Precise bond percolation thresholds on several four-dimensional lattices

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We study bond percolation on several four-dimensional (4D) lattices, including the simple (hyper)cubic (SC), the SC with combinations of nearest neighbors and second nearest neighbors (SC-NN+2NN), the body-centered cubic (BCC), and the face-centered cubic (FCC) lattices, using an efficient single-cluster growth algorithm. For the SC lattice, we find \( p_c = 0.1601312(8) \), which confirms previous results (based on other methods), and find a new value \( p_c = 0.035827(2) \) for the SC-NN+2NN lattice, which was not studied previously for bond percolation. For the 4D BCC and FCC lattices, we obtain \( p_c = 0.074212(2) \) and \( 0.049517(2) \), which are substantially more precise than previous values. We also find critical exponents \( \tau = 2.3135(5) \) and \( \Omega = 0.40(3) \), consistent with previous results, including the recent four-loop series result of Gracey [Phys. Rev. D 92, 025012, (2015)], \( \Omega = 0.4003 \).

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I. INTRODUCTION

Percolation, which was introduced by Broadbent and Hammersley [1] in 1957, is one of the fundamental models in statistical physics [2, 3]. In percolation systems, sites or bonds on a lattice are either occupied with probability \( p \), or not with probability \( 1 - p \). When increasing \( p \) from below, a cluster large enough to span the entire system from one side to the other will first appear at a value \( p_c \). This point is called the percolation threshold.

The percolation threshold is an important physical quantity, because many interesting phenomena, such as phase transitions, occur at that point. Consequently, finding percolation thresholds for a variety of lattices has been a long-standing subject of research in this field. In two dimensions, percolation thresholds of many lattices can be found analytically [4–7], while others cannot and must be found numerically. In three and higher dimensions, there are no exact results, and all thresholds must be determined by approximation schemes or numerical methods. Many effective numerical simulation algorithms [5, 11] have been developed. For example, the “cluster multiple labeling technique” was proposed by Hoshen and Kopelman [8] to determine the critical percolation concentration, percolation probabilities, and cluster-size distributions for percolation problems. Newman and Ziff [10, 11] developed a Monte Carlo algorithm which allows one to calculate quantities such as the cluster-size distribution or spanning probability over the entire range of site or bond occupation probabilities from zero to one in a single run, and takes an amount of time that scales roughly linearly with the number of sites on the lattice.

Much work in finding thresholds has been done with these and other techniques. Series estimates of the critical percolation probabilities for the bond problem and the site problem were presented by Sykes and Essam [12], which can be traced back to 1960s. Lorenz and Ziff [13] performed extensive Monte Carlo simulations to study bond percolation on three-dimensional lattices using an epidemic cluster-growth approach. Determining the crossing probability [2, 14, 15] \( R(p) \) as a function of \( p \) for different size systems, and using scaling to analyze the results is also a common way to find \( p_c \). By examining wrapping probabilities, Wang et al. [16, 17] simulated the bond and site percolation models on several three-dimensional lattices, including simple cubic (SC), the diamond, body-centered cubic (BCC), and face-centered cubic (FCC) lattices. Other recent work on percolation includes [18, 27].

Percolation has been investigated on many kinds of lattices. In three and higher dimensions, the most common of these lattices are the SC, the BCC, and the FCC lattices. Thanks to the techniques mentioned above, precise estimates are known for the critical thresholds for site and bond percolation and related exponents in three dimensions. However, in four dimensions, the estimates of bond percolation thresholds that have been determined for the BCC and FCC lattices are much less precise than the values that have been found for some other lattices. In addition, to the best of our knowledge, the bond percolation threshold on SC lattice with the combinations of nearest neighbors (NN) and second nearest neighbors (2NN), namely (SC-NN+2NN), has not been reported so far. We note that the notation \( 2n+3n \) is also used for NN and 2NN [29].

In this paper, we employ the single-cluster growth method [13] to study bond percolation on several lattices in four dimensions. While confirming previous results of SC lattice, we obtain more precise estimates of percolation thresholds for BCC and FCC lattices. We
also find a new value for bond threshold of the complexneighborhood lattice, SC-NN+2NN.

