Bond and Site Percolation in Three Dimensions

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We simulate the bond and site percolation models on a simple-cubic lattice with linear sizes up to \(L = 512\), and estimate the percolation thresholds to be \(p_c^{\text{(bond)}} = 0.248\,811\,82(10)\) and \(p_c^{\text{(site)}} = 0.311\,607\,7(2)\). By performing extensive simulations at these estimated critical points, we then estimate the critical exponents \(1/\nu = 1.141\,0(15)\), \(\beta/\nu = 0.477\,05(15)\), the leading correction exponent \(y_t = -1.2(2)\), and the shortest-path exponent \(d_{\text{min}} = 1.375\,6(3)\). Various universal amplitudes are also obtained, including wrapping probabilities, ratios associated with the cluster-size distribution, and the excess cluster number. We observe that the leading finite-size corrections in certain wrapping probabilities are governed by an exponent \(c_t \approx -2\), rather than \(y_t \approx -1.2\).

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I. INTRODUCTION

Percolation\[1\] is a cornerstone of the theory of critical phenomena\[2\], and a central topic in probability\[3,4\]. In two dimensions, Coulomb gas arguments\[5,6\] and conformal field theory\[7\] predict the exact values of the bulk critical exponents \(\beta = 5/36\) and \(\nu = 4/3\), which have been confirmed rigorously in the specific case of triangular-lattice site percolation\[8\]. Exact values of the percolation thresholds \(p_c\) on several two-dimensional lattices are also known\[8\]. In particular, it is known rigorously\[9\] that \(p_c = 1/2\) for bond percolation on the square lattice. For all \(d\) greater than or equal to the upper critical dimension\[10\] of \(d_{c1} = 6\), the mean-field values for the exponents \(\beta = 1\) and \(d\nu = 3\) are believed to hold; this has been proved rigorously\[11,12\] for \(d \geq 19\).

For dimensions \(2 < d < 6\) by contrast, no exact values for either the critical exponents or the percolation thresholds are known. Significant effort has therefore been expended on obtaining ever more accurate estimates, especially in three dimensions.

In addition to percolation thresholds and critical exponents, crossing probabilities\[13,14\] also play an important role in studies of percolation. For lattices drawn on a torus, the analogous quantities are wrapping probabilities\[15\], and in two dimensions their values can be determined exactly\[16\]. The three-dimensional case\[17\] has been far less studied however. Precise estimation of wrapping probabilities on the simple-cubic lattice represents one of the central undertakings of the current work.

In addition to their intrinsic importance, wrapping probabilities have proved to be an effective practical means of estimating percolation thresholds\[18,19\]. Using Monte Carlo (MC) simulations and performing a careful finite-size scaling analysis of various wrapping probabilities in the neighborhood of the transition, we obtain very accurate estimates of \(p_c\) for both site and bond percolation. We observe numerically that the leading finite-size corrections for certain wrapping probabilities appear to be governed by an exponent \(y_c \approx -2\), rather than by the leading irrelevant exponent \(y_t \approx -1.2\).

We then estimate the thermal exponent \(y_t = 1/\nu\) by fixing \(p\) to our best estimate of \(p_c\), and studying the divergence with linear size \(L\) of the derivative of the wrapping probability, which is proportional to the covariance of its indicator with the number of bonds. We find this procedure for estimating \(y_t\) preferable to methods in which \(y_t\) is estimated by studying how quantities behave in a neighborhood of \(p\) values around \(p_c\). In particular, we believe the current method produces more reliable error estimates.

The remainder of this paper is organized as follows. The simulation method and the sampled quantities are discussed in Sec. IV. The results for the wrapping probabilities and thresholds are given in Sec. III. Critical exponents and the excess cluster number are discussed in Sec. IV. We then finally conclude with a discussion in Sec. V.

