Surface and bulk criticality in midpoint percolation

Seung Ki Baek,[1,*] Petter Minnhagen,[1] and Beom Jun Kim[2]
[1]*Department of Physics, Umeå University, 901 87 Umeå, Sweden*
[2]*BK21 Physics Research Division and Department of Physics, Sungkyunkwan University, Suwon 440-746, Korea*
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The concept of midpoint percolation has recently been applied to characterize the double percolation transitions in negatively curved structures. Regular d-dimensional hypercubic lattices are investigated in the present work using the same concept. Specifically, the site-percolation transitions at the critical thresholds are investigated for dimensions up to $d=10$ by means of the Leath algorithm. It is shown that the explicit inclusion of the boundaries provides a straightforward way to obtain critical indices, both for the bulk and surface parts. At and above the critical dimension $d=6$, it is found that the percolation cluster contains only a finite number of surface points in the infinite-size limit. This is in accordance with the expectation from studies of lattices with negative curvature. It is also found that the number of surface points, reached by the percolation cluster in the infinite limit, approaches $2d$ for large dimensions d. We also note that the size dependence in proliferation of percolating clusters for $d \geq 7$ can be obtained by solely counting surface points of the midpoint cluster.

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I. INTRODUCTION

Percolation has been extensively studied over the past several decades and remains as an active field of research. In addition to its intrinsic scientific value and its role as one of the basic models of critical phenomena [1], it has contributed to improving our general understanding of statistical physics on various geometries (see, e.g., Ref. [2]), as well as developing efficient numerical algorithms (for a general introduction to percolation, see Ref. [3]). A percolation transition can be manifested in many different ways: a common quantity used in studies of the transition is the largest cluster size, but many other quantities also give a clear signature of the transition, including the cluster size distribution [4,5] and the ratio between the first and second largest cluster sizes [6]. At the same time, percolation is often a question of connectivity, so one obvious question is then how many connections can be randomly broken before the system fails to percolate from one side of the system to the other, or from its middle to the boundary. From this viewpoint, a percolation phenomenon requires a surface in order to be meaningful, just as water has to percolate all the way through the coffee layer in a coffee percolator. Thus, one might ask how the percolation transition is reflected on the actual surface. Specifically, the fraction of surface points belonging to the percolating cluster, $\mathcal{C}_\infty$, can be written as $P_s \sim (p-p_c)^{\beta_s}$ for d-dimensional systems where p is the occupation probability and p_c is its critical value. This formulation is parallel to the bulk criticality, i.e., $P \sim (p-p_c)^{\beta}$ where P is the fraction of bulk points belonging to $\mathcal{C}_\infty$. The exponent β_s is known to be 4/9 from conformal invariance for $d=2$ [7], and the mean-field value, valid for $d \geq 6$, is $\beta_s = 3/2$ [8]. For $d=3$, Monte Carlo simulations have estimated $\beta_s/\nu = 0.9753(3)$ where ν describes the correlation length as $\xi \sim (p-p_c)^{-\nu}$ [9].

The midpoint percolation turns out to be a useful concept to understand percolation transitions in curved structures [10]. This earlier work focused on lattices with negative Gaussian curvatures and it was found that the percolation for such lattices contains two critical thresholds: the first one at which the number of points reached on the surface from the midpoint becomes finite in the limit of the large system size, and the second one, where this number becomes a finite fraction of the surface points. The reason for the occurrence of two percolation thresholds appears to be intimately related to the size of the surface: when the surface-volume ratio is finite, as for the negatively curved lattices, there appear two thresholds. These two separate thresholds coalesce into a single one if the surface-volume ratio vanishes. In a d-dimensional system with size N, this ratio is to leading order $N^{-1/d}$. Thus from this viewpoint, a negatively curved structure with a constant surface-volume ratio is infinite-dimensional.