With regards to the latter system, Malarz and coworkers [29, 33] have carried out several studies on lattices with various complex neighborhoods, that is, lattices with combinations of two or more types of neighbor connections, in two, three and four dimensions. Their results have all concerned site percolation, and are generally given to only three significant digits. Here we show that the single cluster growth method can be efficiently applied to one of these lattices also. Our goal was to find results to about six significant digits, which was not difficult to achieve using the methods given here.

Precise percolation thresholds are needed in order to study the critical behavior, including critical exponents, critical crossing probabilities, critical and excess cluster numbers, etc. Four dimensions is interesting because it is close enough to six dimensions for $6 - \varepsilon$ series analysis to have a hope of yielding good results [34], and in general there is interest in how thresholds depend upon dimensionality [28, 35–38]. The study of how thresholds depend upon lattice structure, especially the coordination number $z$, has also had a long history [39, 40]. Having thresholds of more lattices is useful for extending those generally given to only three significant digits. Here we show results have all concerned site percolation, and are generally given to only three significant digits. Here we show that the single cluster growth method can be efficiently applied to one of these lattices also. Our goal was to find results to about six significant digits, which was not difficult to achieve using the methods given here.

In the following sections, we present the underlying theory, and discuss the simulation process. Then we present and briefly discuss the results that we obtained from our simulations.

II. THEORY

The central property describing the cluster statistics in percolation is $n_s$, defined as the number of clusters (per site) containing $s$ occupied sites or bonds, as a function of the occupation probability $p$. At the percolation threshold $p_c$, $n_s$ is expected to behave as

$$n_s \sim A_0 s^{-\tau}(1 + B_0 s^{-\Omega} + \ldots),$$

where $\tau$ is the Fisher exponent, and $\Omega$ is connected with the leading correction to scaling. Both $\tau$ and $\Omega$ are expected to be universal, namely the same for all lattices of a given dimensionality. The $A_0$ and $B_0$ are constants that depend upon the system (are non-universal). The probability a vertex belongs to a cluster with size greater than or equal to $s$ will then be

$$P_{\geq s} = \sum_{s' \geq s} s' n_{s'} \sim A_1 s^{2-\tau}(1 + B_1 s^{-\Omega} + \ldots),$$

where $A_1 = A_0/(\tau - 2)$ and $B_1 = (\tau - 2)B_0/(\tau + \Omega - 2)$. Multiplying both sides of Eq. (2) by $s^{\tau - 2}$, we have

$$s^{\tau - 2} P_{\geq s} \sim A_1(1 + B_1 s^{-\Omega} + \ldots).$$

It can be seen that there will be a linear relationship between $s^{\tau - 2} P_{\geq s}$ and $s^{-\Omega}$ for large $s$, if we choose the correct value of $\Omega$. This linear relationship can be used to determine the value of percolation threshold, because for $p \neq p_c$ the behavior will be nonlinear.

Taking the logarithm of Eq. (2), we find

$$\ln P_{\geq s} \sim \ln A_1 + (2 - \tau) \ln s + \ln(1 + B_1 s^{-\Omega})$$

$$\sim \ln A_1 + (2 - \tau) \ln s + B_1 s^{-\Omega},$$

for large $s$. Similarly,

$$\ln P_{\geq 2s} \sim \ln A_1 + (2 - \tau) \ln 2s + B_1(2s)^{-\Omega}.$$  \hspace{1cm} (5)

Then it follows that

$$\frac{\ln P_{\geq 2s} - \ln P_{\geq s}}{\ln 2} \sim \frac{(2 - \tau)(\ln 2s - \ln s)}{\ln 2} - \frac{B_1 s^{-\Omega}(2^{-\Omega} - 1)}{\ln 2}$$

$$\sim (2 - \tau) + B_2 s^{-\Omega},$$

where $\ln P_{\geq 2s} - \ln P_{\geq s}$ is the local slope of a plot of $\ln P_{\geq 2s}$ vs. $\ln s$, and $B_2 = B_1(2^{-\Omega} - 1)/\ln 2$. Eq. (6) implies that if we make of plot of the local slope vs. $s^{-\Omega}$ at $p_c$, linear behavior will be found for large $s$, and the intercept of the straight line gives the value of $(2 - \tau)$.