II. SAMPLED QUANTITIES

We study bond and site percolation on a periodic \(L \times L \times L\) simple-cubic lattice with linear system sizes \(L = 8, 12, 16, 24, 32, 48, 64, 128, 256\), and \(512\). For each system size, we produced at least \(2 \times 10^7\) independent samples. Each independent bond (site) configuration is generated by independently occupying each bond (site) with probability \(p\). The clusters in each configuration are...
TABLE I: Fits of the wrapping probabilities $R^{(x)}$, $R^{(y)}$, and $R^{(z)}$, and the ratios $Q_1$ and $Q_2$ for bond percolation. We did not obtain stable fits with $y$ free for $R^{(z)}$.

| $L_{min}$ | $\chi^2$/DF | $y_0$ | $Q_c$ | $p_c$ | $b_1$ | $y_1$ | $b_2$ |
|-----------|-------------|------|-------|-------|-------|-------|-------|
| 16        | 53/40       | 0.2481203(5) | 1.16(1) | 0.86537(1) | -0.36(1) | -0.0423(5) | -1.2 | 0.341(5) |
| 24        | 33/33       | 0.2481198(6) | 1.16(2) | 0.86535(2) | -0.31(2) | -0.040(2) | -1.2 | 0.31(2)  |
| 28/26     | 0.248193(7) | 1.19(3) | 0.86533(2) | -0.31(3) | -0.036(3) | -1.2 | 0.25(5)  |
| 16        | 44/39       | 0.248184(8) | 1.16(1) | 0.86539(3) | -0.36(1) | -0.10(4) | -1.34(9) | 0.50(8) |
| 24        | 31/32       | 0.248188(9) | 1.19(2) | 0.86529(4) | -0.32(3) | -0.10(8) | -1.3(2)  | 0.5(2)   |
| 32        | 28/25       | 0.248196(14) | 1.19(3) | 0.8654(2) | -0.31(3) | -0.02(4) | -1.0(5) | 0.2(3)   |
| 32        | 28/25       | 0.248196(14) | 1.19(3) | 0.8654(2) | -0.31(3) | -0.02(4) | -1.0(5) | 0.2(3)   |
| 48        | 16/18       | 0.248195(14) | 1.14(2) | 0.86350(3) | -0.39(8) | -0.088(9) | -1.2 | -0.3(2)  |
| 64        | 10/11       | 0.248184(11) | 1.12(3) | 0.8634(2) | -1.0(2) | -0.05(4) | -1.2 | -1(1)    |
| 32        | 28/25       | 0.248196(14) | 1.19(3) | 0.8654(2) | -0.31(3) | -0.02(4) | -1.0(5) | 0.2(3)   |
| 48        | 16/19       | 0.248193(14) | 1.14(2) | 0.86346(7) | -0.89(8) | -0.15(4) | -1.22(7) |
| 64        | 10/12       | 0.248182(11) | 1.12(3) | 0.8633(2) | -1.0(2) | -0.05(4) | -1.5(4) |

We sampled the following observables in our simulations:

(a) The number of occupied bonds $N_b$ for bond percolation, and the number of occupied sites $N_c$ for site percolation.

(b) The number of clusters $N_c$.

(c) The size $C_1$ of the largest cluster.

(d) The cluster-size moments $S_m = \sum C |C|^m$ with $m = 0, 2, 4$. The sum runs over all clusters $C$, and $S_0$ is simply the number of clusters.

(e) An observable $S := \max \max d(x_C, y)$ used to determine the shortest-path exponent. Here $d(x, y)$ denotes the graph distance from site $x$ to site $y$, and $x_C$ is the vertex in cluster $C$ with the smallest vertex label, according to some fixed (but arbitrary) vertex labeling.

(f) The indicators $R^{(x)}$, $R^{(y)}$, and $R^{(z)}$, for the event that a cluster wraps around the lattice in the $x$, $y$, or $z$ direction, respectively.

From these observables we calculated the following quantities:

(i) The mean size of the largest cluster $C_1 = \langle C_1 \rangle$, which at $p_c$ scales as $C_1 \sim L^{y_h}$ with $y_h = d_f - \beta/\nu$, where $d_f$ is the fractal dimension.

(ii) The cluster density $\rho = \langle N_c \rangle/L^d$.

(iii) The mean size of the cluster at the origin, $\langle C \rangle = \langle C \rangle_0$, which at $p_c$ scales as $\langle C \rangle \sim L^{2y_h-d}$.

(iv) The dimensionless ratios

$$Q_1 = \frac{\langle C_1 \rangle^2}{\langle C_1 \rangle^2}, \quad Q_2 = \frac{\langle S_2 \rangle^2}{3 \langle S_2 \rangle^2 - 2 \langle S_4 \rangle}.$$  

(v) The shortest-path length $S = \langle S \rangle$, which at $p_c$ scales as $S \sim L^{d_{min}}$ with $d_{min}$ the shortest-path fractal dimension.

