Convergence of threshold estimates for two-dimensional percolation

R. M. Ziff
Michigan Center for Theoretical Physics and Department of Chemical Engineering,
University of Michigan, Ann Arbor, MI 48109–2136

M. E. J. Newman
Department of Physics, University of Michigan, Ann Arbor, MI 48109–1120 and
Santa Fe Institute, 1399 Hyde Park Road, Santa Fe, NM 87501

Using a recently introduced algorithm for simulating percolation in microcanonical (fixed-occupancy) samples, we study the convergence with increasing system size of a number of estimates for the percolation threshold for an open system with a square boundary, specifically for site percolation on a square lattice. We show that the convergence of the so-called “average-probability” estimate is described by a non-trivial correction-to-scaling exponent as predicted previously, and measure the value of this exponent to be 0.90 ± 0.02. For the “median” and “cell-to-cell” estimates of the percolation threshold we verify that convergence does not depend on this exponent, having instead a slightly faster convergence with a trivial analytic leading exponent.

I. INTRODUCTION

Percolation \[\square\] is one of the most fundamental and widely studied systems in statistical physics. Theoretical studies of percolation models and applications of percolation theory to physical systems have spawned thousands of papers over the last few decades. Even so, there are some substantial gaps in our understanding of percolation. For example, we have at present no exact value for the position \(p_c\) of the percolation threshold for site percolation on that simplest of two-dimensional lattices, the square lattice. And in three dimensions we have almost no exact results whatsoever. Because of this, numerical methods have played an important role in the study of percolation. In this paper we consider a class of methods for estimating \(p_c\) for site percolation using finite-size scaling, and show how various estimates of \(p_c\) in this class scale with varying system size in two dimensions.

The methods studied here for measuring \(p_c\) are widely used and are all based upon consideration of the crossing-probability function \(R_L(p) \equiv \mathbb{P}\{\text{crossing}\}\). This function gives the probability that a connected path crosses the system from one boundary segment to another, at site occupation probability \(p\) and system size or length-scale \(L\). Some examples of these estimates are:

1. The renormalization-group (RG) fixed-point estimate \(p_{\text{RG}}(L) = p^*(L)\), where \(p^*\) is the solution to the equation \[\Box\]:

\[
R_L(p) = p. \tag{1}
\]

2. The average value of \(p\) at which crossing first occurs \[\Box\]:

\[
p_{\text{av}}(L) = \langle p \rangle = \int_0^1 p R_L(p) \, dp = 1 - \int_0^1 R_L(p) \, dp, \tag{2}
\]

where the last equality follows from integrating by parts. The prime indicates differentiation with respect to \(p\).

3. The estimate \(p_{RL}(L)\) corresponding to the point where \(R_L(p)\) equals its universal infinite-system value \(R_c \equiv R_\infty(p_c)\) (which is determined by the system shape and boundary conditions) \[\Box\]:

\[
R_L(p) = R_c. \tag{3}
\]

For a square system, where \(R_c = \frac{1}{2}\), this estimate \(p_{0.5}(L)\) corresponds to the median of the distribution \(R(p)\). A related estimate \(p_{h+v}(L)\) for rectangular systems is the value of \(p\) at which the horizontal and vertical crossing probabilities sum to unity \[\Box\]:

\[
R_L^{(h)}(p) + R_L^{(v)}(p) = 1. \tag{4}
\]

This estimate is identical to \(p_{RL}(L) = p_{0.5}(L)\) when the boundary is a perfect square.

4. The estimate \(p_{\text{max}}(L)\) which is the value of \(p\) at which \(R_L'(p)\) reaches a maximum (or equivalently, where \(R_L(p)\) is at its inflection point) \[\Box\]:

\[
R_L'(p) = 0. \tag{5}
\]

5. The cell-to-cell RG estimate, which is the point where two systems of different size have the same value of \(R\) \[\Box\]. One possible choice for this estimate, \(p_{c-e}^{(1)}(L)\), is the value of \(p\) at which

\[
R_L(p) = R_{L-1}(p), \tag{6}
\]

while a second, \(p_{c-e}^{(2)}(L)\), is the point at which

\[
R_L(p) = R_{L/2}(p). \tag{7}
\]
In order to use these estimates to determine the threshold precisely, we need to know the manner in which they converge to \( p_c \) as \( L \to \infty \). While it is possible to simulate very large systems for which finite-size effects may be quite small, the statistics for such simulations are still relatively poor because of the small number of samples that can typically be generated. In most cases, better results can be derived by doing more simulations on smaller systems, and this requires that the finite-size behavior is characterized accurately.

It is usually assumed (based upon very general scaling arguments) that all finite-system estimates of the percolation threshold converge to the bulk value \( p_c \) as

\[
P_{\text{est}}(L) - p_c \sim c L^{-1/\nu}\tag{8}
\]

where \( c \) is a system-dependent constant, and \( \nu \) is the exponent governing the correlation length \( \xi \), such that \( \xi \sim |p - p_c|^{-\nu} \). (For the two-dimensional systems we will be looking at in this paper \( \nu = \frac{4}{3} \).) Well known exceptions to this behavior are a few highly symmetric, self-dual systems, such as bond percolation on a square lattice with a square boundary, and site percolation on a triangular lattice with a rhomboidal boundary; in both these cases \( R_L(p) \) is perfectly symmetric about \( p = \frac{1}{2} \) for all \( L \) and all the estimates above give \( p_c = \frac{1}{2} \) exactly. For these systems, one could consider the constant \( c \) above to be zero.

