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Universality of finite-size corrections to the number of critical percolation clusters

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Abstract

Monte-Carlo simulations on a variety of 2d percolating systems at criticality suggest that the excess number of clusters in finite systems over the bulk value n_c is a universal quantity, dependent upon the system shape but independent of the lattice and percolation type. Values of n_c are found to high accuracy, and for bond percolation confirm the theoretical predictions of Temperley and Lieb, and Baxter, Temperley and Ashley, which we have evaluated explicitly in terms of simple algebraic numbers. Predictions for the fluctuations are confirmed numerically for the first time.

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The standard percolation model [1] involves the random occupation of sites or bonds of a regular lattice. At a critical occupation probability p_c, the mean size of clusters of adjacently occupied sites becomes infinite, initiating the percolation transition. The number $n(p)$ of clusters per site, however, remains finite, and attains a value $n_c = n(p_c)$ with critical behavior $|p - p_c|^{2-\alpha}$ as $p \to p_c$, where $2 - \alpha = 8/3$. Critical exponents like α are universal, having the same value for all systems of a given dimensionality no matter what the lattice or percolation type, essentially because they derive from the large-scale, fractal properties of the percolation clusters.

On the other hand, n_c, like p_c, is a non-universal quantity which varies from system to system. This is because it depends upon the microscopic, lattice-level behavior of the systems. For some systems, n_c is known theoretically [2,3], while for others, it must be determined by Monte-Carlo (MC) means. Accurate values of n_c — a basic property of a percolating system — do not seem to be available for many common lattices. Thus we embarked on a project to determine it for a variety of systems by MC simulation. In the course of this work we found a number of new results which we report upon here.

To obtain accurate values, we performed a very extensive simulations on square (SQ) and triangular (TR) lattices, with both site (S) and bond (B) percolation, and the honeycomb (HC) lattice, for B only. Various orientations and system boundaries were used as shown in Fig. 1. Periodic boundary conditions were used. Systems ranged from 16×16 to 512×512 in size, and between 10^6 to 10^9 samples were generated for each, which required several months of workstation computer time. All but one set of simulations were carried out at the critical point p_c of the respective lattice.

Because simulations must necessarily be done on finite systems, an essential part of such a project is to determine the nature of the finite-size corrections. The use of periodic boundary conditions reduces those corrections to sub-surface terms. In characterizing the remaining corrections, we found that the finite-size corrections to n_c, which are related to the excess number of clusters, appear to follow a simple universal behavior. That is, for a finite system of S sites, we found that the average density of clusters (number per site) behaves as

$$n = n_c + \frac{b}{S} + \ldots \tag{1}$$

where b is a function of the system shape only and thus, apparently, a universal quantity. For example, the results for a system with a square boundary of dimension $L \times L$ are shown in Fig. 2, where we plot $n(S)$ vs. $1/S$. For this boundary shape we considered three systems: S-SQ-I (site percolation on a square lattice with orientation I shown in Fig. 1), B-SQ-I, and B-SQ-II, where II is a square lattice rotated by 45°. The equality of the slopes of the three curves means that b has the same value ≈ 0.8835 for all these systems. Higher-order corrections to (1) are small and not visible above the statistical errors of these simulations.

For rectangular systems of dimension $L \times L'$, we found that b increases monotonically with increasing aspect ratio $r = L'/L$ as shown in Table I. Here, we considered only one type of system for each aspect ratio. Besides B-SQ, we also considered B-TR with the boundary III. With III's rectangular boundary, a normal torus is produced when the periodic boundary conditions are applied, and the effective aspect ratio of the system we used is $\sqrt{3}$. Note that, because $b(r) = b(1/r)$, the value $b(1) \approx 0.8835$ is a minimum for rectangular systems.

Besides rectangular systems, we also considered a 60° rhomboid system with an effective helical or "twisted" periodic boundary conditions (systems IV and V). This type of boundary results when a triangular lattice is represented in the computer by a square lattice with one set of diagonals drawn in. The periodic boundary conditions are applied to the lattice in the squared-off orientation, and an effective helical twist is introduced in the torus when the lattice is transformed back to its true configuration with the triangles equilateral. For such a system with sides $L \times L$, we find $b \approx 0.878$, somewhat smaller than the minimum value above for a rectangular boundaries. (Likewise, 0.878 should be the minimum value of b for all 60° parallelograms.) Note that the effective height-to-width of this system is $\sqrt{3}/2$, although it is not really comparable to a rectangular system of a given aspect ratio because of the twist in the boundary condition.