(vi) The wrapping probabilities

$$R^{(x)} = \langle R^{(x)} \rangle = \langle R^{(y)} \rangle = \langle R^{(z)} \rangle,$$

$$R^{(a)} = 1 - (1 - R^{(x)})(1 - R^{(y)})(1 - R^{(z)}),$$

$$R^{(3)} = \langle R^{(x)} R^{(y)} R^{(z)} \rangle.$$
Here \( R^{(x)} \) gives the probability that a winding exists in the \( x \) direction, \( R^{(a)} \) gives the probability that a winding exists in at least one of the three possible directions, and \( R^{(3)} \) gives the probability that windings simultaneously exist in all three possible directions. Near \( p_c \), we expect each of these wrapping probabilities to behave as \( \sim f((p - p_c)L^\nu) \), where \( f \) is a scaling function.

(vii) The covariance of \( R^{(x)} \) and \( N_b \)

\[
g_{bR}^{(x)} = \langle R^{(x)}N_b \rangle - \langle R^{(x)} \rangle \langle N_b \rangle = p(1-p)\frac{\partial R^{(x)}}{\partial p}. \tag{3}
\]

At \( p_c \), we expect \( g_{bR}^{(x)} \sim L^\nu \). An analogous definition of \( g_{bR}^{(x)} \) with \( N_b \) being replaced with \( N_a \), was used for site percolation.

To derive \( g_{bR}^{(x)} \), one can explicitly differentiate \( \langle R^{(x)} \rangle \) with respect to \( p \), and use the fact that \( \langle N_b \rangle = p|E| \) where \(|E| \) is the total number of edges on the lattice.

The complete set of data for all observables, for both bond and site percolation, is available as Supplemental Material \[20\].

III. ESTIMATING \( p_c \)

A. Bond percolation

We estimate the thresholds of bond and site percolation by studying the finite-size scaling of the wrapping probabilities \( R^{(x)} \), \( R^{(a)} \), and \( R^{(3)} \), and the dimensionless ratios \( Q_1 \) and \( Q_2 \). Around \( p_c \), we perform least-squares fits of the MC data for these quantities by the ansatz

\[
O(\epsilon, L) = O_c + \sum_{k=1}^{2} q_k \epsilon^k L^{k\nu} + b_1 L^\nu + b_2 L^{-2}, \tag{4}
\]

where \( \epsilon = p_c - p \), \( O_c \) is a universal constant, and \( y_i \) is the leading correction exponent. We perform fits with both \( b_1 \) and \( b_2 \) free, as well as fits with \( b_2 \) being set identically to zero. By performing fits with \( y_i \) free we estimate that \( y_i = -1.2(2) \). We also perform fits with \( y_i \) fixed to \( y_i = -1.2 \).

As a precaution against correction-to-scaling terms that we have neglected in our chosen ansatz, we impose a lower cutoff \( L \geq L_{\text{min}} \) on the data points admitted in the fit, and we systematically study the effect on the \( \chi^2 \) value of increasing \( L_{\text{min}} \). In general, our preferred fit for any given ansatz corresponds to the smallest \( L_{\text{min}} \) for which \( \chi^2 \) divided by the number of degrees of freedom (DFs) is \( O(1) \), and for which subsequent increases in \( L_{\text{min}} \) do not cause \( \chi^2 \) to drop by much more than one unit per degree of freedom.

Table \[\ref{tab:fit_results}\] summarizes the results of these fits. From the fits, we can see that the finite-size corrections of \( Q_1 \) and \( Q_2 \) are dominated by the exponent \( y_i \approx -1.2 \). From \( Q_1 \) and \( Q_2 \), we estimate \( p_c = 0.2488119(3) \), and their universal critical values \( Q_{1,c} = 0.8654(2) \) and \( Q_{2,c} = 0.6335(2) \).