In Ref. \[5\], however, it was argued that for non-self-dual systems with a square boundary, such as site percolation on a square lattice (where because of the non-duality the estimates show finite-size effects), the convergence of most of those estimates is faster than given by Eq. (8) (a result that has been verified in many numerical studies). The rest of the estimates above should converge according to the faster behavior

\[
P_{\text{est}}(L) - p_c \sim c L^{-1-1/\nu}, \tag{12}
\]

where the constant \( c \) varies from estimate to estimate. Simulations reported in Ref. \[5\] for systems of size up to \( 1024 \times 1024 \) sites verified this convergence for the estimate \( p_{0.5} \) to high accuracy. The estimates \( p_{c-\epsilon}, p_{\text{max}} \) and \( p_{\text{ave}} \) were studied in Ref. \[5\] using only exact enumeration results for systems of sizes up to \( 7 \times 7 \) which give polynomials for \( R \) (see the appendix), and while the behavior of these results was found to be roughly consistent with (12), the uncertainty due to higher-order corrections was large.

Following the publication of Ref. \[5\], Aharony and Hovi \[14, 15\] argued that the irrelevant scaling variables in the renormalization-group treatment of percolation imply a slower leading-order convergence of \( R_L \) to its infinite-system value, characterized by an exponent \( \omega \), whose value was deduced from the Monte-Carlo work of Stauffer \[13\] to be about \( \omega = 0.85 \). (Note that Aharony and Hovi used \( \theta_1 \) to denote the exponent we call \( \omega \).) A variety of series expansion results from the early 1980s were also analyzed to give values for this exponent ranging from 0.89 to over 1 [14, 15].

The argument given by Aharony and Hovi implies that the leading terms in the expansion of \( R_L(p) \) should in fact be

\[
R_L(p) \sim f_0(x) + L^{-\omega} f_\omega(x) + L^{-1} f_1(x) + \ldots \tag{13}
\]

where

\[
f_\omega(x) = c_1 x + c_2 x^2 + \ldots \tag{14}
\]

and

\[
f_0(x) = a_0 + a_1 x + a_2 x^3 + \ldots \tag{10}
\]

\[
f_1(x) = b_0 + b_1 x + b_2 x^2 + \ldots \tag{11}
\]

with \( a_0 = \frac{1}{2} \) by the symmetry and self-duality of the square boundary. The same symmetry also implies that \( f_0 - \frac{1}{2} \) is an odd function in \( x \) and hence that \( a_n = 0 \) for all even \( n > 0 \), as above. (To see that \( f_0 - \frac{1}{2} \) is odd, note that for the perfectly dual system of bond percolation on a square lattice, \( R - \frac{1}{2} \) is an odd function of \( x \) for all \( L \), including \( L = \infty \), and by universality systems with other underlying lattices must behave the same way in the scaling limit.) In Ref. \[3\] no particular assumption was made about the behavior of \( f_1(x) \), other than its analyticity about \( x = 0 \).

Note that the form of \( f_0(x) \) in Eq. (10) is not entirely universal, because the independent variable \( x \) should incorporate a metric factor which depends upon the underlying lattice [14, 15]. For convenience, however, since we are considering only the one system of site percolation on a square lattice in this paper, we do not include that factor here.

Once the above assumptions, Eqs. (11) and (12) are made, the convergence of the various estimates of \( p_c \) is straightforward to analyze, and one finds that while the RG estimate does indeed converge according to Eq. (8) (a result that has been verified in many numerical studies), the rest of the estimates above should converge according to the faster behavior

\[
P_{\text{est}}(L) - p_c \sim c L^{-1-1/\nu}, \tag{12}
\]
Hovi and Aharony argued that the constant term $c_0$ is zero for a square system, because at $p_c$ there are no correction terms for the square-lattice, bond-percolation system, and corrections due to irrelevant variables should be universal. They also argued that $f_1(x)$ should be even, so that $b_1 = 0$ in (11), also by symmetry and self-duality. They discussed various consequences of these assumptions, and presented numerical evidence that the term containing the exponent $\omega$ is indeed the leading correction term, by showing that the behavior of $R_L(p)$ for large $x$ (that is, for $p \neq p_c$) was better fit with such a term than without it. However, the procedure they used did not allow them to determine the value of $\omega$ accurately, because of the numerical difficulty of finding $R_L(p)$ precisely for all $p$. Furthermore, they did not study the convergence of the other estimates given above.

Recently [16, 17], the present authors have shown that quantities like $R_L(p)$ can be studied efficiently for all $p$ by first finding the crossing probability $R_{L,n}$ in a “microcanonical” system of exactly $n$ occupied sites, and then convolving with a binomial distribution to derive results for the corresponding “canonical” system thus:

$$R_L(p) = \sum_{n=0}^{N} \binom{N}{n} p^n (1-p)^{N-n} R_{L,n},$$

(15)

where $N = L^2$ for site percolation on a square lattice. The microcanonical crossing probability is found using an efficient cluster-joining algorithm employing data structures based on trees and a fast method is employed for checking for percolation on the fly during the progress of the calculation. (While many of the ideas incorporated in this method were put forward previously [18, 19, 20, 21, 22, 23], this was the first time that all of these components were combined in this way, for the purpose of finding $R$ efficiently.) In Ref. [17] we studied the function corresponding to $R$ for the probability of a cluster wrapping around the boundary of a periodic system on a torus. In the present paper, we describe how that method can be implemented for crossing of an open system, and we report results from some large-scale simulations. The results allow us to determine accurately the behavior of all of the estimates above, and to test the theoretical predictions that follow from Eq. (13). As we will see, the appearance of the “irrelevant” term in the scaling of some estimates is confirmed, and a new, more precise value of $\omega$ is found.

The outline of the paper is as follows. In Section II we derive the expected scaling behavior of the various estimates of $p_c$, assuming the form (13). In Section III we describe our numerical method, and in Section IV we present the results of our simulations. In Section V we give our conclusions.

II. CONVERGENCE OF ESTIMATES

If we assume Eq. (13) to be a correct description of the behavior of $R_L(p)$, it is straightforward to deduce the resulting convergence of the various estimates for $p_c$. In the following paragraphs we derive the leading correction term for each estimate, or leading two terms when their powers are close to each other.

