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Universality of the excess number of clusters and the crossing probability function in three-dimensional percolation

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Abstract. Extensive Monte Carlo simulations were performed to evaluate the excess number of clusters and the crossing probability function for three-dimensional percolation on the simple cubic (s.c.), face-centred cubic (f.c.c.), and body-centred cubic (b.c.c.) lattices. Systems $L \times L \times L'$ with $L' \gg L$ were studied for both bond (s.c., f.c.c., b.c.c.) and site (f.c.c.) percolation. The excess number of clusters $\tilde{b}$ per unit length was confirmed to be a universal quantity with a value $\tilde{b} \approx 0.412$. Likewise, the critical crossing probability in the L' direction, with periodic boundary conditions in the $L \times L$ plane, was found to follow a universal exponential decay as a function of $r = L'/L$ for large r. Simulations were also carried out to find new precise values of the critical thresholds for site percolation on the f.c.c. and b.c.c. lattices, yielding $p_c(\text{f.c.c.}) = 0.199\,2365 \pm 0.000\,0010$, $p_c(\text{b.c.c.}) = 0.245\,9615 \pm 0.000\,0010$. We also report the value $p_c(\text{s.c.}) = 0.311\,6080 \pm 0.000\,0004$ for site percolation.

1. Introduction

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 occupied sites becomes infinite, while the number of clusters $n(p)$ per site or per unit volume remains finite with $n_c = n(p_c)$.

The value of n_c depends on the microscopic characteristics of each system, and because of this it is a non-universal quantity. For two-dimensional (2D) systems, precise numerical values of n_c for bond and site percolation on the square and triangular lattices were found by Ziff *et al* [2], whose results for bond percolation confirmed the theoretical predictions of Temperley and Lieb [3] and Baxter *et al* [4]. In three dimensions, there are no theoretical predictions for n_c, and its values for different systems apparently have not been reported in literature.

In [2], it was also found that the *excess* number of clusters $b \equiv \lim_{L\to\infty} LL'(n(L, L') - n_c)$, with $r = L'/L =$ fixed, where $n(L, L')$ is the number of clusters per unit area in a finite system of size $L \times L'$ with periodic boundary conditions, is a universal quantity that depends only upon aspect ratio r. (Note that in [2], the authors defined n as clusters per site rather than per unit area, but the result for b is the same.) This universality is consistent with the theoretical arguments of Privman and Fisher [5], and has also been discussed by Aharony and Stauffer [6], and by Müller [7] for the Ising model. Kleban and Ziff [8] introduced an

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Table 1. Values of p_c for bond and site percolation on the b.c.c., f.c.c. and s.c. lattices from present (*) and other recent work. The numbers in parentheses represent the errors in the last digit(s).

System	p_c	Reference	Value used here
b.c.c. (bond)	0.180 3	[1]	
	0.180 2(2)	[30]	
	0.180 2875(10)	[23]	0.180 287 5
b.c.c. (site)	0.246	[1]	
	0.245 8(2)	[30]	
	0.245 9615(10)	*	
f.c.c. (bond)	0.119	[1]	
	0.120 0(2)	[30]	
	0.120 1635(10)	[23]	0.120 163 5
f.c.c. (site)	0.198	[1]	
	0.199 4(2)	[30]	
	0.199 2365(10)	*	0.199 236 5
s.c. (bond)	0.248 8	[1]	
	0.248 7(2)	[30]	
	0.248 8(2)	[31]	
	0.248 75(13)	[32]	
	0.248 814(3)	[33]	
	0.248 812(2)	[26]	
	0.248 8126(5)	[23]	0.248 812 6
s.c. (site)	0.311 6	[1]	
	0.311 4(4)	[30]	
	0.311 605(10)	[26]	
	0.311 604(6)	[33]	
	0.311 605(5)	[21]	
	0.311 600(5)	[34]	
	0.311 6081(13)	[27]	
	0.311 6080(4)	[9]	

excess number per unit length $\tilde{b} \equiv \lim_{r\to\infty} b(r)/r = \lim_{L\to\infty} L^2(n(L, L') - n_c)$ for long cylindrical systems $L' \gg L$, and derived exact results for both $b(r)$ and $\tilde{b}$ in 2D systems. Again, however, no theoretical predictions for b in three dimensions exist.