Let b be the average number of surface points reached from the midpoint in a d-dimensional hypercubic lattice having a linear size L. The quantity b has a size dependence of the form $b \sim L^{\kappa}$ at criticality. The exponent κ can be related to the bulk exponent β and the surface exponent β_s as follows:

$$\kappa = (d-1) - (\beta + \beta_s)/\nu. \tag{1}$$

This follows since the probability that the percolation cluster at criticality contains the midpoint, in the large-L limit, is independent of how many surface points it contains. Thus, the fraction between the number of surface points and the total number of points of the percolating cluster becomes $L^{\kappa}/L^{d-1} \sim L^{-\beta/\nu} L^{-\beta_s/\nu}$, where $L^{-\beta_s/\nu}$ is proportional to P_s and $L^{-\beta/\nu}$ is proportional to P (see Sec. III A below). Consequently, the exact value $\beta_s = 4/9$ for $d=2$ implies that $\kappa = 9/16 = 0.5625$[11]. A second case where the exponent b can be obtained analytically is $d=6$, for which Eq. (1) gives $\kappa = 0$ with the known values for the exponents [8]. This implies that only a finite number of points on the surface are reached from the midpoint at criticality. A third example is the Cayley tree with coordination number z, which is a negatively curved lattice and hence can be regarded as corresponding to

*Corresponding author; garuda@tp.umu.se

$d=\infty$. This structure has the lower and upper critical thresholds at $p_{c1}=1/(z-1)$ and $p_{c2}=1$, respectively [10], and there exist indefinitely many percolating clusters between these two thresholds [12]. One can calculate the average number of surface points reached from the midpoint at the lower threshold p_{c1} which gives $b=z/(z-1)$. Since there is no size dependence, this means that $\kappa=0$. The implication is that one only reaches a finite number of surface points from the midpoint for all dimensions $d \geq 6$.

One might also imagine a gradual reduction in the magnitude of the curvature until the structure becomes an ordinary d-dimensional lattice. Since both of the thresholds coalesce for a regular lattice, $p_c=p_{c1}=p_{c2}$, we are left with the following possibilities at criticality: b can be either a positive constant as it is for p_{c1} in case of the Cayley tree, or an increasing function of L as it is at p_{c2}. In this work, we find that the divergent behavior of b indeed becomes weaker as d increases, and reaches the limit of $b=$const. at the upper critical dimension, $d=6$ in accordance with the expectation above. We also show that the surface observable, b, provides us with a direct way of quantifying the percolation transition in general dimensions. In Sec. II, we describe the Leath algorithm used throughout this work. In Sec. III, we analyze the numerical results and discuss the critical behavior. Finally, Sec. IV gives a summary.

II. LEATH ALGORITHM

The measurement of b is well suited for the Leath algorithm [4,5], which is basically a burning algorithm to create a cluster starting from the midpoint. The collection of burned sites at each realization will be called a midpoint cluster, and abbreviated as $\mathcal{C}_m$. It suffices to count the number of surface points which are contained in $\mathcal{C}_m$. This makes the algorithm in the present case easier to use than in most earlier works since we need no explicit treatment to exclude the boundary. Let us consider a d-dimensional hypercubic lattice having the length of each edge as $L=2^n$ with an integer n. For convenience, we will impose the periodic boundary condition in this lattice. Each point will be assigned a coordinate with d components. Fixing one of the components, one gets a $(d-1)$-dimensional *surface* across the system which serves as our effective boundary layer: we do not allow the midpoint cluster to grow beyond this layer. In this way, we effectively get an odd number of lattice sites in each direction which uniquely defines the midpoint.

As for the actual implementation of the burning algorithm, one may choose between two options: depth-first and breadth-first methods. The former can be easily made using recursion as follows.

(1) Assign the "boundary" state to the points constituting the boundary layers, and set all the other points as "unexamined."

(2) Set the midpoint as "occupied."

(3) For each of the neighboring unexamined points of this occupied one, (a) with probability p, mark the neighbor as occupied and repeat Step 3 with respect to this newly occupied point. (b) With probability $1-p$, mark the neighbor as "stopped."

The midpoint cluster consists of the resulting occupied points and its growth will stop when it is completely surrounded by points marked as either stopped or boundary.

In spite of the ease of implementation, this method requires that the program remember the state of every lattice point, which severely restricts accessible system sizes. For this reason, the other option, i.e., the breadth-first method is better suited for the present context. The program is then only required to remember the outmost shell of $\mathcal{C}_m$. This can be implemented in the following way.

(1) Prepare a queue and an array, both initialized as empty. The queue stores actively burning points with its possible directions to proceed, while the array stores points which cannot be burned again, i.e., either "stopped" or currently "active."

(2) Add the midpoint to the queue, with every direction allowed, and record the midpoint as well as its state as active in the array.

(3) Retrieve an element from the queue. The queue becomes shortened by one in length on the retrieval. Also delete this active point from the array.