1. The RG fixed-point: The relevant terms of Eq. (1) are

$$\frac{1}{x} + a_1 x + a_3 x^3 + \ldots = p_c + xL^{-1/\nu},$$

which implies

$$p_{RG}(L) = p_c + \left[ p_c - \frac{1}{a_1} - \frac{a_3(p_c - \frac{1}{a_1})^3}{a_1^3} + \ldots \right] L^{-1/\nu} + O(L^{-2/\nu}).$$

(17)

The term in brackets is the value of $x$ that is the solution to $f_0(x) = p_c$.

2. Average-probability estimate: Eq. (2) gives

$$p_{av}(L) = 1 - L^{-1/\nu} \int_{x_0}^{x_1} f_0(x) + L^{-\omega} f_\omega(x) + L^{-1} f_1(x) \, dx,$$

(18)

where $x_0 = -p_c L^{1/\nu}$ and $x_1 = (1 - p_c) L^{1/\nu}$, which are the values of $x$ at $p = 0$ and 1 respectively. Noting that, since $f_0(x)$ is odd about $f_0(0) = \frac{1}{2}$ and approaches 1 as $x \to \infty$, we have

$$L^{-1/\nu} \int_{x_0}^{x_1} f_0(x) \, dx \sim L^{-1/\nu} x_1 = 1 - p_c,$$

(19)

and we then get

$$p_{av}(L) = p_c + L^{-\omega - 1/\nu} \int_{-\infty}^{\infty} f_\omega(x) \, dx + L^{-1/\nu} \int_{-\infty}^{\infty} f_1(x) \, dx,$$

(20)

where we have extended the limits of the integrals to $\pm \infty$. This result is also implied by Eq. (40) of Ref. [12], for $n = 1$. The order of the next correction depends upon the higher-order corrections to (13).
leading order by the presence of the exponent \( \omega \).

Thus, the scaling of these results, so the leading scaling does not change if \( \lambda \)

b. In doing so, we must ensure that all pointers followed are subsequently changed to point

to the root of their own cluster. The net result of such a bond belong are identified by following pointers

clusters are always made subclusters of larger ones, and all clusters have been joined by the addition of the bond.

We represent this by adding a pointer from the root site of one of the clusters to the root site of the other. Smaller

clusters are always made subclusters of larger ones, and all pointers followed are subsequently changed to point
directly to the root of their own cluster. The net result is an algorithm that can calculate \( \bar{R}_{L,n} \) (and many other

observable quantities) for all values of \( n \) in average running time which is of the order the area of the lattice, or
\( O(L^2) \) for a square lattice.

In our previous calculations using this algorithm we measured the probability of the existence of a cluster
that wraps around the periodic boundary conditions of a toroidal lattice. In this paper we are interested instead
in the existence (or not) of a cluster that spans an open system along one given direction. There are (at least) three
efficient methods for detecting spanning of this kind, two of which are described in detail in Ref. [17] and all of which

Thus, the scaling of \( p_{RG} \), \( p_{0.5} \), and \( p_{c} \) is unaffected to leading order by the presence of the exponent \( \omega \). How-

ever, \( p_{av} \) and \( p_{\text{max}} \) are affected by \( \omega \) to leading order, scaling as \( L^{-\omega-1/\nu} \), slightly slower than predicted in Ref. [2] (order \( L^{-1/\nu} \)). Note that \( b_1 \) does not enter in any of

these results, so the leading scaling does not change if \( b_1 \) is equal to zero, as argued to be the case in Ref. [2].

\[ \frac{1}{2} + a_1 x + b_0 L^{-1} + c_1 x L^{-\omega} + \ldots = \frac{1}{2}, \]

which implies

\[ p_{0.5}(L) = p_c - \frac{b_0}{a_1} L^{-1-1/\nu} + O(L^{-1-\omega-1/\nu}). \]

4. Maximum estimate: Eq. (3) gives

\[ 6a_3 x + 2b_2 L^{-1} + (2c_2 + 6c_3 x) L^{-\omega} + \ldots = 0, \]

which implies

\[ p_{\text{max}}(L) = p_c - \frac{c_2}{3a_3} L^{-\omega-1/\nu} - \frac{b_2}{3a_3} L^{-1-1/\nu} + O(L^{-2\omega-1/\nu}). \]

5. Cell-to-cell estimate: Eq. (3) gives

\[ a_0 + a_1 (p - p_c) L^{1/\nu} + b_0 L^{-1} + c_1 (p - p_c) L^{1/\nu - \omega} + \ldots = a_0 + a_1 (p - p_c) (L - 1)^{1/\nu} + b_0 (L - 1)^{-1} + c_1 (p - p_c) (L - 1)^{1/\nu - \omega} + \ldots \]

which implies

\[ p_{c-\text{c}}^{(1)}(L) = p_c + \frac{b_0}{a_1} \nu L^{-1-1/\nu} + O(L^{-1-\omega-1/\nu}). \]

Likewise, for \( p_{c-\text{c}}^{(2)} \) we have

\[ p_{c-\text{c}}^{(2)}(L) = p_c + \frac{b_0}{a_1 (1 - 2^{-1/\nu})} L^{-1-1/\nu} + O(L^{-1-\omega-1/\nu}). \]

III. PROCEDURE

We have performed simulations to test the scaling hypotheses above using the algorithm described in Refs. [16]
and [17]. Briefly, sites are occupied one by one in random order starting with an empty lattice. Occupied sites form
contiguous clusters, each of which is identified uniquely by the site label of a chosen single site within the
cluster, which we call the “root site.” Other (non-root) sites within a cluster possess pointers that point either directly
to the root site, or to other sites within the cluster such that by following a succession of pointers one can get
from any site to the root. A newly added site is considered to be a cluster of size one, which is its own root site,
and bonds are then added between it and any adjacent occupied sites. The clusters to which sites at either end
of such a bond belong are identified by following pointers from them to their corresponding root sites, and if the
root sites found are different we conclude that two different clusters have been joined by the addition of the bond.
We represent this by adding a pointer from the root site of one of the clusters to the root site of the other. Smaller
clusters are always made subclusters of larger ones, and all pointers followed are subsequently changed to point
directly to the root of their own cluster. The net result is an algorithm that can calculate \( \bar{R}_{L,n} \) (and many other
observable quantities) for all values of \( n \) in average running time which is of the order the area of the lattice, or
\( O(L^2) \) for a square lattice.
we have used in the present work. In the first method, we use the same pointer-based trick that we used in Ref. [16] to detect wrapping with periodic boundary conditions, but start out with an \((L+1) \times (L+1)\) lattice in which one horizontal row of sites is fixed to be permanently empty and one vertical one is fixed occupied. Occurrence of a wrapping cluster in such a system is then exactly equivalent to occurrence of a spanning cluster in the horizontal direction in an open system with dimensions \(L \times L\).