In this paper, we determine n_c and $\tilde{b}$ for various 3D rectangular solid systems of dimensions $L \times L \times L'$ with $L' \gg L$. We consider bond percolation on the simple cubic (s.c.), body-centred cubic (b.c.c.), and face-centred cubic (f.c.c.) lattices, and site percolation on the f.c.c. lattice.

A prerequisite to finding the value of n_c for each of these systems is knowing the critical occupational probability p_c to high accuracy. Previously, accurate values were found for bond percolation on all three lattices and site percolation on the s.c. lattice only, as summarized in table 1. To round out these values, we carried out simulations to determine p_c for site percolation on the b.c.c. and f.c.c. lattices to high accuracy—although we used only the latter in the study of the excess cluster number, since the universality was clearly confirmed with the four systems that we studied. In another work [9], we have studied site percolation on the s.c. lattice, and also report this result in table 1.

The simulations for finding n_c were also used to study the critical crossing probability for the 3D systems. The crossing probability function $\pi(\Gamma)$ of a system of shape Γ gives

the probability that at least one cluster connects two disjoint pieces of the boundary $\partial\Gamma$, and has been of much recent interest following the realization that it is a fundamental, universal property of percolation, independent of the underlying lattice type, and subject to conformal invariance [10–13]. In two dimensions, Cardy [11] derived an explicit expression for the vertical crossing probability π_v of rectangular systems $L \times L'$, with open boundaries in the horizontal direction, and Watts [14] derived an expression for the probability of vertical but not horizontal crossing for this system. The π_v for 2D systems with periodic (and other) boundary conditions was studied by Hovi and Aharony [15]. A number of systems were also studied by various groups including Hu *et al* [16], Hsu *et al* [17], Gropengiesser and Stauffer [18], and Vicsek and Kertész [19]. In three dimensions, work has been restricted to simple cubical boundaries $L \times L \times L$, with crossing studied between two opposite planes and various boundary conditions on the sides [16, 20, 21].

Here we find π_v for the $L \times L \times L'$ systems for all L' by measuring the distribution of the maximum height of clusters connected to the base of the rectangular system. (A similar method was used in [22] for 2D systems.) We consider crossing in the L' direction for systems with periodic boundary conditions in the $L \times L$ plane, and show that π_v is a universal function of $r = L'/L$ for large L.

In the following three sections we report on the determination of the new values of p_c, the determination of n_c and $\tilde{b}$, and the determination of $\pi_v(r)$. The results are summarized and discussed further in the conclusions section.

2. Percolation thresholds

Precise values for the thresholds for bond percolation on all three lattices, and for site percolation on the s.c. lattice, have been found elsewhere. Here we also determine accurate values for site percolation on the f.c.c. and b.c.c. lattices. A summary of our results and other recent results is given in table 1.

The procedure we used to find p_c was similar to that we used for bond percolation in [23]. We grew individual clusters by a Leath-type algorithm and identified the critical point using an epidemic scaling analysis. A virtual lattice of 2048^3 sites was simulated, using the block-data method first described in [24]. There were only two minor changes made to the simulation of [23] so that it could be used to study site percolation. First, as the clusters were grown, the sites were either occupied with a probability, p, or left vacant with a probability, $1 - p$. If a site was determined to be vacant, then (unlike in bond percolation) it was never revisited as a potential growing site. The other difference is the cut-off for the growth of these clusters was set to 2^{19} (524 288) wetted sites, as opposed to 2^{20} (1048 576) and 2^{21} (2097 152) in [23].