While we do not have a proof that b is universal, we can make the following heuristic arguments to support that hypothesis. Eq. (1) can be written

$$N \approx n_c S + b \tag{2}$$

where $N = nS$ is the total number of clusters in the system. This equation shows that b is effectively the excess number of clusters over the expected bulk value, $n_c S$. As such, it represents large clusters whose size is of the order of the size of the system. While the number and distribution of small, "microscopic" clusters is non-universal, the distribution of these larger clusters is universal. One can also relate b to the average number w of clusters wrapping around the toroidal system, which too is a universal quantity. Consider taking one $2L \times 2L$ system, unwrapping the periodic boundary conditions, cutting it into four $L \times L$ systems, and then re-applying the periodic boundary conditions to each of these. The number of clusters $N(L)$ should roughly satisfy $N(2L) - w = 4(N(L) - w)$, since the density of non-wrapping clusters will be about the same, and this formula is consistent with (2) with $w = b$ (here, $S = L^2$). A similar argument shows that b should increase as the aspect ratio $r = L'/L$ increases, since there are then more wraparound clusters, consistent with what we have observed.

The values of n_c that we found from plots like Fig. 2 are listed in Table II. The results for the bond percolation systems are consistent with theoretical predictions that have been made for these systems. For B-SQ, where $p_c = 1/2$, Temperley and Lieb [2] showed

$$n_c^{B\text{-}SQ} = \frac{1}{2}\left[Z\frac{\partial I_1}{\partial Z}\right]_{Z=1} = \frac{1}{2}\left[-\cot\mu\frac{\partial I_1}{\partial \mu}\right]_{\mu=\pi/3} \tag{3}$$

where $Z = 2\cos\mu$ and

$$I_1 = \frac{1}{4\mu}\int_{-\infty}^{\infty} \operatorname{sech}\Big(\frac{\pi\alpha}{2\mu}\Big)\ln\Big(\frac{\cosh\alpha - \cos 2\mu}{\cosh\alpha - 1}\Big)\mathrm{d}\alpha\ , \tag{4}$$

and reported the numerical estimate 0.0980_7. In fact, we have found that this rather complicated integral result can be evaluated explicitly [4]. First, integrate (4) by parts to obtain

$$I_1 = \frac{4\sin^2\mu}{\pi}\int_0^{\infty} \frac{\tan^{-1}\big(\tanh\frac{\pi\alpha}{4\mu}\big)\coth\frac{\alpha}{2}}{\cosh\alpha - \cos 2\mu}d\alpha \tag{5}$$

and then differentiate to find:

$$\left.\frac{\partial I_1}{\partial \mu}\right|_{\mu=\pi/3} = \frac{8\sqrt{3}}{\pi}\int_0^\infty \frac{\tan^{-1}\left(\tanh\frac{3\alpha}{4}\right)\sinh\alpha}{(2\cosh\alpha+1)^2}d\alpha$$
$$-\frac{27}{\pi^2}\int_0^\infty \alpha\cosh\frac{\alpha}{2}\,\mathrm{csch}\,3\alpha\,d\alpha\ . \qquad (6)$$

Substituting $\alpha = -2\log z$ in the first integral above, we can reduce it to a form that can be evaluated with the help of Mathematica [5], yielding $2\sqrt{3}-3$. Likewise, the second integral in (6) can also be evaluated, and leads to the simple final result

$$n_c^{B\text{-}SQ} = \frac{3\sqrt{3}-5}{2} \approx 0.098\,076\,211\ . \qquad (7)$$

Further details are given in [4]. Our numerical results in Table II are consistent with this prediction to all significant figures. Likewise, for B-TR, where $p_c^{B\text{-}TR} = 2\sin(\pi/18)$ is the solution to $p^3-3p+1=0$ [6], Baxter, Temperley and Ashley [3] showed that

$$n_c^{B-TR} = \left[-\frac{\csc 2\phi}{4}\frac{\partial I_2}{\partial\phi}\right]_{\phi=\pi/3} + \frac{3}{2} - \frac{2}{1+p_c^{B\text{-}TR}} \qquad (8)$$

where

$$I_2 = \frac{3}{2}\int_{-\infty}^\infty \frac{\sinh(\pi-\phi)x\,\sinh\frac{2}{3}\phi x}{x\sinh\pi x\,\cosh\phi x}dx\ , \qquad (9)$$

and estimated $n_c \approx 0.1118$ by numerical integration and also from the 16-term series available at that time. Again, we have explicitly evaluated this expression [7,8], and after many manipulations find simply

$$n_c^{B\text{-}TR} = \frac{35}{4} - \frac{3}{p_c^{B\text{-}TR}} \approx 0.111\,844\,275 \qquad (10)$$

which is in agreement with our observations.