In the second method, two complete rows of sites at the top and bottom of an open \((L+2) \times (L+2)\) lattice are fixed permanently empty, and two columns of \(L\) sites on the left and the right sides of the lattice are fixed occupied. The two columns of occupied sites form two initial clusters on the lattice. By following pointers \(\times 1039\) two initial clusters on the lattice. By following pointers, we can detect when a spanning cluster occurs. Performing this check after the addition of each site to the lattice, we can detect when a spanning cluster is detected, as spanning must also occur for all higher values of \(n\). This produces about a 40% saving in running time.

In the third method, which was used for the major-

Since in the present calculation we are only interested in the existence or not of a system-spanning cluster, we can stop the simulation once a spanning cluster is de-\n
The remaining estimate, \(p_{av}\), could be found directly by performing a numerical integral over \(R_L(p)\). A better method is to use the following exact formula:

\[
p_{av} = 1 - \int_0^1 R_L(p) \, dp
\]

\[
= 1 - \sum_{n=0}^{N} \frac{n}{N} R_{L,n} \int_0^1 p^n (1-p)^{N-n} \, dp
\]

\[
= 1 - \frac{1}{N+1} \sum_{n=0}^{N} R_{L,n}.
\] (29)

Using Eq. (28) this can also be written directly in terms of \(P_{L,n}\) as

\[
p_{av} = 1 - \frac{1}{N+1} \sum_{n=0}^{N} \sum_{n'=0}^{n} P_{L,n^{'}} = \frac{1}{N+1} \sum_{n=0}^{N} n P_{L,n},
\] (30)

which means that the canonical average position of the percolation threshold is \(N/(N+1)\) times the microcanonical average \((1/N) \sum_{n} n P_{L,n}\) and no convolution is necessary to find its value. Higher moments of the distribution \(R'\) can be found in a similar fashion. For the second moment, for example, we have

\[
\langle p^2 \rangle = \int_0^1 p^2 R_L(p) \, dp
\]

\[
= 1 - \frac{2}{(N+1)(N+2)} \sum_{n=0}^{N} (n+1) R_{L,n}
\]

\[
= \frac{1}{(N+1)(N+2)} \sum_{n=0}^{N} n(n+1) P_{L,n}.
\] (31)

To find where \(R''_L(p) = 0\) for the estimate \(p_{max}\), we make use of the following result:

\[
R''_L(p) = \sum_{n=0}^{N} \binom{N}{n} p^n (1-p)^{N-n} R_{L,n} \times \frac{n(n-1)}{p^2} - \frac{2n(N-n)}{p(1-p)} + \frac{(N-n)(N-n+1)}{(1-p)^2}.
\]

(32)

The above three results, along with Eq. (13), demonstrate further the advantage of calculating \(R_L(p)\) through the microcanonical \(R_{L,n}\): quantities like \(R_L(p)\) and \(R''_L(p)\) can be calculated exactly at all \(p\), while \(p_{av}\) can be found without introducing any error through numerical integration.

In the more familiar binary search method for finding \(R_L(p)\), \(p\) is increased or decreased to narrow the bounds on one’s estimate of position of the percolation point for a given realization of the disorder. This search
process is stopped after some number \(m\) of iterations, typically about 15, giving to a resolution of \(2^{-m}\) on the estimate for \(p_c\). Thus, \(R_L(p)\) is evaluated at only a finite set of points, and this adds some uncertainty to the calculation, beyond the basic statistical error. Given a finite set of points, and this adds some uncertainty to the calculation, beyond the basic statistical error. Given that our microcanonical method is also much faster than binary search due to its efficient cluster-merging and percolation-checking, there seems no reason to use other methods.

### IV. RESULTS OF SIMULATIONS

Simulations were carried out for \(L = 7, 8, 16, 32, 64, 128, 256\). The results are given in Table I along with exact results from exhaustive enumeration of states for small systems with \(L \leq 7\). The polynomials from which \(\langle p \rangle\) are derived are listed in the appendix. We also conducted some simulations at \(L = 7\) to compare numerical and exact results, and the agreement was found to be perfect within the statistical accuracy of the simulations. The pseudo-random number generator used for the simulations was the four-tap feedback generator known as R9689 or gfar4 (23).

Error analysis for the simulation data indicates that the estimates of \(p_c\) are accurate to about six figures, and the values of \(R(p_c)\) are accurate to four or five figures, as indicated the table. We also simulated 2.4 \times 10^7 samples for a system of size \(L = 512\), but the statistical accuracy of the results was insufficient to add anything to the present analysis.

Consider the results for the estimate \(p_{\text{max}}\), whose convergence is non-monotonic. Its value starts below \(p_c\) for small systems, then goes above \(p_c\) as lattice size passes though \(L \approx 100\), and presumably converges to \(p_c\) from above as \(L \to \infty\). Indeed, according to Eq. (24), \(p_{\text{max}}\) has two correction terms with closely-spaced scaling exponents \(-\omega - 1/\nu \approx -1.65\) (using the value of \(\omega\) from below) and \(-1 - 1/\nu = -1.75\); it appears that these terms contribute more or less equally in the range of system sizes that we are considering. The observed behavior is consistent with Eq. (24) if \(b_0 < 0\), \(c_0 > 0\), and the two are are roughly comparable in magnitude. (Note that \(a_3 < 0\) because \(f_0(x)\) is at a maximum at \(x = 0\).) It is not possible to fit the exponents of Eq. (24) reliably to these data.