(4) For every possible neighbor from the retrieved point, make a search in the array unless it belongs to the boundary layers.

(a) If it is absent, (i) with probability p, add this to the array as active. Also add this to the queue with preventing it from propagating back. (ii) With probability $1-p$, add this to the array as "stopped."

(b) If it is found as active, tell the corresponding element in the queue not to propagate toward this direction.

(c) If it is found as stopped, this neighbor is not penetrable. Do nothing.

(5) Go to Step 3.

Note that we need not predefine the connection structure since one can easily compute neighboring coordinates from a given point in regular structures. As recommended in earlier works [13–15], we have employed hashing [16] in Step 4, but not included the data blocking method [13] nor the generation of a random number from each site index [14,17]. We choose the burning probability p from the previously known site-percolation thresholds, and the values used are tabulated in Table. I. Since p_c decreases with d, the actually generated cluster is much smaller than the effective lattice size in a high dimension. We also note how efficiently the Leath algorithm performs with respect to memory usage. For example, our implementation with 2 200 megabytes memory can readily simulate a case where boundaries are away from the midpoint by 31 lattice spacings in a six-dimensional hypercube around the known threshold, $p_c \approx 0.109017$ [15]. If we loaded every lattice point on memory, the memory requirement should roughly amount to 2^{36} integers, a significant portion of which would be simply redundant since the burning probability is low. The depth-first method has been used in this work only for simulating small system sizes, as well as performance checks of the breadth-first method.

III. RESULTS

Using the above algorithms, we have generated more than 10^6 samples for each L and d obtainable within our re-

TABLE I. Occupation probabilities used in this work and values of exponents obtained in this work in comparison to previously known results. For $d=2$ and $d\geq 6$, the known values of β/ν and β_s/ν are exact. The last column is for a consistency check of our analysis where the sum should be $d-1$ according to Eq. (1). The discrepancy at $d=7$ signals the proliferation of percolating clusters, as explained in the text.

d	p_c (known)	β/ν (X)	β/ν (known)	κ (Y)	β_s/ν (Z)	β_s/ν (known)	$X+Y+Z$
2	0.5927460[a]	0.1044(2)	5/48[e]	0.563(1)	0.33345(10)	1/3[m]	1.001(1)
3	0.3116081[b]	0.478(2)	0.474(6)[f]	0.554(7)	0.974(2)	0.970(6)[f]	2.01(1)
			0.477(4)[g]				
			0.4770(2)[h]				
			0.481(1)[i]			0.975(4)[i]	
						0.9754(4)[n]	
			0.4774(1)[j]			0.9753(3)[j]	
4	0.196889[c]	0.945(5)	0.9528(14)[b]	0.410(1)	1.64(2)		3.00(2)
			0.953(7)[c]				
5	0.1407966[d]	1.5(1)	1.462(16)[k]	0.11(7)	2.408(5)		4.0(2)
			1.46(1)[c]				
6	0.109017[d]	1.9(1)	2[l]	0.06(2)	2.8(3)	3[o]	4.8(4)
7	0.0889511[d]	2.0(1)	2[l]	0.06(8)	3.08(1)	3[o]	5.1(2)

[a]Reference [18].
[b]Reference [19].
[c]Reference [14].
[d]Reference [15].
[e]Reference [20].
[f]Reference [21].
[g]Reference [13].
[h]Reference [22].
[i]Reference [23].
[j]Reference [9].
[k]Reference [24].
[l]Reference [25].
[m]Reference [7].
[n]Reference [26].
[o]Reference [8].

sources. Our numerical results are presented in Figs. 1 and 2 and Table I. After recording the number of surface points reached by each midpoint cluster, we carry out the following analysis.

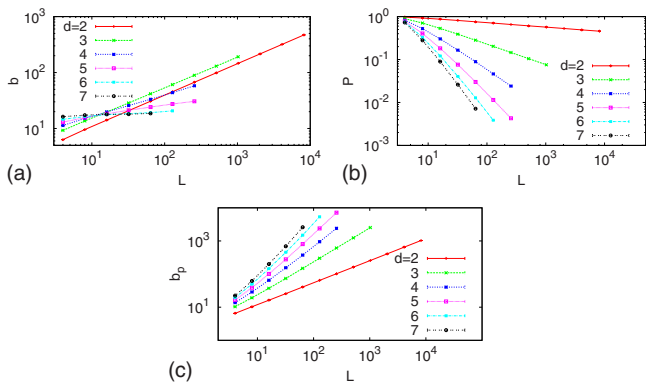

FIG. 1. (Color online) Data obtained by the Leath algorithm from $d=2$ to 7. (a) The average number of surface points, b, reached by the midpoint cluster. (b) The average probability for the midpoint cluster to reach the boundary, which is identified with P, the density of the percolating cluster. (c) The average number of surface points contained in a percolating midpoint cluster, b_p, for different sizes L. Error bars are shown in all the figures, but usually comparable to the symbol sizes.

