcal{G}})$ as $\mathcal{G}$ and the set of directed edges $\mathcal{E}(\tilde{\mathcal{G}}) \subseteq \mathcal{V} \otimes \mathcal{V}$ where each undirected edge $(i, j) \in \mathcal{E}(\mathcal{G})$ of the original graph $\mathcal{G}$ is replaced by a pair of directed edges $i \to j$ and $j \to i$. Then the matrix H of the eigensystem (6) has the components labeled by the directed edges of $\tilde{\mathcal{G}}$,

$$H_{u,v} = \delta_{jj'}(1 - \delta_{li}), \quad u \equiv i \to j, \quad v \equiv j' \to l, \tag{7}$$

where the second term in the product accounts for the nonbacktracking condition $i \neq l$. Matrix H was originally introduced by Hashimoto [35] to generate nonbacktracking walks on a digraph. This matrix can also be interpreted as the adjacency matrix of the oriented line (di)graph (OLG) [38] associated with the digraph $\tilde{\mathcal{G}}$. To simplify the notations, we will associate the Hashimoto matrix $H \equiv H_{\mathcal{G}}$ in Eq. (7) directly with the graph $\mathcal{G}$.

In the presence of cycles, the probabilities Q_{jl} and $Q_{jl'}$ for different branches leading to $l \neq l'$ may no longer be independent. Both branches could lead to the same finite or infinite cluster. As a result of these correlations, the probability that both $j \to l$ and $j \to l'$ lead to finite clusters is generally smaller than the product of corresponding probabilities computed independently. Respectively, a nontrivial solution of Eq. (4) may already exist for some $p < p_c(\mathcal{G})$. This implies that in the presence of cycles, the maximum eigenvalue $\lambda_{\max}$ of Eq. (6) would give a lower bound on the percolation threshold, $p_c(\mathcal{G}) \geq 1/\lambda_{\max}(H)$, which is the first part of the inequality (3).

It is easy to check that the spectral radius $\rho(A)$ of the graph adjacency matrix A [which by definition equals the spectral radius of the graph, $\rho(\mathcal{G}) \equiv \rho(A_{\mathcal{G}})$] cannot be smaller than any eigenvalue λ of H corresponding to a nontrivial solution $\epsilon_{ij} \geq 0$ of Eq. (6), which implies $\lambda \geq 0$. Indeed, for a nonempty graph, A is a symmetric non-negative matrix with some nonzero matrix elements [thus $\rho(A) > 0$] and we need to check only the case $\lambda > 0$. Starting with the corresponding nontrivial solution $\epsilon_{ij} \geq 0$, we introduce vertex variables $x_j \equiv \sum_{i:i\sim j} \epsilon_{ij}$ and $y_j \equiv \sum_{l:j\sim l} \epsilon_{jl}$ where summation is over all edges incident to and incident from j, respectively. Summing Eq. (6) over all j neighboring with i, we obtain

$$y_i = A_{ij} y_j - x_i, \tag{8}$$

where the second term in the rhs accounts for nonbacktracking condition $l \neq i$. Now, by assumption the solution $\epsilon_{ij} \geq 0$ is such that $\epsilon_{i_0 j_0} > 0$ for some edge (i_0, j_0). Equation (6) then also implies that $\epsilon_{j_0 l_0} > 0$ for some $l_0 \sim j_0$, so that at the vertex j_0 both $x_{j_0} > 0$ and $y_{j_0} > 0$. If we multiply Eq. (8) by y_i and sum over all i, we get

$$\lambda ||y||^2 = y_i A_{ij} y_j - y_i x_i < y_i A_{ij} y_j \leq \rho(A) ||y||^2, \tag{9}$$

where $||y||^2 \equiv y_i^2 > 0$. This proves [cf. Eq. (3)] the following theorem.

Theorem 1.—The spectral radius of the adjacency matrix $A_{\mathcal{G}}$ of any connected nonempty graph $\mathcal{G}$ is strictly larger than the maximum eigenvalue of the Hashimoto matrix $H_{\mathcal{G}}$ corresponding to a nonzero eigenvector with non-negative components, $\rho(A_{\mathcal{G}}) > \lambda_{\max}(H_{\mathcal{G}})$.

Results for quasitransitive graphs: The discussion of the MF equations (6) was at the "physical" level of rigorousness. We argued that the percolation threshold for an arbitrary infinite connected graph should be bounded from below by the inverse maximum positive eigenvalue $\lambda_{\max}(H)$ of Eq. (6) corresponding to $\epsilon_{ij} \geq 0$, and we proved that this bound is in turn larger than the inverse spectral radius of the graph.