For \( R^{(x)} \) and \( R^{(a)} \), fixing \( y_i = -1.2 \) and including both the \( b_1 \) and \( b_2 \) terms we find that \( b_1 \) is consistent with zero, while \( b_2 \) is clearly nonzero. Furthermore, if we set \( b_2 = 0 \) and leave \( y_i \) free, we find \( y_i \approx -2 \). This suggests that either the amplitudes of the leading corrections of \( R^{(x)} \) and \( R^{(a)} \) vanish identically, or at least that they are sufficiently small that they cannot be detected from our data. Due to these weak finite-size corrections, the values of \( p_c \) fitted from \( R^{(x)} \) and \( R^{(a)} \) are much more stable than those obtained from \( Q_1 \) and \( Q_2 \). From \( R^{(x)} \) and \( R^{(a)} \), we estimate \( p_c = 0.2488118(2) \). For \( R^{(3)} \), we report only the fits with corrections \( b_1 L^{-1.2} + b_2 L^{-2} \). If \( y_i \) is left free the fits become unstable, regardless of whether the \( b_2 L^{-2} \) term is included. From \( R^{(3)} \), we estimate \( p_c = 0.24881185(15) \) which is consistent with the value obtained from \( R^{(x)} \) and \( R^{(a)} \). From these fits, we estimate the universal wrapping probabilities to be \( R_{c}^{(x)} = 0.25778(6) \), \( R_{c}^{(a)} = 0.45997(8) \) and \( R_{c}^{(3)} = 0.08041(8) \).

In Fig. \[\ref{fig:results}\] we illustrate our estimate of \( p_c \) by plotting...
TABLE II: Fits of the wrapping probabilities $R^{(x)}$, $R^{(a)}$, and $R^{(3)}$, and the ratios $Q_1$ and $Q_2$ for site percolation. For $R^{(x)}$ we obtain unstable results when $y_i$ is free.

| $L_{\text{min}}$ | $\chi^2/\text{DF}$ | $p_c$ | $y_1$ | $Q_c$ | $q_1$ | $b_1$ | $y_2$ | $b_2$ |
|------------------|----------------|--------|-------|-------|-------|-------|-------|-------|
| 32               | 19/16          | 0.311 606 9(2) | 1.14(2) | 0.865 05(2) | −0.22(2) | 0.062(2) | −1.2 | 0(3) |
| 48               | 11/11          | 0.311 607 0(2) | 1.11(3) | 0.865 09(3) | −0.25(3) | 0.054(6) | −1.2 | 0.2(2) |
| 32               | 19/16          | 0.311 606 9(2) | 1.15(2) | 0.865 06(3) | −0.22(2) | 0.063(4) | −1.1(2) | - |
| 48               | 10/11          | 0.311 607 1(2) | 1.11(3) | 0.865 12(4) | −0.25(3) | 0.09(2) | −1.2(2) | - |
| 32               | 10/11          | 0.311 607 3(2) | 1.12(6) | 0.865 27(5) | −0.24(6) | 0.09(10) | −1.8(3) | - |
| 64               | 3/6            | 0.311 607 6(2) | 1.12(4) | 0.633 3(1) | −0.56(9) | 0.02(3) | −1.2 | 5.1(7) |
| 48               | 13/11          | 0.311 607 2(1) | 1.14(2) | 0.633 06(4) | −0.52(4) | 0.9(1) | −1.52(3) | - |
| 64               | 2/6            | 0.311 607 6(2) | 1.12(4) | 0.633 29(8) | −0.56(9) | 0(2) | −1.9(2) | - |

$R^{(x)}$ and $R^{(a)}$ vs $L$. Precisely at $p = p_c$, as $L \to \infty$ the data should tend to a horizontal line, whereas the data with $p \neq p_c$ will bend upward or downward. Figure 1 shows that our estimate of $p_c$ lies slightly below the central value 0.248 812 6 reported in [21].

In Fig. 2 we plot the data at $p = 0.248 811 8$ for $R^{(x)}$ and $R^{(a)}$ vs $L^{-1.2}$, and for $Q_1$ and $Q_2$ vs $L^{-1.2}$. The figure strongly suggests that the correction $L^{-1.2}$ dominates in $Q_1$ and $Q_2$, but vanishes (or is very weak) in $R^{(x)}$ and $R^{(a)}$.  

B. Site percolation

For site percolation, we again estimate $p_c$ by fitting $Q_1$ and $Q_2$, $R^{(x)}$, $R^{(a)}$, and $R^{(3)}$ with Eq. (1). The fitting procedure is similar to that of bond percolation, and the results are summarized in Table I. From the table, we can see that the fits of $Q_1$ and $Q_2$ are less stable for site percolation than for bond percolation. The ratio of $\chi^2$ per DF remains large until $L_{\text{min}} \geq 32$ for $Q_1$ and $L_{\text{min}} \geq 48$ for $Q_2$, and the resulting estimates of $p_c$ range from 0.311 606 9(2) to 0.311 607 7(3).

