Leaf-free percolation in two and three dimensions

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We introduce the leaf-free percolation model, which we define to be the standard bond percolation model conditioned on the absence of leaves (vertices of degree one). We study leaf-free percolation on the square and simple-cubic lattices via Monte Carlo simulation, using a worm-like algorithm. By studying wrapping probabilities, we precisely estimate the critical thresholds to be $0.355 247 5(8)$ (square) and $0.185 022(2)$ (simple-cubic). Our estimates for the thermal and magnetic exponents are consistent with those for percolation, implying that the phase transition of leaf-free percolation belongs to the standard percolation universality class.

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I. INTRODUCTION

As a fundamental model in equilibrium statistical mechanics, and a cornerstone of the theory of critical phenomena, percolation [1,2] has attracted tremendous attention over many years. Numerous exact results are available in two dimensions, including exact thresholds on specific lattices [3,4], and the critical exponents $\beta = 5/36$ and $\nu = 4/3$ predicted by Coulomb-gas arguments [5] and conformal field theory [6]. For dimensions above 2 and below the upper critical dimension ($d_c = 6$) [8], no exact results are known for either the thresholds or the critical exponents. At and above the upper critical dimension, the mean-field values $\beta = 1$ and $d\nu = 3/2$ [9,10] are believed to hold.

One of the main goals of percolation theory in recent decades has been to understand the geometric structure of percolation clusters, following the pioneering work by Stanley in 1977 [11]. Recently in [12], the authors studied the geometric structure of percolation clusters by classifying the bridges present in clusters into two types: branches and junctions. A bridge was defined to be a branch iff at least one of the two clusters produced by its deletion is a tree. It was found that the leaf-free clusters, obtained by deleting the branches from percolation clusters, have the same fractal dimension and hull dimension as the original percolation clusters. This observation motivates us to study the phase transition of a modified percolation model, in which we explicitly condition on the absence of leaves. We refer to this model as the leaf-free percolation (LFP) model.

Explicitly, on a given graph $G = (V, E)$, the LFP model selects random bond configurations $A \subseteq E$ with distribution

$$P(A) \propto v^{|A|} \prod_{i \in V} 1(d_A(i) \neq 1),$$

where $d_A(i)$ denotes the degree of vertex $i$ in the spanning subgraph $(V, A)$, and $v$ is the bond weight. The conditioning on the absence of leaves implies that edges are no longer occupied independently in the LFP model. We therefore construct a worm-like algorithm in order to efficiently simulate the model. Using this algorithm, we simulate the LFP model on the square and simple-cubic lattices with periodic boundary conditions. We estimate the critical threshold $\nu_c$ by studying the finite-size scaling of wrapping probabilities. Wrapping probabilities are believed to be universal, and have been successfully applied to the estimate of critical thresholds of several percolation models [13,14]. By simulating precisely at our estimated $\nu_c$, we then estimate the thermal exponent $\gamma_t = 1/\nu$ and magnetic exponent $y_h = d - \beta/\nu$. Our results for critical exponents and universal amplitudes strongly suggest that the phase transition of the LFP model belongs to the standard percolation universality class.

The remainder of this paper is organized as follows. Sec. II introduces the worm-like algorithm and the observables measured in our simulations. Numerical results are summarized and analyzed in Section III. A brief discussion is then given in Section IV.

II. ALGORITHM AND OBSERVABLES

A. Worm algorithm

To simulate the LFP model, we construct a variant of the worm algorithm [15]. The key idea underlying the worm algorithm is to first enlarge the configuration space by including “defects”, and move these defects via random walk.
It is most simple to define the algorithm on an arbitrary (finite and connected) graph $G = (V, E)$. For the LFP model, defects correspond to leaves. We therefore introduce an enlarged space of worm configurations

$$S = \{(A, u, v) \in E \times V^2 : d_A(i) \neq 1 \text{ for } i \neq u, v\}.$$ 

The worm-like algorithm proceeds as follows. We use $\Delta$ to denote symmetric difference of sets.

1. Set $(A, u, v) \mapsto (A, v, u)$
2. Choose uniformly random $w \in V$ and set $(A, u, v) \mapsto (A, w, v)$ if $d_A(u) \neq 1$ and $d_A(w) \neq 1$.
3. Do the following:
   
   (a) Uniformly at random, choose $w \sim u$

   (b) Propose $(A, u, v) \mapsto (A \Delta uw, w, v)$, and accept with probability $\min[1, v^{|A \Delta uw| - |A|}]$, provided $(A \Delta uw, w, v) \in S$.