A. Bulk criticality

Let us consider a lattice at an occupation probability p, where one or more clusters are distributed over the system. Among them, our algorithm always picks only one cluster, $\mathcal{C}_m$, the midpoint cluster. When p reaches p_c, a percolation cluster $\mathcal{C}_\infty$ will appear among many clusters in the system. It may or may not contain the midpoint. In case that the mid-

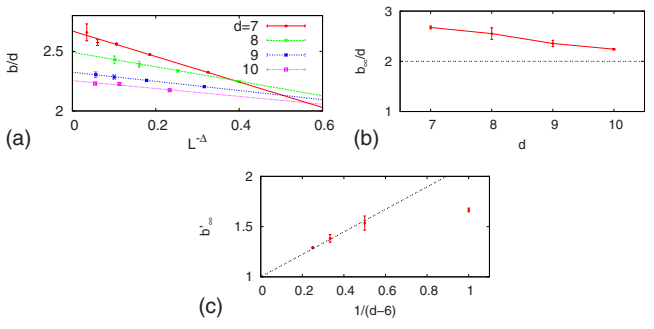

FIG. 2. (Color online) (a) Measurements of b/d for dimensions from $d=7$ to 10, where b is fitted by Eq. (5). The correction exponents are estimated as $\Delta(d=7)=0.5(1)$, $\Delta(d=8)=0.8(2)$, $\Delta(d=9)=0.7(4)$, and $\Delta(d=10)\gtrsim 1$. (b) The limiting number of surface points, $b(L\to\infty)$, divided by d. (c) The number of surface points reached, when percolation along the surface is prohibited, as a function of $1/(d-6)$. Linear extrapolation suggests that $b'_\infty(d\to\infty)\approx 1$.

point happens to be contained in $\mathcal{C}_\infty$, our algorithm shows that the generated cluster, $\mathcal{C}_m$, actually percolates the system, i.e., reaches the boundary. If $\mathcal{C}_\infty$ does not contain the midpoint, on the other hand, our algorithm picks up only a nonpercolating cluster with no surface points. In short, the frequency of touching the boundary in our algorithm simply means the probability for a percolating cluster $\mathcal{C}_\infty$ to contain the midpoint. Moreover, since the midpoint is one of the lattice points in the bulk, the probability that it is contained within the percolating cluster $\mathcal{C}_\infty$ is the same as for any other bulk point. This probability is given by the density of lattice points in $\mathcal{C}_\infty$ and consequently has the size scaling $P \sim L^{d_f-d}=L^{-\beta/\nu}$ where d_f is the fractal dimension of the percolating cluster. This means that one can estimate β/ν by counting how frequently $\mathcal{C}_m$ with a given size L reaches the boundary since when it touches, it does belong to the percolating cluster with certainty and vice versa. We generally expect a size scaling of an observable Q at criticality as

$$Q = AL^{\Upsilon}(1 + BL^{-\Delta} + \cdots) + C, \tag{2}$$

where A, B, and C are L-independent constants and $\Delta > 0$ characterizes the correction to the leading scaling behavior. In case of P, we know that $\Upsilon = -\beta/\nu$. Furthermore, since $P(L \to \infty)$ in fact vanishes, we can safely set C as zero in this case. Therefore, one arrives at