Making use of duality, we also studied the B-HC system at the same time as B-TR. Our value of n_c for this lattice given in Table II agrees with prediction $n_c^{B\text{-}HC} = n_c^{B\text{-}TR} + (p_c^{B\text{-}TR})^3 \approx 0.153\,733\,341$, which follows from the results of [16] written in terms of clusters of wetted sites per site on the TR lattice. Note that for all bond percolation systems, we count the number of clusters of all wetted sites, which includes both clusters of connected sites and "null" clusters of isolated sites with no occupied bonds attached to them. Having the above exact results for n_c was very useful for finding b to high accuracy for these systems.

Previous numerical results are also consistent with our findings. For B-SQ, Nakanishi and Stanley [9] found 0.98075 by simulation. Domb and Pearce [10] found $n_c = 0.0173(3)$ by series analysis, where here n_c is the number of bond clusters per bond. To put (7) in this form, one must subtract the concentration of isolated sites (1/16) and then divide by two, the number of bonds per site. This yields

$$n_c^{B\text{-}SQ}(\text{per bond}) = \frac{24\sqrt{3}-41}{32} \approx 0.017\,788\,106, \tag{11}$$

and shows that the results of [10] are slightly low. Surprisingly, we have found little comparison with or discussion of the results of [2] and [3] in the percolation literature — a notable exception being [11], where in fact we first became aware of [2].

For S-SQ, where $p_c = 0.592\,746\,0(5)$ [12], we find

$$n_c^{S\text{-}SQ} = 0.027\,5931 \pm 0.000\,0003\ , \tag{12}$$

but could not find any published values to compare this with. A simple Padé analysis [13] of the 25-th order series for $n(p)$ given in [14], with no attempt made to account for the branch-point singularity at p_c, yields $n_c = 0.027\,54(4)$, the error representing the variation for [N,D] = [12,13], [13,12],....

For S-TR lattice, where $p_c = 1/2$, we find

$$n_c^{S\text{-}TR} = 0.017\,6255 \pm 0.000\,0005\ . \tag{13}$$

This result is consistent with the previous MC value 0.017 630(2) of Margolina et al. [15] but not the early low-order series value 0.0168(2) [10]. As in the S-SQ case, no theoretical prediction for this quantity exists. Note that the value of $n_c^{S\text{-}TR}$ is quite close to $n_c^{B\text{-}SQ}$ of (11), which is reasonable because the matching site lattice to the B-SQ system is quite similar to the S-TR system, both having coordination number 6 and $p_c = 1/2$.

We also considered S-SQ at $p = 0.5$, well below p_c. Our MC results give

$$n^{S\text{-}SQ}(0.5) = 0.065\,770\,3 \pm 0.000\,000\,2 \ . \tag{14}$$

This quantity relates to a simple question of graph theory [17]: how many clusters of 1's exist on a matrix filled randomly with 0's and 1's of equal concentration? Here finite-size effects were observed in lattices from 32×32 to 512×512 in size (i.e., $b = 0$), presumably because the dimension of a typical cluster was smaller than 32. In this case, a straightforward Padé analysis of Conway and Guttmann's series [14] yields a result of nearly the same accuracy: $0.065\,769\,6(6)$.

The fluctuations σ^2 in the number of clusters from sample to sample, determined by $\langle(\Delta N)^2\rangle = \langle N^2\rangle - \langle N\rangle^2 = S\sigma^2$ for large S, are given in Table II. Like n_c, σ^2 is a function of the lattice and percolation type and thus non-universal, but still independent of the boundary condition and shape. The value 0.164 found for B-SQ, for example, was found for square systems with both orientations, rectangular systems of aspect ratio 2 and 4, and also a square system with open boundaries. These values of σ were also used to obtain the statistical error bars in n_c, which are given by $\sigma(SN_{runs})^{-1/2}$ where N_{runs} is the number of samples. Note that previously, only rough measurements of fluctuations were made [18].

For the B-SQ case, the theory of [2] yields a prediction for the fluctuations of a quantity $H \equiv C_G + S_G$, where C_G is the number of components (clusters plus isolated sites — the same as N above) and S_G is the number of independent cycles in the system:

$$\frac{\langle(\Delta H)^2\rangle}{S} = \left[\left(\cot\mu\frac{\partial}{\partial\mu}\right)^2 I_1\right]_{\mu=\pi/3} \tag{15}$$

The numerical results given in [2] (p. 280) imply the value $0.196_2 - 0.037_7 = 0.158_5$ for this quantity. After many intermediate steps, we have evaluated the resulting integral expressions explicitly and find [4]

$$\frac{\langle(\Delta H)^2\rangle}{S} = \frac{8\sqrt{3}-25}{2} + \frac{18}{\pi} \approx 0.157\,781\,182 \ . \tag{16}$$