The fits of the wrapping probabilities are better behaved, as was the case for bond percolation. For $R^{(3)}$, fixing $y_i = -1.2$ and including both the $b_1$ and $b_2$ terms, we find that $b_1$ is consistent with zero, while $b_2$ is clearly nonzero. Furthermore, if we set $b_2 = 0$ and leave $y_i$ free, we find $y_i \approx -2$. This suggests that the amplitude of the leading correction of $R^{(3)}$ is smaller than the resolution of our fits, and might possibly be zero. The fits of the $R^{(a)}$ data, however, quite clearly indicate the presence of the $b_1 L^{-1.2}$ term. For $R^{(a)}$, we report only the fits with corrections $b_1 L^{-1.2} + b_2 L^{-2}$; if $y_i$ is left free the fits become unstable, regardless of whether the $b_2 L^{-2}$ term is included. As for $R^{(a)}$, the amplitude $b_1$ appears to take a nonzero value. These observations suggest that the leading correction $L^{-1.2}$ does not generically vanish for all wrapping probabilities, but rather that the amplitudes in some cases are smaller than the resolution of our simulations.

Comparing the various fits, we estimate $p_c = 0.311 607 7(2)$ for site percolation, which is consistent with the previous result 0.311 607 7 (4) [22]. In addition, we estimate the universal wrapping probabilities to be $R^{(x)} = 0.257 82(6)$, $R^{(a)} = 0.459 99(8)$, and $R^{(3)} = 0.080 46(6)$, which are consistent with those estimated from bond percolation. In Fig. 3 we show plots of $R^{(x)}$ and $R^{(a)}$ which illustrate our estimate of $p_c$.

IV. RESULTS AT $p_c$

In this section, we estimate the critical exponents $y_i$, $y_h$, and $d_{\text{min}}$, as well as the excess cluster number. Fixing $p$ at our estimated thresholds for bond and site percolation, we study the covariances $g_{bR}$ and $g_{sR}$, the mean
size of the largest cluster $C_1$, the mean size of the cluster at the origin, $\chi$, the shortest-path length $S$, and the cluster density $\rho$. The MC data for $g_{bR}(x)$, $g_{sR}(x)$, $C_1$, $\chi$ and $S$ are fitted by the ansatz

$$A = L^{y_s}(a_0 + b_1 L^{-1.2} + b_2 L^{-2})$$

We perform fits using different combinations of the two corrections $b_1 L^{-1.2}$ and $b_2 L^{-2}$ and compare the results.

### A. Estimating $y_t$

We estimate $y_t$ by studying the covariances $g_{bR}(x)$ and $g_{sR}(x)$ both of which scale as $\sim L^{y_t}$ at the critical point. We find this procedure for estimating $y_t$ preferable to methods, such as that employed in [22], in which $y_t$ is estimated by studying how quantities behave in the neighborhood of $p_c$ as the system deviates from criticality. In particular, we believe the current method produces more reliable error estimates.

We fit the data for $g_{bR}(x)$ at $p = 0.2488118$ and $g_{sR}(x)$ at $p = 0.3116077$ to Eq. [22], and the results are shown in Table III. The estimate of $y_t$ from $g_{sR}(x)$ produces a smaller error bar than that from $g_{bR}(x)$. From these fits we take our final, somewhat conservative, estimate to be $y_t = 1.1410(15)$.

In Fig. [3] we plot $(\ln g_{bR}(x) - y_t \ln L)$ and $(\ln g_{sR}(x) - y_t \ln L)$ vs $\ln L$ using three different values of $y_t$: our estimate, as well as our estimate plus or minus three standard deviations. Using the true value of $y_t$ should produce a horizontal line for large $L$. In the figure, the data using $y_t = 1.1365$ and $y_t = 1.1455$ respectively bend upward and downward, suggesting that the true value of

![Fig. 2: Plots of $Q_1$ and $Q_2$ vs $L^{-1.2}$ (top), and $R^{(x)}$ and $R^{(s)}$ vs $L^{-2}$ (bottom), with $p = 0.2488118$, for bond percolation. The solid lines are simply to guide the eye.](image1)