Yet some questions remain: Eigensystem (6) has a nonsymmetric matrix H. Under what conditions do we expect to get a real-valued eigenvalue $\lambda_{\max}(H) \geq 1$ which would correspond to a valid percolation threshold? Could we obtain $\lambda_{\max}(H)$ as a solution of some finite eigenvalue problem, or at least as a limit of some sequence of such problems? If yes, what are the convergence conditions? As an example, Theorem 2 states that for any finite tree, Eq. (6) gives $\lambda_{\max}(H) = 0$. Of course, this makes perfect sense since these equations are exact on any tree, and the probability to have an infinite cluster on a finite tree is zero. However, the downside is that, at least in the case of an infinite tree graph, it is not sufficient to consider percolation on finite subgraphs.

In the following, we concentrate on the special case of infinite connected quasitransitive graphs, and we show that the maximum real eigenvalue $\lambda_{\max}(H)$ of the corresponding Hashimoto matrix (7) is finite, lies in the physical range $\lambda_{\max}(H) \geq 1$, and can be obtained by solving a single finite-dimensional spectral problem.

Let us first consider the eigensystem (6) for a finite graph $\mathcal{G}$. While the Hashimoto matrix $H_{\mathcal{G}}$ in Eq. (7) is nonsymmetric, it is finite dimensional and has non-negative matrix elements. The properties of the maximal real-valued eigenvalue $\lambda_{\max}$ of such matrices is addressed by the Perron-Frobenius theory of non-negative matrices [39–41]. In particular, an eigenvalue corresponding to a non-negative eigenvector always exists and it equals the spectral radius of H, $\lambda_{\max}(H) = \rho(H)$, although in general one could have $\rho(H) = 0$.

For any $m \times m$ matrix H with non-negative matrix elements, a sufficient condition for having $\rho(H) > 0$ is expressed [41] in terms of the digraph $\mathcal{D}_H$ with the adjacency matrix corresponding to nonzero elements of the square matrix H. Namely, there is a directed edge $u \to v$ whenever $H_{uv} > 0$ (or a loop $u \to u$ in the case of a diagonal matrix element $H_{uu} > 0$). In the case of the Hashimoto matrix, this graph is the OLG associated with the original graph [see the discussion below Eq. (7)]. The spectral radius of H is positive, $\rho(H) > 0$, if the digraph

$\mathcal{D}_H$ is *strongly connected*. This requires that for any pair of vertices u, v, there must be a directed path $(u_0 = u, u_1, \ldots, u_f \equiv v)$ connecting u and v such that $u_{s-1} \to u_s$, $s = 1, \ldots, f$ is in the edge set of $\mathcal{D}_H$. In such a case, we also know that the eigenvalue $\lambda_{\max} = \rho(H)$ is nondegenerate, it is the only one with the magnitude equal to the spectral radius, $|\lambda| = \rho(H)$, and the corresponding eigenvector has all positive components [39–41].

We prove the following theorem.

Theorem 2.—For any finite connected graph $\mathcal{G}$, the spectral radius of the Hashimoto matrix $H_\mathcal{G}$ is zero if and only if $\mathcal{G}$ contains no cycles. Otherwise, $\rho(H_\mathcal{G}) \geq 1$. The eigenvector corresponding to $\lambda \equiv \lambda_{\max} = \rho(H_\mathcal{G})$ is non-negative.

The interpretation is simple: On a finite tree, any non-backtracking walk eventually terminates at a *leaf* (a degree-one vertex) with no outgoing edges; thus Eq. (6) with $\lambda \neq 0$ has only trivial solutions $\epsilon_{ij} = 0$. With one or more cycles present, recursively plucking off any leaves, we arrive at a *backbone* graph $\mathcal{B}$ with minimum degree $d_{\min}(\mathcal{B}) \geq 2$; the corresponding Hashimoto matrix $H_\mathcal{B}$ is strongly connected and its spectral radius is limited from below by $\rho(H_\mathcal{B}) \geq d_{\min}(\mathcal{B}) - 1 \geq 1$. Putting the leaves back recovers the original graph but does not affect the spectral radius of the Hashimoto matrix. The full proof is given in the Supplemental Material [42].

We are not aware of an extension of the Perron-Frobenius theory to infinite matrices. However, in the case of a quasitransitive graph which only has a finite set of inequivalent vertices, it is reasonable to expect that the solution $\epsilon_{ij} \geq 0$ of Eq. (6) has the same symmetry as the original graph. Namely, for any pair of directed edges $i \to j$ and $i' \to j'$ which can be mapped to each other by an automorphism of $\mathcal{G}$, we request

$$\epsilon_{ij} = \epsilon_{i'j'}. \tag{10}$$

Such an ansatz reduces Eq. (6) to a finite-dimensional eigensystem. Depending on the details, the corresponding matrix M may have elements which are greater than one, or nonzero elements along the diagonal. As we discuss in the Supplemental Material [42], the nonzero elements of M uniquely correspond to nonzero elements of the Hashimoto matrix $H_{\mathcal{G}/\Gamma}$ corresponding to the quotient graph $\mathcal{G}/\Gamma$ with respect to the group Γ of automorphisms of $\mathcal{G}$. When the original infinite graph is connected, $\mathcal{G}/\Gamma$ necessarily has cycles. We prove the following theorem.