The rest of the estimates are all monotonic, and lead to reasonably straight lines when viewed on a logarithmic plot of \(|p_{\text{est}} - p_c|\) vs. \(L\), reflecting the leading power-law behavior. To provide a more sensitive representation of our data, we calculate successive slopes between pairs of points for systems of size \(L/2\) and \(L\), giving values \(-\log|p_{\text{est}}(L) - p_c| - \log|p_{\text{est}}(L/2) - p_c|/\log 2\) for the leading exponent for the various estimates \(p_{\text{est}}(L)\). For these calculations we used the value \(p_c = 0.5927462\) given in Ref. [41], which is consistent with the data presented here, but of somewhat higher precision than these data would yield.

In Fig. 1 we show the plots of the successive slopes for estimates \(p_{\text{av}}(L), p_{\text{c(c)}}(L),\) and \(p_{\text{av}}(L)\), as a function of \(L^{-\omega}\) with \(\omega = 0.9\). According to Eqs. (24) and (24), both of these estimates should converge with a leading exponent of \(-1 - 1/\nu\) and a next-order term of order \(-1 - 1/\nu - \omega\), which implies that the successive slopes should fall on a straight line when plotted as a function of \(L^{-\omega}\), with intercept of 1.75. This behavior is indeed seen in Fig. 1 with measured intercepts of 1.754 and 1.763 respectively. (Note that agreement is not highly sensitive to the value of \(\omega\); if the data were plotted as a function of \(L^{-1}\), the fit to linearity would not be much worse.)

The successive slopes for \(p_{\text{av}}(L)\) do not fall on as good a straight line as the other estimates, presumably because the exponents \(-\omega - 1/\nu\) and \(-1 - 1/\nu\) of the two leading terms in the convergence are closely spaced (see Eq. (24)). Extrapolation to \(L = \infty\) is still possible however, and we

| \(L\) | \(N_S\) | \(p_{\text{av}} = \langle p \rangle\) | \(p_{0.5}\) | \(p_{\text{c(c)}}\) | \(p_{\text{max}}\) | \(\sqrt{\langle (\Delta p)^2 \rangle}\) | \(R_L(p_c)\) |
|---|---|---|---|---|---|---|---|
| 2 (exact) | 0.61803399 | 0.53333333 | 0.54119610 | 0.57735027 | 0.22110832 | 0.5792507 |
| 3 (exact) | 0.61926013 | 0.55238095 | 0.55929632 | 0.6207447^{(1)} | 0.58030237 | 0.18137908 | 0.567036 |
| 4 (exact) | 0.61935542 | 0.56400919 | 0.56972413 | 0.6195837^{(1)} | 0.58439952 | 0.15483466 | 0.5555884 |
| 5 (exact) | 0.61890529 | 0.57114567 | 0.57581007 | 0.6135606^{(1)} | 0.58675948 | 0.1358442 | 0.5475384 |
| 6 (exact) | 0.61658709 | 0.57585067 | 0.57907276 | 0.6092087^{(1)} | 0.58825653 | 0.12151246 | 0.541467 |
| 7 (exact) | 0.61511736 | 0.57919147 | 0.58235130 | 0.6060759^{(1)} | 0.58926561 | 0.11027224 | 0.5367513 |
| 7.0 \times 10^{10} | 0.61511800 | 0.57912049 | 0.58235190 | 0.6060812^{(1)} | 0.58926550 | 0.11027200 | 0.536749 |
| 8.0 \times 10^{10} | 0.6137656 | 0.5814866 | 0.5842394 | 0.608314^{(2)} | 0.58997550 | 0.10119250 | 0.532998 |
| 16.0 \times 10^{9} | 0.6069022 | 0.5878189 | 0.5898858 | 0.59882^{(2)} | 0.59201040 | 0.06337610 | 0.518117 |
| 32.0 \times 10^{9} | 0.6016319 | 0.5914246 | 0.5918352 | 0.59482^{(2)} | 0.59260260 | 0.03872030 | 0.509335 |
| 64.0 \times 10^{9} | 0.5981485 | 0.5923179 | 0.5924657 | 0.59341^{(2)} | 0.59273910 | 0.02337930 | 0.504890 |
| 128.0 \times 10^{9} | 0.5958937 | 0.5926087 | 0.5926613 | 0.59295^{(2)} | 0.59275770 | 0.01397030 | 0.502476 |
| 256.0 \times 10^{9} | 0.5946742 | 0.5927013 | 0.5927208 | 0.59280^{(2)} | 0.59275360 | 0.00833430 | 0.50124 |

TABLE I: Various estimates of \(p_c\) from the simulations \((L \geq 7)\), where \(N_S\) is the number of samples, and from exact expressions \((L \leq 7)\). The cell-to-cell estimate is \(p_{c(c)}^{(1)}\) for superscript (1) and \(p_{c(c)}^{(2)}\) for superscript (2). Errors in the numerical results are generally in the last digit quoted.
find an intercept at $1/\nu + \omega = 1.65 \pm 0.02$, clearly different from the value of 1.75 for the other estimates, implying $\omega = 0.90 \pm 0.02$, the figure we have used above. The error bars are smaller than the size of the symbols for all $L$ except $L = 256$, as shown in the plot. Note that although $\omega$ is used in the abscissa of Fig. [1], its value has little effect on the determination of $\omega$ from the intercept of $p_{av}(L)$. We can also compare the coefficients for the leading behavior of estimates to their predicted values. For example, the predicted value of the leading coefficient for $p_{0.5}$, Eq. [24], is $b_0/a_1 = 0.423$, using values of $b_0 = 0.322$ (see below) and $a_1 = 0.765 \pm 0.02$. This compares favorably with the value measured here of 0.436. And for $p_{c-c}$, the coefficient from Eq. [27], $b_0/[a_1(1 - 2^{-1/\nu})]$, should have a value of 1.04, which compares favorably with the measured value 1.02. Note that if we take the linear combination of these two estimates (whose finite-size corrections are opposite in sign), $(p_{0.5} + \alpha p_{c-c}^{(2)})/(1 + \alpha)$ where $\alpha = 1 - 2^{-1/\nu}$, the leading correction terms are predicted to cancel one another and the combination should have leading scaling of $L^{-1 - \omega - 1/\nu} = L^{-2.65}$. And indeed this combination is seen to converge very quickly in our numerical results, with values 0.592968, 0.592739, 0.592745, and 0.592746 for $L = 32, 64, 128$, and 256 respectively. The plot of these figures vs. $L^{-2.65}$ given in Fig. [2] shows linear behavior expected, with an intercept at $p = 0.5927464(5)$, consistent with the best current figure of $p_c = 0.5927462(1) \pm 0.02$. Thus, by taking a combination of estimates, we can improve the convergence rate for the open system to the point where it becomes competitive with that of the periodic system, in which the estimate with the best convergence has exponent $-1/\nu$. This cancellation of leading order corrections between the two terms is expected to be universal.