4. If new state is leaf-free, measure observables.

At a given time step, we do either of the first three proposals, respectively with probability $1/4, 1/4$ and $1/2$.

We note that, unlike the case of the worm algorithm for the Ising model, there is no particular reason for using two defects in our algorithm, and in fact the above algorithm can be easily modified to use any fixed number of defects; including one defect. We also note that it is somewhat of a misnomer to refer to the above algorithm as a worm algorithm; for a state $(A, u, v) \in S$, it will not be true in general that $u$ and $v$ are connected by occupied bonds, and so in general there is no worm as such. This is in contrast to worm algorithms for Eulerian subgraphs (e.g. Ising high temperature graphs), where the handshaking lemma demands that the two defects be connected.

### B. Sampled quantities

We simulated the LFP model on the $L \times L$ square lattice for system sizes up to $L = 1024$, and on the $L \times L \times L$ cubic lattice for system sizes up to $L = 96$. For each system size, approximately $10^8$ samples were produced.

Given a leaf-free bond configuration, we sampled the following observables.

1. The number of occupied bonds $N_b$.
2. The size of the largest cluster $C_1$.
3. The cluster-size moments $S_m = \sum C |C|^m$ with $m = 2, 4$, where the sum is over all clusters $C$.
4. The indicators $R^{(x)}, R^{(y)}, R^{(z)}$ for the event that a cluster wraps around the lattice in the $x, y, z$ direction, respectively.

From these observables, we calculated the following quantities:

1. The mean size of the largest cluster $C_1 = \langle C_1 \rangle$, which scales as $\sim L^{y_1}$ at the critical point $v_c$.
2. The mean size of the cluster at the origin, $\chi = \langle S_\text{c} \rangle / L^d$, which at $v_c$ scales as $\sim L^{2y_2-d}$.
3. The dimensionless ratios

$$Q_1 = \frac{\langle C_1^2 \rangle}{\langle C_1 \rangle^2}, \quad Q_2 = \frac{\langle 3S_\text{c}^2 - 2S_\text{c} \rangle}{\langle S_\text{c}^2 \rangle}.$$  

4. The probability that a winding exists in the $x$ direction $R^{(x)} = \langle R^{(x)} \rangle$. In two dimensions, we also measured $R^{(y)} = \langle R^{(y)} \rangle$, and in three dimensions measured $R^{(z)} = \langle R^{(z)} \rangle$. $R^{(d)}$ gives the probability that windings simultaneously exist in all $d$ possible directions.

5. The covariance of $R^{(x)}$ and $N_b$

$$g^{(x)}_{bR} = \langle R^{(x)} N_b \rangle - \langle R^{(x)} \rangle \langle N_b \rangle,$$

which is expected to scale as $\sim L^{y_2}$ at the critical point.

### III. RESULTS

#### A. Fitting methodology

We began by estimating the critical point $v_c$ by performing a finite-size scaling analysis of the ratios $Q_1, Q_2$ and wrapping probabilities $R^{(x)}, R^{(d)}$. The MC data for these quantities were fitted to the ansatz

$$O(\epsilon, L) = O_c + \sum_{k=1}^2 q_k \epsilon^k L^{ky_k} + b_1 L^{y_1} + b_2 L^{y_2},$$

where $\epsilon = v_c - v$, $y_1$ and $y_2$ are respectively the leading and sub-leading correction exponents, and $O_c$ is a universal constant.

We then performed extensive simulations at our best estimate of $v_c$, in order to estimate the critical exponents $y_1$ and $y_2$. These exponents were obtained by fitting $g^{(x)}_{bR}$, $C_1$ and $\chi$ to the ansatz

$$O(L) = L^{y_2} (a_0 + b_1 L^{y_1} + b_2 L^{y_2}),$$

where $y_2$ equals $y_1$ for $g^{(x)}_{bR}$, $y_1$ for $C_1$ and $2y_2 - d$ for $\chi$. In all fits reported below we fixed $y_2 = -2$, which corresponds to the exact value of the sub-leading correction exponent $[\mathbb{C}]$.