![Fig. 3: Plots of $R^{(x)}(p,L)$ (top) and $R^{(s)}(p,L)$ (bottom) vs $L$ for fixed values of $p$, for site percolation. In both cases, the curves correspond to our preferred fit of the MC data for $R(p,L)$ by ansatz [22]: the dashed curve corresponds to setting $p = 0.3116077$. The shaded blue strips indicate an interval of $1\sigma$ above and below the estimates $R^{(x)}_c = 0.25782(6)$ and $R^{(s)}_c = 0.45999(8)$.](image2)
TABLE IV: Fits of $C_1$ and $\chi$. The superscripts $b$ and $s$ denote bond and site percolation, respectively.

| $L_{\text{min}}$ | $\chi^2$/DF | $y_h$ | $a_0$ | $b_1$ | $b_2$ |
|------------------|---------------|--------|--------|--------|--------|
| $C_1^b$          |               |        |        |        |        |
| 16               | 3/4           | 2.52286(5) | 0.9394(3) | -0.014(6) | 0.22(4) |
| 24               | 3/3           | 2.52289(7) | 0.9393(4) | -0.009(11) | 0.2(1)  |
| 24               | 5/4           | 2.52298(3) | 0.9388(2) | 0.009(2)  | -       |
| 32               | 3/3           | 2.52294(4) | 0.9390(2) | 0.005(3)  | -       |
| $\chi^s$         |               |        |        |        |        |
| 16               | 4/4           | 2.5230(3)  | 1.1257(5) | 0.14(1)  | 0.18(7) |
| 24               | 3/3           | 2.52300(5) | 1.1262(7) | 0.12(2)  | 0.3(2)  |
| 24               | 6/4           | 2.52308(3) | 1.1251(3) | 0.15(4)  | -       |
| 32               | 4/3           | 2.52305(3) | 1.1255(4) | 0.151(6) | -       |
| $C_1^s$          |               |        |        |        |        |
| 16               | 5/3           | 2.52299(3) | 0.4716(7) | 0.024(2) | -0.44(2) |
| 24               | 5/3           | 2.52300(5) | 0.4712(2) | 0.024(4) | -0.45(4) |
| $\chi^s$         |               |        |        |        |        |
| 32               | 0.9/2         | 2.52291(5) | 0.2841(2) | -0.001(7) | -1.15(9) |
| 48               | 0.7/1         | 2.52294(9) | 0.2840(4) | -0.007(18)| -1.3(3)  |
| 32               | 0.9/3         | 2.52292(1) | 0.2840(6) | -        | -1.16(1) |
| 48               | 0.9/2         | 2.52291(2) | 0.2840(8) | -        | -1.17(5) |

$y_h$ does indeed lie within $3\sigma$ of our estimate. The data with $y_h = 1.141$ appear to be consistent with an asymptotically horizontal line. We note that while the curve appears to be increasing around the point at $L = 512$ for bond percolation, it instead slightly decreases for site percolation, suggesting that in fact this movement is dominated (or even entirely caused) by noise.

B. Estimating $y_h$

We estimate $y_h$ by studying the divergence of $C_1$ and $\chi$ as $L$ increases with $p$ fixed to our best estimates of $p_c$. We fit the MC data for $C_1$ and $\chi$ with Eq. (5), with the exponent $y_A$ then corresponding to $y_h$ and $2y_h - d$, respectively. The results are reported in Table IV. We use superscripts $b$ and $s$ to distinguish bond and site percolation. For $C_1^b$ and $\chi^s$, the amplitude $b_1$ is quite small, while $b_1$ in $\chi^b$ and $C_1^s$ is clearly present. In the fits of $\chi^s$ with one correction term $b_1 L^{-1.2}$, the ratio of $\chi^2$ per DF remains large until $L_{\text{min}} \geq 64$. We therefore show the fits with the correction $b_2 L^{-2}$ instead. Comparing these fits, we estimate $y_h = 2.52295(15)$.

In Fig. 5, we plot $(\ln C_1^b - y_h \ln L)$ and $(\ln C_1^s - y_h \ln L)$ vs $\ln L$ using three different values of $y_h$: our estimate, as well as our estimate plus or minus three standard deviations. As $L$ increases, the data with $y_h = 2.52250$ and $2.52340$ respectively slope upward and downward, while the data with $y_h = 2.52295$ are consistent with an asymptotically horizontal line.