At p_c, $S_G = C_G$, but because of the cross term $\langle C_G S_G\rangle$ in $\langle(\Delta H)^2\rangle$, the above result cannot be used to obtain a prediction for $\sigma^2 = \langle(\Delta C_G)^2\rangle/S$. However, one can show that S_G is equal to the number of components on the dual lattice $C_{\tilde{G}}$, which can be measured at the same time as clusters on C_G. (It also follows that H is equal to the total number of hulls that can be drawn on the system, minus 1 if there is wraparound in both directions [19].) Indeed, for B-SQ percolation on rectangular systems, we find that $\langle(\Delta H)^2\rangle = 0.1578(1)$, in perfect agreement with (15). If C_G and $C_{\tilde{G}}$ were uncorrelated, then $\langle(\Delta H)^2\rangle/S$ would equal $2\sigma^2 = 0.328$. This implies that realizations with more clusters on the regular lattice tend to have fewer clusters on the dual lattice, and *vice versa*, as one might expect. The fluctuations of H have finite-size corrections that behave as $\approx L^{-2}$, while the fluctuations σ^2 of clusters alone was found to follow an unusual behavior $\approx L^{-1.25}$.

We have also measured $\langle(\Delta H)^2\rangle/S$ for the B-TR case, where now $C_{\tilde{G}}$ are components on the B-HC lattice, and find 0.2207(1). We have not related this result to theory [3]; although we can evaluate the next derivative of I_2 [7], we have not found the additional terms analogous to the last two terms in (8).

Thus, we have shown that the theory of [2] can be applied to cluster fluctuations if one includes the dual-lattice clusters in the measurements. We have found surprisingly simple expressions for the integrals of the theories of [2,3], which we have also verified numerically to high precision. And we have presented evidence that the excess number of clusters is a universal quantity, much like the crossing probability that has been of much interest recently [19–24]. Recently, Aharony and Stauffer [25] have presented theoretical arguments for the universality of b, and furthermore, Kleban [26] has derived explicit expressions for b using conformal invariance methods, which support this universality hypothesis.

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FIGURES

FIG. 1. Different lattices and boundary shapes used in the MC studies. Systems I, II and III have rectangular boundaries and lead to normal tori when the periodic boundaries are applied. IV and V have a rhomboid boundary, but the periodic boundary conditions are applied when the lattice is in a squared-off form, leading to a helical or twisted boundary.

FIG. 2. A plot of $n = N/S$ vs. $1/S$ for the $L \times L$ S-SQ-I (filled square), B-SQ-I (open square) and B-SQ-II (open diamond) systems at p_c. The curves are offset vertically for clarity; the actual intercepts are $n_c^{S\text{-}SQ}$ for the upper curves, and $n_c^{B\text{-}SQ}$ for the lower two curves. This plot illustrates that b (the slope) is the same for all three systems.

TABLES

TABLE I. Measured values of the universal finite-size correction constant $b = N - n_c S$, grouped by universality class (system shape and boundary condition). Numbers in parentheses show the errors in the last digit(s).

system	boundary	b
S-SQ-I	square	0.8832(3)
B-SQ-I	square	0.8838(5)
B-SQ-II	square	0.8835(8)
B-TR-III	$1 \times \sqrt{3}$ rectangle	0.946(2)
B-SQ-II	1×2 rectangle	0.991(2)
B-SQ-II	1×4 rectangle	1.512(3)
S-TR-IV	1×1 rhombus	0.8783(8)
B-TR-IV	1×1 rhombus	0.878(1)
B-HC-V	1×1 rhombus	0.877(1)

TABLE II. MC results for cluster concentration n_c and fluctuations σ^2 for the various systems studied, grouped by system type, along with known values of p_c [6,12]. These quantities are non-universal, but independent of the system boundary, as seen here for the B-SQ and B-TR cases.

system	boundary	p_c	n_c	σ^2
S-SQ-I	square	0.592 746	0.027 5981(3)	0.05385
S-TR-IV	1×1 rhombus	0.5	0.017 6255(5)	0.0309
B-SQ-I	square	0.5	0.098 0763(8)	0.1644
B-SQ-II	square	0.5	0.098 0765(10)	0.1644
B-SQ-II	1×2 rectangle	0.5	0.098 076	0.1642
B-SQ-II	1×4 rectangle	0.5	0.098 1	0.163
B-TR-III	$1 \times \sqrt{3}$ rect.	0.347 296	0.111 846(2)	0.183
B-TR-IV	1×1 rhombus	0.347 296	0.111 843(2)	0.1827
B-HC-V	1×1 rhombus	0.652 705	0.153 735(2)	0.267