As a precaution against correction-to-scaling terms that we failed to include in the fit ansatz, we imposed a lower cutoff $L \geq L_{\text{min}}$ on the data points admitted in the fit, and we systematically studied the effect on the
χ^2 value of increasing L_{min}. Generally, the preferred fit for any given ansatz corresponds to the smallest L_{min} for which the goodness of fit is reasonable and for which subsequent increases in L_{min} do not cause the χ^2 value to drop by vastly more than one unit per degree of freedom. In practice, by “reasonable” we mean that χ^2/DF ≲ 1, where DF is the number of degrees of freedom.

We analyze the data on the square lattice in Sec. III B and Sec. III C. The results on the simple cubic lattice are shown in Sec. III D.

B. Square lattice near v_c

We first study the critical behavior of R(x), R(d) and Q_1, Q_2 near v_c. Fig. 1 plots R(x) and Q_1 versus v. Clearly, R(x) suffers from only very weak corrections to scaling.

We begin by considering R(x). Setting b_2 = 0 and leaving y_i free, we were unable to obtain stable estimate of y_i. The fits with two correction terms included (fixing y_i = −1) show that both b_1 and b_2 are consistent with zero for L_{min} = 64. In fact, the data of R(x) for L_{min} = 128 can be well fitted even with fixed b_1 = b_2 = 0. We also perform fits with only one of b_1L^{-1} or b_2L^{-2} included. Comparing the fits, we estimate v_c = 0.355 247 5(5) and y_t = 0.752(3). The latter is clearly consistent with 3/4 for two-dimensional percolation. We also estimate the universal amplitude R_c(x) = 0.521 2(2), consistent with the exact value 0.521 058 290.

The fits of R(d) show that it suffers even weaker finite-size corrections. The amplitudes b_1 and b_2 are both consistent with zero for L_{min} = 16. Again, we also perform fits in which we include only one of these corrections, and also fits in which we include neither. We then estimate v_c = 0.355 247 4(5), y_i = 0.753(3) and R_c(d) = 0.351 7(1), the latter of which is consistent with the exact value 0.351 642 855 for standard percolation.

Finally, we fit the data for Q_1 and Q_2. The fits predict a leading correction exponent y_i = −1.58(5) and −1.7(1) respectively. We note that this is consistent with the exact value −3/2 for two-dimensional percolation. We estimate v_c = 0.355 247 6(8) from Q_1 and v_c = 0.355 247 5(8) from Q_2. Both of their fits produce y_t = 0.751(3). We also estimate the universal amplitudes Q_1,c = 1.041 46(10) and Q_2,c = 1.148 7(2), both of which are consistent with the estimates for standard percolation.

Our estimates for v_c, y_t and the universal wrapping probabilities are summarized in Tab. I, where we also report the known results for standard percolation. This clearly shows that the phase transition of leaf-free percolation belongs to the standard percolation universality class.

C. Square lattice at v_c

To obtain final estimates of y_i and y_h, we performed high-precision simulations at a single value of v corresponding to our estimated threshold v_c = 0.355 247 5, and fitted the data for g_{bR}^{(x)}, C_1 and χ to Fig. 2. The leading correction exponent was set to y_i = −3/2.

The fits of g_{bR}^{(x)} show that both the amplitudes b_1 and b_2 are consistent with zero. The data for g_{bR}^{(x)} can be well fitted (χ^2/DF < 1 for L_{min} = 24) even without any corrections. From the fits, we estimate y_t = 0.750(1), which is consistent with the estimate in Sec. III D but with improved precision.

The fits of C_1 and χ show a non-zero b_1 if only the leading correction term is included in the fits. For comparison, we also performed fits including only the b_2L^{-2} term, and including both corrections. Both of these fits suggest y_h = 1.895 8(1), which is fully consistent with the exact result y_h = 91/48 for two-dimensional percolation. As further illustration, Fig. 2 shows a plot of L^{-3/4}g_{bR}^{(x)} and L^{-91/48}C_1 versus L^{-3/2}.

D. Simple-cubic lattice

We also performed an analogous study of leaf-free percolation on the simple-cubic lattice.