C. Estimating $d_{\text{min}}$

We estimate the shortest-path fractal dimension $d_{\text{min}}$ by studying the quantity $S$ at our estimated thresholds.
TABLE V: Fits of $S$. The superscripts $b$ and $s$ denote bond and site percolation, respectively.

| $L_{\text{min}}$ | $\chi^2$/DF | $d_{\text{min}}$ | $a_0$ | $b_1$ | $b_2$ |
|------------------|--------------|-----------------|-------|-------|-------|
| 24               | 2/3          | 1.375 26(5)     | 1.814 9(5) | $-0.65(2)$ | $-3.8(2)$ |
| 32               | 1/2          | 1.375 33(7)     | 1.814 2(7)  | $-0.59(5)$ | $-4.4(4)$ |
| 48               | 0/2          | 1.375 30(9)     | 1.815 1(1)  | $-0.63(9)$ | $-4(1)$  |
| 16               | 5/4          | 1.375 80(2)     | 1.383 4(2)  | $-3.32(5)$ | $2.72(3)$ |
| 24               | 4/4          | 1.375 77(3)     | 1.383 6(3)  | $-3.45(2)$ | $2.82(3)$ |
| 32               | 4/2          | 1.375 76(5)     | 1.383 7(4)  | $-3.45(3)$ | $2.9(3)$  |

TABLE VI: Fits of $\rho$. The superscripts $b$ and $s$ denote bond and site percolation, respectively.

| $L_{\text{min}}$ | $\chi^2$/DF | $\rho_c$ | $b$  | $b_0$ |
|------------------|--------------|----------|------|-------|
| 10               | 3/5          | 0.272 932 83(1) | 0.679(3) | 0.1(6) |
| 24               | 1/4          | 0.272 932 83(1) | 0.674(6) | 3(4)  |
| 10               | 2/7          | 0.272 932 83(1) | 0.678 9(6) | -     |
| 24               | 2/6          | 0.272 932 83(1) | 0.679(2) | -     |
| 12               | 4/6          | 0.052 438 218(3) | 0.674 5(5) | 0.02(8) |
| 16               | 4/5          | 0.052 438 218(3) | 0.674 7(8) | $-0.02(21)$ |
| 24               | 4/4          | 0.052 438 218(3) | 0.674 2(2) | $0.2(10)$ |
| 12               | 4/7          | 0.052 438 218(3) | 0.674 6(2) | -     |
| 16               | 4/6          | 0.052 438 218(3) | 0.674 6(3) | -     |
| 24               | 4/5          | 0.052 438 218(3) | 0.674 6(5) | -     |

The MC data for $S$ are fitted to Eq. (1) with the exponent $y_A$ replaced by $d_{\text{min}}$, and the results are reported in Table V. We again use the superscripts $b$ and $s$ to distinguish bond and site percolation. In the fits, both $b_1$ and $b_2$ are clearly observable for $S^b$ and $S^s$. And when we set $b_2 = 0$, the ratio of $\chi^2$ per DF remains relatively large. We also did the fits by replacing the correction with $b_2$ by a constant term $c_0$ in Eq. (1), and obtained $d_{\text{min}}(\text{bond}) = 1.375 55(6)$ and $d_{\text{min}}(\text{site}) = 1.375 59(6)$. Comparing these fits, we estimate $d_{\text{min}} = 1.375 6(3)$.

To illustrate this estimate, Fig. 6 shows a log-log plot of $S$ versus $L$.

D. Excess number of clusters

The cluster density tends to a finite limit $\rho_c = \lim_{L \to \infty} \lim_{p \to p_c} \rho$ at criticality. While the value of $\rho_c$ is non-universal, the excess cluster number $b := \lim_{L \to \infty} \lim_{p \to p_c} L^d (\rho - \rho_c)$ is universal [28]. To estimate $b$, we study $\rho$ with $p$ fixed to our estimated thresholds for bond and site percolation and fit the data to the ansatz

$$\rho = \rho_c + L^{-3}(b + b_1 L^{-2}) .$$

The resulting fits are summarized in Table VI, where we again use superscripts $b$ and $s$ to differentiate the bond and site cases. We report fits both with $b_1$ free and with $b_1 = 0$. We find that $\rho_c$ can be well fitted to (1) with $b_1 = 0$ fixed. Leaving $b_1$ free, we find that $b_1$ is consistent with zero, suggesting that the leading correction exponent might be even smaller than $-2$. We also performed fits in which the leading correction exponent was fixed to $-1.2$ and $-3$, and in both cases the resulting estimates of $\rho_c$ and $b$ were consistent with those reported in Table VI. Leaving the leading correction exponent free produces unstable fits however. Comparing these fits, we estimate $b = 0.675(2)$.