The results for $p_{RG}$ and the standard deviation $\sigma = \sqrt{(\langle 2p \rangle^2) - \langle p \rangle^2}$ converge to the infinite system value with exponent $1/\nu = -0.75$ as shown in Fig. [2] where we plot the successive slopes as a function of $1/L$. The convergence of the standard deviation of the distribution is predicted in Ref. 12 and also follows from the equations of Section II. The intercepts are at 0.749 and 0.763 respectively. We also show in Fig. [2] a plot of the type introduced by Stauffer, in which $p_{RG}$ is shown as a function of $\sigma$, allowing extrapolation to infinite system size to be carried out without knowledge of the value of $\nu$. This plot shows nearly linear behavior, with the last three points ($L = 64, 128$, and 256) well fit by the line $p_{RG} = 0.5927465 + 0.231512\sigma$ with $R^2 = 0.9999979$. The intercept is in excellent agreement with the known value of $p_c$, although this agreement is perhaps fortuitous, considering the slow convergence of the RG estimate.

The last column of Table [I] gives the crossing probability at $p_c$. The considerations in Section II imply that $R_L(p_c) \sim 1 + b_0/L$ with no contributions from the irrelevant scaling variable $R_L(p_c) = 0.320/L - 0.44/L^2 + \ldots$, yielding $b_0 = 0.320 \pm 0.001$. This is nearly identical to the value 0.319 given in Ref. 12 (where larger systems, but with lower statistics, were generated) and the value 0.31 ± 0.01 of Ref. 12.

V. CONCLUSIONS

We have studied the finite-size scaling of estimates of the percolation threshold $p_c$ derived from the crossing probability $R_L(p)$ for site percolation on the square lattice. Our numerical results confirm that different estimates converge to $p_c$ with a variety of scaling exponents as predicted by the scaling theory developed in Refs. 12.
In particular, we have shown that the average threshold estimate $p_{\text{av}}$ converges with a nontrivial exponent $L^{-\omega-1/\nu}$ whose origins lie in the irrelevant variables in the renormalization group treatment of the problem, and our results for this estimate provide us with a direct measurement of that exponent. We find $\omega = 0.90 \pm 0.02$, somewhat higher than the value of about 0.85 found previously [14] but consistent with the (wide) bounds set by series studies [14, 15]. Our result is in good agreement with a renormalization-group result of $\omega = 0.915$ found by Burkhardt [27, 32]. More extensive simulations could be done to give $\omega$ to higher precision.

Of the estimates considered here, $p_{\text{av}}$ is the only one that shows the effect of the irrelevant exponent clearly. The estimates $p_{0.5}$ and $p_{c-c}$ are confirmed to converge as $L^{-1-1/\nu}$, as proposed previously [3]. The maximum estimate $p_{\text{max}}$ is found to exhibit non-monotonic behavior, which can be explained by competition between correction terms with closely spaced exponents $-1 - 1/\nu$ and $-\omega - 1/\nu$.

The numerical results reported here were found using a microcanonical simulation method which allows one to calculate $R_L(p)$ easily for any $p$ [14, 17]. The various estimates can then be found quickly to any desired degree of precision by applying appropriate formulas, Eqs. (1–7). This method proves particularly advantageous for the estimate $p_{\text{av}}$, since this estimate depends on knowing $R_L(p)$ for all values of $p$, the determination of which by most other methods requires a great deal of work. From the microcanonical data, $p_{\text{av}}$ can be found without any calculational bias using Eq. (22).

Having characterized the convergence rates of our various threshold estimates, one can go back to older literature and find many instances where an anomalous rate of convergence was seen but not fully understood or recognized. For example, Reynolds et al. [2] derived an estimate of $p_c$ which is equivalent to our $p_{\text{av}}$ from numerical data for the one-way crossing probability which they denoted $R_1$. Assuming this estimate to scale as Eq. (8), they plotted their results against $L^{-1/\nu}$ (their Fig. 13). The resulting plot is seen to fall on a nearly vertical line, consistent with higher-order behavior. Fitting their data with the supposed $L^{-1/\nu}$ scaling, they deduced a best estimate of $p_c = 0.5931$ in the large system-size limit. If however one assumes instead the $L^{-\omega-1/\nu}$ scaling derived here, the intercept of their data becomes $p_c \simeq 0.5927$, which is much closer to the current best estimate of this quantity.

Yonezawa et al. [4] plotted a quantity essentially equivalent to our $p_{0.5}$ as a function of $L^{-1/\nu}$, and found apparent agreement with this assumed $L$-dependence (their Figs. 7 and 8). The expected $L^{-1-1/\nu}$ behavior is evidently too weak to be distinguished from $L^{-\omega-1/\nu}$ within the errors on their numerical data. Similarly, Hu et al. [25] believed the cell-to-cell estimate $p_{c-c}^{(1)}$ to be insensitive to $L$; again, the precision of their work did not allow them to observe the higher-order scaling predicted by Eq. (27).