We again began by fitting the data for R(x), R(d) and Q_1, Q_2 to the ansatz Fig. 1 in order to estimate v_c. In each...
case, leaving $y_t$ free resulted in unstable fits. Instead, we fixed $y_t = -1.2$, which is numerically estimated in [13] to be the leading correction exponent for three-dimensional percolation. For comparison, we performed fits with different combinations of the terms $b_1 L^{-1.2}$ or $b_2 L^{-2}$ present. The best estimates were obtained from $R(x)$, which yield $v_c = 0.185022(2)$ and $y_t = 1.143(8)$. We also estimated the universal amplitudes $R_c(x) = 0.261(3)$ and $R_c(d) = 0.083(4)$. The universal amplitudes for $Q_1$ and $Q_2$ cannot be precisely estimated due to the strong finite-size corrections.

Simulating at our estimated $v_c$, we then fitted the data for $g_{bR}(x)$, $C_1$, $\chi$ to the ansatz (5) to estimate $y_t$ and $y_h$. Both the two correction terms were included in the fits. The fits of $g_{bR}$ yields $y_t = 1.142(7)$. From $C_1$ we estimate $y_h = 2.513(5)$. However, we find that it is difficult to estimate $y_h$ from $\chi$ due to the strong finite-size corrections.

Our estimates for the critical threshold, critical exponents and wrapping probabilities on the simple-cubic lattice are summarized in Tab. I. The agreement with the corresponding values for standard three-dimensional percolation [13] strongly suggests the LFP model is in the percolation universality class. As further illustration, Fig. 4 shows plots of $L^{-y_t} g_{bR}(x)$ and $L^{-y_h} C_1$ versus $L^{y_t}$, using percolation exponent values taken from [13].

**FIG. 2:** Plots of $L^{-3/4} g_{bR}$ and $L^{-91/48} C_1$ versus $L^{-3/2}$. The straight lines are simply to guide the eye.

**FIG. 3:** Plots of $R(x)$ and $Q_1$ versus $v$ for the LFP model on the simple-cubic lattice.

**FIG. 4:** Plot of $L^{-1.1415} g_{bR}$ and $L^{-2.52295} C_1$ versus $L^{-1.2}$. The straight lines are simply to guide the eye.

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**IV. DISCUSSION**

We investigate in this paper the critical behavior of the leaf-free percolation model, which is obtained from the standard bond percolation model by conditioning on the absence of leaves. Monte Carlo simulations of the LFP model were carried out on the square and simple-cubic lattices with periodic boundary conditions. By studying wrapping probabilities, we estimated the critical thresholds $v_c = 0.3552475(8)$ (square) and $v_c = 0.185022(2)$ (simple-cubic). The critical exponents $y_t$ and $y_h$ were found to be consistent with those for standard percolation, which indicates that the phase transition of the LFP model belongs to the percolation universality class.

Rather than conditioning on the absence of degree 1 vertices, as we have considered in the current work, one


\begin{table}
\centering
\begin{tabular}{|c|c|c|c|c|c|c|c|}
\hline
$d$ & Model & $v_c$ & $y_t$ & $y_h$ & $R_{\varepsilon}^{(s)}$ & $R_{\varepsilon}^{(d)}$ & $Q_{1,c}$ & $Q_{2,c}$ \\
\hline
2 & LFP & 0.3552475(8) & 0.751(1) & 1.8958(1) & 0.5212(2) & 0.3517(1) & 1.04146(10) & 1.1487(2) \\
2 & Percolation [6, 17, 18, 20] & 1 & 3/4 & 91/48 & 0.521058290 & 0.351642855 & 1.04148(1) & 1.14869(3) \\
3 & LFP & 0.185022(2) & 1.143(8) & 2.513(5) & 0.261(3) & 0.083(4) & - & - \\
3 & Percolation [13, 21] & 0.3312244(1) & 1.1415(15) & 2.52295(15) & 0.25780(6) & 0.08044(8) & 1.1555(3) & 1.5785(5) \\
\hline
\end{tabular}
\caption{Summary of our estimates for the thresholds $v_c$, critical exponents $y_t$ and $y_h$, and wrapping probabilities for the LFP model. A comparison with standard bond percolation is also included.}
\end{table}

could more generally condition on the absence of any specified set of vertex degrees. A very familiar example is to condition on the absence of odd vertices, in which case one obtains the high-temperature expansion of the Ising model. Dimer monomer/dimer, and fully-packed loop models also fit into this framework. It would be of interest to understand systematically how the choice of forbidden vertex degrees affects the resulting universality class.

It would also be of interest to extend the current study to the Fortuin-Kasteleyn random cluster model.

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