III. SIMULATION RESULTS AND DISCUSSIONS

The basic algorithm of single-cluster growth method is as follows. An individual cluster starts to grow at the seeded site that is located on the lattice. We choose the origin of coordinates for the seeded site, though any site on the lattice can be chosen under periodic boundary conditions. From this site, a cluster is grown to neighboring sites by occupying the connecting bonds with a certain probability $p$ or leaving them unoccupied with probability $1-p$. All of these clusters are allowed to grow until they terminate in a complete cluster, or when they reach an upper size cutoff, their growing is halted.

To grow the clusters, we check all neighbors of a growth site for unvisited sites, which we occupy with probability $p$, and put the newly occupied growth site on a first-in, first-out queue. To simulate bond percolation, we simply occupy them. (For site percolation, unoccupied visited sites are blocked from ever being occupied in the future.) The single-cluster growth method is similar to the Leath algorithm [9].

We utilize a simple programming procedure to avoid clearing out the lattice after each cluster is formed: the lattice values are started out at 0, and for cluster $n$, any site whose value is less than $n$ is considered unoccupied. When a site is occupied in the growth of a new cluster, it is assigned the value $n$. This procedure saves a great deal of time because we can use a very large lattice, and do not have to clear out the whole lattice after every cluster, many of which are quite small and grow very quickly.

The size of the cluster can be identified by the number of occupied sites it contains. Then the number of clusters
whose size (number of sites) fall in a range of \((2^n, 2^{n+1} - 1)\) for \(n = 0, 1, 2, \cdots\) is recorded in the \(n\)th bin. If a cluster is still growing when it reaches the upper cutoff, it is counted in the last bin. The cutoff was \(2^{17}\) occupied sites for the SC lattice, \(2^{16}\) for SCC and SC-NN+2NN, and \(2^{15}\) for the BCC lattice. The cutoff had to be lower in the latter case because of the expanded nature of the BCC lattice represented on the SC lattice.

While the single-cluster growth method requires separate runs to be made for different values of \(p\), it is not difficult to quickly zero in on the threshold to four or five digits, and then reserve the longer runs for finding the sixth digit. It is also simple to analyze the results as shown here — one does not need to study things like the intersections of crossing probabilities for different size systems or create large output files of intermediate microcanonical results to find estimates of the threshold. The output files here are simply the 15 to 17 values of the bins for each value of \(p\) described above.

The simulations on the SC lattice, SC-NN+2NN lattice, BCC lattice, and FCC lattice were carried out for system size \(L \times L \times L \times L\) with \(L = 128\), and with periodic boundary conditions. For each lattice, we produced \(10^6\) independent samples. Then the number of clusters greater than or equal to size \(s\) could be found based on the data from our simulation, and the corresponding quantities, such as the local slope \((\ln P_{\geq s} - \ln P_{\geq 2s})/\ln 2\), and \(s^\tau P_{\geq s}\), could be easily calculated.

Figs. 1 and 2, respectively, show the plots of the local slope and \(s^\tau P_{\geq s}\) vs. \(s^{-\Omega}\) for the SC lattice under different values of \(p\). When \(p\) is away from \(p_c\), no matter if it is larger or smaller than \(p_c\), the curves show a deviation from linearity. When \(p\) is very near to \(p_c\), we can see better linear behavior for large \(s\). The linear behavior here is in good agreement with the theoretical predictions of Eqs. (6) and (7).

Based on these simulation results, for bond percolation on the SC lattice in four dimensions, we conclude

SC:
\[
p_c = 0.1601312(6), \quad \tau = 2.3135(7), \quad \Omega = 0.40(3).
\]

Here numbers in parentheses represent errors in the last digit(s), determined from the observed statistical errors.