$$PL^{\beta/\nu} \approx A + B'L^{-\Delta} \tag{3}$$

with $B' \equiv AB$. Since plotting $PL^{\beta/\nu}$ against $L^{-\Delta}$ should give a straight line for correct exponents, we can determine the exponents from the goodness of fit. For $d=2$, for example, we get $\beta/\nu = 0.1044(2)$ together with $\Delta = 1.4(2)$, when choosing the chi-square significance level as $\alpha = 10\%$, and this result agrees well with the exact value, $\beta/\nu = 5/48 \approx 0.1042$ (see Ref. [20] and references therein). We have employed this method for lattices of dimension $2 \le d \le 7$ and the results are presented in Table I [Fig. 1(b)]. Whenever the data fail to exceed the chi-square critical value (CV) for $\alpha = 10\%$, we remove the smallest system size and then repeat the procedure. As seen in Table I, the resolution of our data tends to deteriorate somewhat with increasing dimension (see e.g., the values for $d=5$). This is presumably caused by the fact that the correction term in Eq. (3) is not enough to absorb all the deviations from the leading behavior when L is too small. Since the deviations increase with the dimension, we are restricted to using fewer sizes of L at a larger dimension. To some extent, the deviation is also caused by the fact that the number of available data sets decreases with large β/ν, making the statistics worse. Finally we note that the deviation of β/ν from the predicted values in case of the upper critical dimension, $d=6$, could possibly also be attributed to the logarithmic correction [27].

B. Surface criticality

As for the bulk critical exponent β, we use the surface data in order to obtain κ. This time the observable is b, the number of surface points reached by the midpoint cluster $\mathcal{C}_m$ [Fig. 1(a)]. As discussed in Sec. I, the constant C is expected to be a nonvanishing constant for $d \ge 6$ since it corresponds to the number of surface points reached in the infinite-size limit. Thus, according to Eq. (2), we assume the size scaling as

$$(b - C)L^{-\kappa} \approx A + B'L^{-\Delta}, \tag{4}$$

which is of the same form as Eq. (3) apart from the additional constant, C. As a practical data-fitting procedure, we find the smallest C that gives a sufficiently high CV to pass $\alpha = 10\%$. This procedure yields $\kappa = 0.563(1)$ for $d=2$, which is entirely consistent with the exact result $\kappa = 9/16 = 0.5625$. The result for $2 \le d \le 7$ are given in Table I. One way to obtain β_s/ν is then to use Eq. (1) and the determined values for β/ν and κ. However, we will here use this connection as a consistency check as shown in the last column in Table I. Instead, we use the alternative method of counting the average number of surface points reached by the midpoint cluster which actually do reach the boundary. This means that we only sample over the cases when $\mathcal{C}_m$ does percolate [Fig. 1(c)]. For $d=2$, this gives $\beta_s/\nu = 0.33345(10)$, which is close to the exact value, 1/3. Table I shows β_s/ν estimated in this way for $2 \le d \le 7$. To our knowledge, the values for four and five dimensions are reported for the first time in this work. It is notable that for $d=6$ both β_s/ν and β/ν deviate somewhat from the theoretical predictions but are still inside the estimated bounds. Nonetheless, the consistency check $\beta/\nu + \beta_s/\nu + \kappa = d-1$ is well born out for $2 \le d \le 6$, verifying the internal consistency of our method and analysis (the last column in Table I). We stress that the three exponents β/ν, β_s/ν, and κ in the present work are all obtained by just counting the number of surface points reached by the midpoint percolation cluster at criticality.

The case of $d=7$ in Table I is of special interest because $\beta/\nu + \beta_s/\nu + \kappa = 5.1(2) < d-1 = 6$. This means that the relation $L^{\kappa}/L^{d-1} \sim L^{-\beta/\nu}L^{-\beta_s/\nu}$ breaks down in this case. The reason is that the percolating cluster at criticality is no longer unique for $d \ge 7$ [28]. This is usually referred to as the breakdown of the hyperscaling relation [3]. Suppose that the number of percolation cluster scales as L^x, then the relation changes to $L^{\kappa}/L^{d-1} \sim L^{-x}L^{-\beta/\nu}L^{-\beta_s/\nu}$ so that the consistency relation becomes $\beta/\nu + \beta_s/\nu + \kappa = d-1-x$. The reason is that the chance that the midpoint belongs to one of the percolating clusters is still given by L^{d_f-d}, but now $L^{-\beta/\nu}$ gives the probability that a lattice point belongs to *any* percolating cluster. Consequently, the chance for the midpoint to be contained in one of percolating clusters is $L^{-x}L^{-\beta/\nu}$ from which $\beta/\nu + \beta_s/\nu + \kappa = d-1-x$ follows. The number of percolating clusters is expected to scale as L^{d-6} for $d \ge 6$ [28]. The consistency relation for $d > 6$ then becomes $\beta/\nu + \beta_s/\nu + \kappa = 5$. As seen in Table I, this relation is born out by our results for $d=7$. We also observe that, provided that the mean-field values hold for the critical indices β/ν and β_s/ν for $d \ge 6$, and in addition the critical index $\kappa = 0$ for $d \ge 6$ (as implied by our results), then it follows from the consistency relation that $x = d-6$. Conversely, if we take the growth of the percolation clusters, L^{d-6}, for granted, then we obtain $\kappa = 0$ from the consistency relation. This also implies that the fractal dimension of a single percolating cluster becomes $d_f = d-x-\beta/\nu = 4$ for $d \ge 6$ [28]. It is interesting to note that the exponent x, describing how the number of percolating clusters grows with a