Our estimate of $b$ is determined on the periodic $L \times L \times L$ simple cubic lattice; on the $L \times L$ square lattice $b = 0.8835(8)$ [28]. The excess cluster number was studied in [21] on an $L \times L \times L'$ lattice with $L' \gg L$. Naively, extrapolating their results to $L' = L$ gives an estimate of $b \approx 0.412$ which is significantly below our estimate. We also note that our estimate of the number of clusters $\rho_c = 0.272 932 83(1)$ differs slightly from the estimate $\rho_c = 0.272 931 0(5)$ reported in [21].

V. DISCUSSION

We study in this paper standard bond and site percolation on the three-dimensional simple-cubic lattice with periodic boundary conditions. Using extensive Monte Carlo simulations and finite-size scaling analysis, we report the estimates: $p_c = 0.24881182(10)$ (bond) and $p_c = 0.311 607 7(2)$ (site). The bulk thermal and magnetic exponents are estimated to be $y_t = 1.140(5)$ and $y_h = 2.52295(15)$, the shortest-path fractal dimension to be $d_{\text{min}} = 1.375 6(3)$, and the leading irrelevant exponent to be $y_t = -1.2(2)$. The universal value of the excess cluster number is estimated to be $b = 0.675(2)$.

We emphasize that the reported estimates of $\rho_c$ are obtained by studying wrapping probabilities, which are found to have weaker corrections to scaling than dimensionless ratios constructed from moments of magnetic quantities such as $C_1$ and $S_0$. In particular, we find evidence suggesting that the leading correction exponent in certain wrapping probabilities ($R(x)$ and $R(y)$ for bond percolation, $R(z)$ for site percolation) may be $\approx -2$ rather than $-1.2$, although the reasons are not clear. The universal values of the wrapping probabilities we studied are estimated to be: $R^{(x)} = 0.25780(6)$,
We obtain less of whether a winding exists in the third direction. It is clear that a winding exists in two given directions, regardless of whether a winding exists in the third direction but not in the other two directions; and in words, \( R^c(1) \) is the probability that a winding exists in two given directions but not in the third; and \( R^c(3) \) is the probability that a winding exists in two given directions, regardless of whether a winding exists in the third direction. We obtain \( R^c(1) = 0.075 \) (14), \( R^c(2) = 0.050 \) (14), and \( R^{(x,y)} = 0.131 \) (29(12)).

Table VII summarizes the estimates presented in this work. For comparison, we also provide an (incomplete) summary of previous estimates.

\[
\begin{array}{cccccccccc}
\text{Ref.} & p_c (\text{bond}) & p_c (\text{site}) & y_t = 1/\nu & y_t = d_f & d_{\text{min}} & y_t & R^{(1)} & R^{(2)} & R^{(3)} & b \\
\hline
[21] & 0.248812(6) & 0.311608(4) & 1.121(2) & 2.523(4) & & & & & & \\
[22] & 0.2490(2) & 0.3115(3) & 1.141(2) & 2.523(4) & & & & & & \\
[24] & 0.2488120(5) & 0.3116077(4) & 1.1456(7) & 2.5226(1) & & & & & & \\
[25] & 0.2488120(5) & 0.3116077(4) & 1.1456(7) & 2.5226(1) & & & & & & \\
[26] & 0.248811(2) & 0.311607(2) & 1.1410(15) & 2.52295(15) & 1.3756(3) & 1.142(6) & 1.3756(3) & 1.142(6) & 0(2) & \\
\end{array}
\]

The final error bars reported in [22] were also underestimated, taking insufficient account of systematic errors.

\( R^{(a)} = 0.59598(8) \), and \( R^{(3)} = 0.08044(8) \), by comparing the results for bond and site percolation.

\[
R^c(1) = \langle R^c(x) (1 - R^c(y)) (1 - R^c(z)) \rangle = \frac{1}{3} (2R^c(a) + R^c(3) - 3R^c(x)) ,
\]

\[
R^c(2) = \langle R^c(x) R^c(y) (1 - R^c(z)) \rangle = \frac{1}{3} (3R^c(x) - 2R^c(3) - R^c(a)) ,
\]

\[
R^{(x,y)} = \langle R^c(x) R^c(y) \rangle = \frac{1}{3} (3R^c(x) + R^c(3) - R^c(a)) .
\]

\[ R^{(x,y)} = 0.13129(12) .\]

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