Theorem 3.—Consider an infinite connected quasitransitive graph $\mathcal{G}$ with the group of automorphisms Γ. The invariant ansatz (10) with $\epsilon_{ij} \geq 0$ gives a valid solution of the MF Eq. (6). The corresponding eigenvalue $\lambda = \rho(M)$ satisfies the inequalities

$$\lambda_{\max}(H_\mathcal{G}) = \rho(M) \geq \rho(H_{\mathcal{G}/\Gamma}) \geq 1. \tag{11}$$

Finally, we give a constructive proof of the first part of the inequality (3).

Theorem 4.—The percolation threshold for any infinite connected quasitransitive graph $\mathcal{G}$ is bounded from below by the inverse maximum eigenvalue of the corresponding Hashimoto matrix corresponding to a non-negative eigenvector, $p_c(\mathcal{G}) \geq 1/\lambda_{\max}(H_\mathcal{G})$.

The approach is to construct a tree graph $\mathcal{T}$ which is locally indistinguishable from the original graph $\mathcal{G}$, except that a closed walk on $\mathcal{G}$ goes over to a walk connecting equivalent points on $\mathcal{T}$. This is done by the repeated application of *single cycle unwrapping* (SCU).

Definition 1 (SCU).—Given a connected graph $\mathcal{G}$ and a bond $b \equiv (u, v) \in \mathcal{E}(\mathcal{G})$, such that the two-terminal graph $\mathcal{G}' \equiv (\mathcal{V}(\mathcal{G}), \mathcal{E}(\mathcal{G})\backslash b)$ with source at v and sink at u is connected, define the cycle-unwrapped graph $\mathcal{C}_b\mathcal{G}$ as the series composition of an infinite chain of copies $\mathcal{G}'_i$, $i \in \mathbb{Z}$ of the graph $\mathcal{G}'$, with the source of $\mathcal{G}'_i$ connected to the sink of the $\mathcal{G}'_{i+1}$.

The SCU is illustrated in Fig. 2. Notice that for a graph with more than one cycle, unwrapping at b removes one cycle but creates an infinite number of copies of the remaining cycles. Nevertheless, for a locally finite graph, we prove that a countable number of SCUs is needed to remove all cycles. Further, we prove (see Supplemental Material [42]) that an SCU does not change the maximum eigenvalue of the Hashimoto matrix, $\lambda_{\max}(H_\mathcal{G}) = \lambda_{\max}(H_{\mathcal{C}_b\mathcal{G}})$, whereas the percolation threshold cannot go up. Overall, this gives a constructive proof of Theorem 4.

In conclusion, we suggested a spectral MF lower bound for the threshold of site percolation on an infinite graph. This bound accounts for local structure of the graph and should be asymptotically exact for graphs with no short cycles. This bound goes over to the known lower bound (2) for degree-regular graphs and otherwise improves on Eq. (2). We also demonstrated that the inverse spectral radius of the graph which was suggested previously as an estimate for the percolation threshold is always strictly smaller than our lower bound. In the case of a quasitransitive graph, a graph-theoretical analog of a translationally invariant system, we proved that the bound is in a physically meaningful range and can be found as a solution of a finite spectral problem. This result is directly applicable for site percolation on any periodic lattice [43].

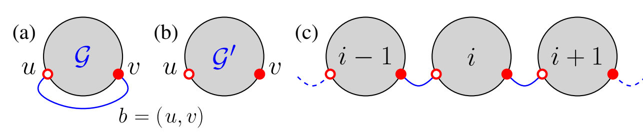

FIG. 2 (color online). Illustration of SCU. (a) A graph $\mathcal{G}$ with a nonbridge bond $b \equiv (u, v)$ highlighted. (b) The two-terminal graph $\mathcal{G}'$. (c) The resulting graph $\mathcal{C}_b\mathcal{G}$ is a series composition of an infinite chain of copies of $\mathcal{G}'$.

Our results can be easily extended to the cases of Bernoulli (bond), combined site-bond, or nonuniform percolation, where the probabilities to have an open vertex may differ from site to site. A similar technique can also be used to prove the conjecture on the location of the threshold for vertex-dependent percolation on directed graphs [44].

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Note added.—Recently, we were alerted to a following Letter by Newman, Karrer, and Zdeborova [45], who arrived at some of the same results using different arguments.

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