lattice size at criticality for $d \geq 6$ can be obtained by just counting the number of surface points reached by the midpoint cluster.

Next we assume that the inferred result $\kappa=0$ for $d \geq 6$ is correct. Then Eq. (4) reduces to

$$b \approx b_\infty + B' L^{-\Delta}, \tag{5}$$

where $b_\infty \equiv A+C$. This says that $b(L \to \infty)$ approaches a constant denoted as b_∞. We have estimated this constant up to $d=10$, using the critical probabilities reported in Ref. [15] [Fig. 2(a)]. The correction exponent Δ shows a tendency to increase as d grows so that the convergence to b_∞ becomes more rapid. Figure 2(b) suggests that the limiting value of b_∞ for large d could possibly be $2d$. In order to investigate this further, we note that $b'(L)=p_c b(L-1)$ corresponds to the number of points reached on the surface *provided* that percolation along the surface is prohibited. In Fig. 2(c), we have plotted $b'_\infty \equiv b'(L \to \infty)$ against $1/(d-6)$, where we assume that $d-6$ is a fundamental parameter in the problem. Linear extrapolation suggests that the limiting value for $d \to \infty$ is close to $b'_\infty=1$. Since p_c approaches $1/(2d-1)$ for large d, this result also implies that $b_\infty \approx 2d$, even though the precision is not sufficient to make any firm conclusion. Note that $2d$ is just the number of faces in a d-dimensional hypercube, so that one can say that C_m reaches every face of the surface in one point on the average. However, any individual realization of the midpoint percolation cluster will of course reach a variety of points on each face and some not at all.

In a previous study, it was shown that the cluster grows on the *average* by one site per step for large enough dimensions, suggesting a connection to the self-avoiding random walk (SAW) [15]: A cluster that grows with *precisely* one site per step traces out a SAW. From this perspective, it is interesting to note that our quantity b'_∞ corresponds to the average number of points that a SAW walker starting from the midpoint reaches on the surface. Since a SAW walker always has a finite chance of getting stuck in any dimension $d<\infty$, this means that $b'_\infty<1$ for SAW, whereas we have found $b'_\infty>1$ for the midpoint percolation cluster at criticality. However, the chance of getting stuck vanishes for the SAW walker in the limit of $d \to \infty$, which means that $b'_\infty=1$ in this limit. This agrees with our corresponding result for percolation, as well as with the result in Ref. [15], suggesting some similar feature between an unhindered SAW and the midpoint cluster at criticality in the limit of large d. However, the cluster created by SAW and the midpoint percolation cluster at criticality have quite different structures in all dimensions including the limit of $d \to \infty$ since the SAW cluster has fractal dimension $d_f=2$ for high d whereas that of the midpoint percolation cluster is $d_f=4$ as verified in the present paper. One may note that if one only takes the backbone of the percolating cluster, the backbone indeed has a fractal dimension $d_f^{(b)}=2$ for $d>6$ [3], which strengthens the similarity.

IV. SUMMARY

We studied the percolation transitions in dimensions from $d=2$ to 10 by the Leath algorithm. In particular, it was shown that one can obtain various critical properties by just counting the number of points reached on the surface from the midpoint. To this end, we checked that our midpoint percolation yielded consistent results with known ones, and estimated exponents characterizing the surface criticality as well as the bulk one. We found that the divergent behavior of b becomes weaker in higher dimensions as anticipated from the Cayley tree, so that it scales as $L^{9/16}$ for $d=2$ but converges to a constant in the infinite-size limit for $d \geq 6$. We also confirmed that the percolation cluster ceases to be unique for $d \geq 6$. In addition, our results suggests that the number of surface points reached approaches the value of $2d$ in the limit of large d. Provided that percolation along the surface excluded, this corresponds to the simple result that precisely one surface point is reached at criticality.

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