The simulation results for other three lattices, i.e., the plots of the local slope and \(s^\tau P_{\geq s}\) vs. \(s^{-\Omega}\) for the SC-NN+2NN, BCC, and FCC lattices under different values of \(p\) are shown in Figs. 1 and 2. From these figures, we can see similar behavior as the SC lattice. In order to avoid unnecessary repetition, we do not discuss the data one by one, and directly show the deduced values of \(p_c\) and the two exponents below:

SC-NN+2NN:
\[
p_c = 0.035827(1), \quad \tau = 2.3138(12), \quad \Omega = 0.40(3).
\]

BCC:
\[
p_c = 0.074212(1), \quad \tau = 2.3133(9), \quad \Omega = 0.41(3).
\]

FCC:
\[
p_c = 0.049517(1), \quad \tau = 2.3135(9), \quad \Omega = 0.41(3).
\]

From these values, we have obtained precise estimates of the percolation threshold, and also confirmed the universality of the Fisher exponent \(\tau\).

When the probability \(p\) is away from \(p_c\), a scaling function needs to be included. Then the behavior can be represented as
\[
P_{\geq s} \sim A_2 s^{\tau - 2} f(B_2 (p - p_c) s^{\sigma}), \tag{7}
\]
in the scaling limit of \(s \to \infty\) and \(p \to p_c\). The scaling function \(f(x)\) can be expanded as a Taylor series,
Combining Eqs. (7) and (8) leads to
\[ B_2(p - p_c) s^\sigma \sim 0.035825 \]
where \( C_2 = B_2 f'(0). \) We assume \( f(0) = 1, \) so that \( A_2 = A_1. \)

Combining Eqs. (7) and (8) leads to
\[ s^{\tau - 2} P_{\geq s} \sim A_2 + D_2(p - p_c) s^\sigma. \]
where \( D_2 = A_2 C_2. \) Eq. (9) predicts that \( s^{\tau - 2} P_{\geq s} \) will converge to a constant value at \( p_c \) for large \( s, \) while it deviates from a constant value when \( p \) is away from \( p_c. \) This provides another way to determine the percolation threshold. Figs. 3–12 show the plots of \( s^{\tau - 2} P_{\geq s} \) versus \( s^\tau \) for the SC, SC-NN+2NN, BCC and FCC lattices, respectively. For these plots, we use the value of \( \sigma = 0.4742, \) which is provided in Ref. [34]. The estimations of percolation thresholds are shown below, and they are consistent with the values obtained above.

SC: \( p_c = 0.1601314(6). \)
SC-NN+2NN: \( p_c = 0.035827(2). \)
BCC: \( p_c = 0.074212(2). \)
FCC: \( p_c = 0.049517(2). \)

Our final estimates of percolation thresholds for all the lattices calculated in this paper are summarized in Table 1, where we also make a comparison with those of previous studies where available. It can be seen that for the
SC lattice, our result is completely consistent with the existing ones within the error range, including the recent more precise result of Mertens and Moore [23]. For the BCC and FCC lattices, we find significantly more precise values of $p_c$ than van der Marck [28], who gave only two digits of accuracy. And we give for the first time a value of $p_c$ for the SC-NN+2NN lattice, which was not studied before for bond percolation.

Table I also shows the coordination number $z$ for each lattice. The values of $p_c$ decrease with the coordination number $z$ as one would expect. Finding correlations between percolation thresholds and lattice properties has a long history in percolation studies [39, 41–43]. In Ref. [31] it was found that the site thresholds for several 3D lattices can be fitted by a simple power-law in the coordination number $z$

$$p_c(z) \sim z^{-\gamma_4},$$  

with $\gamma_4 = 0.790(26)$ in 3D. Similar power-law relations for various systems were studied by Galam and Mauger [40], van der Marck [28], and others, usually in terms of $(z - 1)^{-\gamma_4}$ rather than vs. $z^{-\gamma_4}$. Making a log-log plot of the 4D data of Table I along with the bond threshold $p_c = 0.2715(3)$ for the 4D diamond lattice [28], which has coordination number $z = 5$, in Fig. 13 we find $\gamma_4 = 1.087$. Deviations of the thresholds from this line are within about 2%. We note that the data for site percolation thresholds of these lattices, taken from [28], do not show such a nice linear behavior as do the bond thresholds.
FIG. 11. Plot of $s\tau - 2 P_{\geq s}$ vs. $s\tau$ for the BCC lattice under different values of $p$.