It should be emphasized that the convergence behavior discussed here is specific to a two-dimensional system with a square or rhomboidal open boundary, with crossing defined as a path from one specified side to its opposite. Because of the symmetry of this system, some terms cancel out, allowing various higher-order corrections to become dominant. For different boundaries (such as rectangular ones), and for higher dimensional systems, the behavior will generally be different. In those cases, most of our estimates will scale as the conventional $L^{-1/\nu}$, except perhaps the estimates $p_{c-c}$ and $p_{R_c}$. (To employ the latter, $R_c$ must be known, but we have exact values only for rectangular and conformally related two-dimensional...
systems \cite{29}. Study of these other systems is a subject for future research.

Another approach to measuring \(p_c\) is to use periodic rather than open boundary conditions. A partially periodic system in two dimensions is a cylinder, and crossing in this system was studied in Ref. \cite{12}. The fully periodic system in two dimensions is a cylinder, and crossing probability function scaling exponents. Another approach to measuring \(p_c\) is to use periodic rather than open boundary conditions. A partially periodic system in two dimensions is a cylinder, and crossing in this system was studied in Ref. \cite{12}. The fully periodic system in two dimensions is a cylinder, and crossing probability function scaling exponents.

In conclusion, it is clear that the convergence of estimates for the critical occupation probability \(p_c\) in percolation systems is highly dependent upon the nature of the estimate, as well as the shape and boundary conditions of the system, and that the shrewd use of this fact can allow one to make very accurate estimates of \(p_c\) and scaling exponents.

**APPENDIX A: EXACT ENUMERATION RESULTS**

In Table II we give the exact expressions for the crossing probability function \(R_L(p)\) for site percolation on a square lattice of size \(L \times L\), for crossing from one given side of the square to the opposite side (such as left to right). The results for \(L = 2\) to \(5\) were given previously by Reynolds et al. \cite{3}. Those for \(L = 6\) and \(L = 7\) were calculated previously for the work reported in Ref. \cite{3}, but reported in a different format (results were given for \(R_L'(p)\) rather than \(R_L(p)\) itself). From the results here, one can with reasonable ease calculate the various estimates of \(p_c\) given in Table I using a symbolic manipulation program such as Maple or Mathematica. A file containing these polynomials in forms readable by such programs is available by email from the authors.

An alternative way to represent these results is as a series in \(p^qN^{-n}\) where \(q = 1 - p\) and \(N = L^2\). The transformation can be achieved by substituting \(p \rightarrow 1/(1+r)\), multiplying by \((1+r)^Np^N\), expanding, and replacing \(r \rightarrow q/p\) again. The results are given in Table II.

This is also the form that Reynolds et al. \cite{2} used in their series for \(R_2\) through \(R_5\). From the present point of view, these series are interesting because they are in precisely the form of Eq. \(14\), so that the coefficient \(c_{L,n}\) of \(p^qN^{-n}\) above is related to the microcanonical crossing probability \(R_n\) simply by

\[
R_L(p) = \frac{c_{L,n}}{N^n} = \frac{c_{L,n} n!(N - n)!}{N^n}. \tag{A1}
\]

That is, \(c_{L,n}\) represents the number of configurations with \(n\) occupied sites that satisfy the crossing criterion, out of a total of \(\binom{N}{n}\) possible configurations of the \(n\) occupied sites among the \(N = L^2\) sites of the lattice. For example, of the \(16!/(6!10!) = 8008\) possible configurations of \(6\) occupied sites on a \(4 \times 4\) lattice, exactly \(390\) are percolating by crossing in one direction (from the third term in \(R_4(p, q)\)), yielding a microcanonical probability \(R_{4,6} = 390/8008 = 0.048701\ldots\) Likewise, for \(n = 16\) occupied sites on the \(4 \times 4\) system, there is exactly one percolating system out of one total system.

Thus, the polynomials given in Table II represent the microcanonical \(R_{L,n}\) for \(L\) up to 7.

| \(L\) | \(R_L(p)\) |
|---|---|
| 2 | \(2p^2 - p^7\) |
| 3 | \(3p^3 + 4p^4 - 6p^5 - 9p^6 + 14p^7 - 6p^8 + p^9\) |
| 4 | \(4p^4 + 12p^5 + 6p^6 + 28p^7 + 22p^8 + 48p^9 + 66p^{10} + 108p^{11} + 10p^{12} + 4p^{13} - 20p^{14} + p^{16}\) |
| 5 | \(5p^5 + 24p^6 + 12p^7 - 62p^8 - 92p^9 - 41p^{10} + 274p^{11} + 42p^{12} + 474p^{13} - 1336p^{14} + 172p^{15} - 197p^{16} + 4791p^{17} - 9015p^{18}\) |
| \(\ldots\) | \(\ldots\) |
| 7 | \(7p^7 + 60p^8 + 150p^9 - 18p^{10} - 490p^{11} + 885p^{12} - 318p^{13} + 146p^{14} + 305p^{15} - 158p^{16} + 558p^{17} - 652p^{18} + 4315p^{19}\) |

\begin{table}[h]
\centering
\begin{tabular}{|c|c|}
\hline
\(L\) & \(R_L(p)\) \\
\hline
2 & \(2p^2 - p^7\) \\
3 & \(3p^3 + 4p^4 - 6p^5 - 9p^6 + 14p^7 - 6p^8 + p^9\) \\
4 & \(4p^4 + 12p^5 + 6p^6 + 28p^7 + 22p^8 + 48p^9 + 66p^{10} + 108p^{11} + 10p^{12} + 4p^{13} - 20p^{14} + p^{16}\) \\
5 & \(5p^5 + 24p^6 + 12p^7 - 62p^8 - 92p^9 - 41p^{10} + 274p^{11} + 42p^{12} + 474p^{13} - 1336p^{14} + 172p^{15} - 197p^{16} + 4791p^{17} - 9015p^{18}\) \\
\hline
\end{tabular}
\caption{Exact results for \(R_L(p)\) expressed as polynomials in \(p\), for \(L = 2 \ldots 7\).}
\end{table}

\begin{thebibliography}{10}
\bibitem{1} D. Stauffer and A. Aharony, *Introduction to Percolation Theory*, 2nd edition, Taylor and Francis, London (1994).
\bibitem{2} P. J. Reynolds, H. E. Stanley, and W. Klein, “Large-cell Monte Carlo renormalization group for percolation,” *Phys. Rev. B* **21**, 1223–1245 (1980).
\bibitem{3} S. Kirkpatrick in *Proceedings of the Les Houches Summer...
School on Ill-Condensed Matter, North-Holland, Amsterdam (1980).