FIG. 12. Plot of $s\tau - 2 P_{\geq s}$ vs. $s\tau$ for the FCC lattice under different values of $p$.

### IV. CONCLUSIONS

In this paper, by employing the single-cluster growth algorithm, bond percolation on SC, SC-NN+2NN, BCC, and FCC lattices in four dimensions was investigated. The algorithm allowed us to estimate the percolation thresholds with high precision with a moderate amount of calculation. For the BCC and FCC lattices, our results are about three orders of magnitude more precise than previous values, and for SC-NN+2NN lattice, we find a value of the bond percolation threshold for the first time. In addition, the results indicate that the percolation thresholds $p_c$ decrease monotonically with the coordination number $z$, quite accurately according to a power law of $p_c \sim z^{-74}$, with the exponent $\gamma_4 = 1.087$.

There remain many lattices where thresholds are not known, or where they are known only to low significance, and the methods described here can be used to find them with high accuracy in a straightforward manner. For example, the bond thresholds on the many complex neighborhood lattices of Malarz and co-workers have not been determined before, and knowing these thresholds may be useful for various applications.

Another result of this paper was a precise measurement of the exponent $\tau$, which we were able to do using the finite-size scaling behavior of Eq. (6), which requires the knowledge of $\Omega$ although the results for $\tau$ are not very sensitive to the precise value of $\Omega$. Averaging the results over the four lattices, we find $\tau = 2.3135(5)$. This is consistent with previous Monte Carlo values of 2.3127(6)\textsuperscript{17}, 2.313(2)\textsuperscript{45}, 2.313(2)\textsuperscript{48}, the recent Monte Carlo result of Mertens and Moore, 2.3142(5)\textsuperscript{23}, and also close to the recent four-loop series result 2.3124 of Gracey\textsuperscript{34}. In concurrent work, Deng et al. find that the fractal dimension in 4D equals $d_f = 3.0446(7)$, which implies by the scaling relation $\tau = 1 + d/d_f = 2.3138(3)$\textsuperscript{49}. Our

| Table I. Estimations of bond percolation thresholds for the four-dimensional percolation models. |
|---|
| lattice | $z$ | $p_c$ (Present) | $p_c$ (Previous) |
| SC | 8 | 0.1601312(8) | 0.16005(15)\textsuperscript{44} |
| | | 0.160130(3) \textsuperscript{45} | 0.1601314(13) | 0.1601310(10) | 0.16013122(6) |
| BCC | 16 | 0.074212(2) | 0.074(1) \textsuperscript{28} |
| FCC | 24 | 0.049517(2) | 0.049(1) \textsuperscript{28} |
| SC-NN+2NN | 32 | 0.035827(2) | —– |

FIG. 13. A log-log plot of percolation thresholds $p_c$ vs. coordination number $z$ for the lattices simulated in this paper (square symbols) and the diamond lattice (circle) provided in Ref. \textsuperscript{28}. The slope gives an exponent of $\gamma_4 = 1.087$ in Eq. (10), and the intercept of the line is at $\ln p_c = 0.435$.\textsuperscript{}}
value 2.3135(5) is a good average of all these measurements.

We have also found a fairly accurate value of the corrections-to-scaling exponent $\omega$, with the result $0.40(3)$, which also gives a value of $\omega = \Omega f$ = 1.22(9). We determined $\Omega$ by adjusting its value until we found a straight line in plots like Figs. 1 and 2 — while simultaneously trying to find $p_c$ and $\tau$. Having three different kinds of plots for each lattice helped in this simultaneous determination of these three parameters. Previous Monte-Carlo values of $\Omega$ were 0.31(5) [60], 0.37(4) [47], and 0.5(1) [48]. Gracey found the series extrapolation of 0.4008 [34], which is virtually identical to our central value, 0.40.

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