[4] A. P. Young and R. B. Stinchcombe, “A renormalization group theory for percolation problems,” J. Phys. C 8, L535–540 (1975).

[5] R. M. Ziff, “Spanning probability in 2D percolation,” Phys. Rev. Lett. 69, 2670–2673 (1992).

[6] F. Yonezawa, S. Sakamoto, and M. Hori, “Percolation in two-dimensional lattices. I. A technique for the estimation of thresholds,” Phys. Rev. B 40, 636–649 (1989).

[7] R. P. Langlands, C. Pichet, P. Pouliot, and Y. Saint-Aubin, “On the universality of crossing probabilities in two-dimensional percolation,” J. Stat. Phys. 67, 553–574 (1992).

[8] R. P. Langlands, P. Pouliot, and Y. Saint-Aubin, “Conformal invariance in two-dimensional percolation,” Bull. Am. Math. Soc. 30, 1–61 (1994).

[9] R. M. Ziff, “Effective boundary extrapolation length to account for finite-size effects in the percolation crossing function,” Phys. Rev. E 45, 2547–2554 (1992).

[10] A. Aharony and J.-P. Hovi, “Comment on ‘Scaling probability in 2D percolation,’” Phys. Rev. Lett. 72, 1941 (1994).

[11] C.-K. Hu, C.-Y. Lin, and J.-A. Chen, “Universal scaling functions in critical phenomena,” Phys. Rev. Lett. 75, 193–196 (1995).

[12] J.-P. Hovi and A. Aharony, “Scaling and universality in the spanning probability for percolation,” Phys. Rev. E 53, 235–253 (1996).

[13] D. Stauffer, “Search for logarithmic factors near the two-dimensional percolation threshold,” Phys. Lett. A 83, 404–405 (1981).

[14] J. Adler, M. Moshe, and V. Privman, “New method for analyzing confluent singularities and its application to two-dimensional percolation,” Phys. Rev. B 26, 1411–1415 (1982).

[15] J. Adler, M. Moshe, and V. Privman, “Corrections to scaling for percolation,” Ann. Israel Phys. Soc. 5, 397–423 (1983).

[16] M. E. J. Newman and R. M. Ziff, “Efficient Monte Carlo algorithm and high-precision results for percolation,” Phys. Rev. Lett. 85, 4104–4107 (2000).

[17] M. E. J. Newman and R. M. Ziff, “A fast Monte Carlo algorithm for site or bond percolation,” Phys. Rev. E 64, 016706 (2001).

[18] C.-K. Hu, “Histogram Monte Carlo renormalization-group method for percolation problems,” Phys. Rev. B 46, 6592–6595 (1992).

[19] H. Gould and J. Tobochnik, An Introduction to Computer Simulation Methods, 2nd edition, p. 444, Addison-Wesley, Reading, MA (1996).

[20] J. E. de Freitas, L. S. Lucena, and S. Roux, “Percolation as a dynamical phenomenon,” Physica A 266, 81–85 (1999).

[21] L. N. Shchur and O. A. Vasilyev, “Number of bonds in the site-diluted lattices: Sampling and fluctuations,” preprint cond-mat/0005443.

[22] R. E. Tarjan, “Efficiency of a good but not linear set union algorithm,” J. Assoc. Comp. Mach. 22, 215–225 (1975).

[23] N. Jan, T. Lookman, and D. Stauffer, “Kinetic gelation with and without initiators: A two-dimensional Monte-Carlo study,” J. Phys. A 16, L117–L122 (1983).

[24] J. Machta, Y. S. Choi, A. Lucke, T. Schweizer, and L. M. Chayes, “Inverted cluster algorithm for Potts models,” Phys. Rev. E 54, 1332–1345 (1996).

[25] R. M. Ziff, “Four-tap shift-register-sequence random-number generators,” Computers in Physics 12, 385–392 (1998). An implementation of this random number generator is available as the subroutine gsl_rng_gfsr4 in the GNU scientific library, available from http://sources.redhat.com/gsl/ref/gsl-ref_10.html.

[26] R. M. Ziff, “Reply to ‘Comment on Spanning Probability in 2D percolation’,” Phys. Rev. Lett. 72, 1942 (1994).
[27] T. W. Burkhardt, “Critical and tricritical exponents of the Potts lattice gas,” *Z. Physik B* **39**, 159–162 (1980).

[28] C.-K. Hu, C.-N. Chen, and F. Y. Wu, “Histogram Monte Carlo position-space renormalization group: Applications to the site percolation,” *J. Stat. Phys.* **82**, 1199–1206 (1996).

[29] J. L. Cardy, “Critical percolation in finite geometries,” *J. Phys. A* **25**, L201–206 (1992).

[30] H. T. Pinson, “Critical percolation on the torus,” *J. Stat. Phys.* **75**, 1167–1177 (1994).

[31] C.-K. Hu, “Reply to ‘Comment on Universal scaling functions in critical phenomena’,” *Phys. Rev. Lett* **76**, 3875 (1996).

[32] In fact, Hovi and Aharony found that the data for $p_{av}$ in their Fig. 1 could be fit best using a value of $\omega \approx 0.90$, but for the data of their Fig. 5 $\omega = 0.85$ gave the better fit.