The simulation yielded the fraction of clusters $P(s, p)$ that grew to a size greater than or equal to s sites. When p is near p_c, one expects $P(s, p)$ to behave as

$$P(s, p) \sim A s^{2-\tau} f((p - p_c)s^{\sigma}) \approx A s^{2-\tau}[1 + C(p - p_c)s^{\sigma} + \cdots] \qquad (1)$$

where τ and σ are universal exponents [25]. Here we assumed the values $\tau = 2.189$ and $\sigma = 0.445$, consistent with other 3D work [23, 26, 27]. As in [23], plots of $s^{\tau-2}P(s, p)$ versus s^{σ} for site percolation of the b.c.c. and f.c.c. lattices were used to find the value of the percolation threshold, which corresponds to horizontal behaviour for large L on such a plot. In all, we generated 1.5×10^7 clusters for the f.c.c. lattice and 2.2×10^7 for the b.c.c. lattice for a range of values of p requiring several weeks of workstation computer time.

The results are plotted in figure 1 and imply the following values for the critical thresholds:

$$\begin{aligned} p_c(\text{b.c.c.}) &= 0.245\,9615 \pm 0.000\,0010 \\ p_c(\text{f.c.c.}) &= 0.199\,2365 \pm 0.000\,0010. \end{aligned} \tag{2}$$

These results are consistent with (and more than 1000 times more precise than) previous work, as shown in table 1.

3. Values of n_c and the finite-size correction $\tilde{b}$

Using the values of the critical thresholds given in table 1, we carried out simulations to measure the number of clusters for bond percolation on each of the 3D lattices and site percolation on the f.c.c. lattice. Clusters were grown successively from every unvisited site by a growth algorithm [28] on a 3D square bar, $L \times L \times L'$ with $L' \gg L$. Periodic boundary conditions were assumed in each horizontal plane. (Here, vertical is taken to be the L' direction.) The first cluster was started in the upper left-hand corner of the first plane ($z = 0$) at the point $(0, 0, 0)$. From this corner, a cluster was grown to the nearest-neighbouring sites as defined for each system by the unit vectors in [23], occupying the connecting bonds or neighbouring sites with a probability, p_c, and leaving them unoccupied with a probability, $1 - p_c$. After the first cluster was grown, a new cluster was seeded from the first unoccupied site in the left-most column, and grown until it died. After all sites of the first plane were tested, the growing plane was moved to $z = 1$, and so on. Because the previous planes were completely occupied, their data could be discarded and the memory recycled. Furthermore, the clusters never extended up to a plane of distance $z = 32L$ from the growing plane. As a consequence, a system of size $L \times L \times 32L$ could be used to effectively simulate a $L \times L \times \infty$ system by wrapping around in the third direction.

We ran simulations to $L' = 2 \times 10^9$, with $L = 4$, 5, 6, 7, 8, 10, and 12 for the s.c. lattice, $L = 4$, 6, 8, 10 and 12 for the f.c.c. lattice (both site and bond), and $L = 4$, 6, 8, 10, 12, and 16 for the b.c.c. lattice. In total, we grew 1.06×10^{12} clusters for the b.c.c. lattice, 1.88×10^{12} clusters for the s.c. lattice, 1.44×10^{12} clusters for bond percolation on the f.c.c. lattice, and 3.32×10^{11} for site percolation on the f.c.c. lattice, which required several additional months of computer time.

In figure 2, we display a representative 4×4 plane of each of the three lattices, showing how the lattices were oriented in our simulations and how the unit dimension was defined. For modelling the s.c. lattice, the plane shown in figure 2(a) is repeated for the whole length of the cylinder, while for the other two lattices, the plane shown in the figure is repeated on every other plane. In the case of the s.c. lattice, all of the available sites in the plane are considered active, for the f.c.c. lattice, only half of the underlying cubic-lattice sites are active, and for the b.c.c. lattice, only a quarter of the cubic-lattice sites are active. Note that the unit dimension that we define for the b.c.c. and f.c.c. lattices is neither the unit cell dimension nor the nearest-neighbour distance, but half of the unit cell dimension.

Now, for a finite system of volume V with periodic boundary conditions, analogous to what was found in [2] for two dimensions, we expect

$$n = n_c + \frac{b}{V} + \frac{c}{V^2} + \cdots \tag{3}$$

where b, representing the excess number of clusters in this finite system, is universal, a function of the shape only. Here we studied $L \times L \times L'$ systems, where $L' \gg L$, with the volume given by $V = L^2 L'$. For systems of this shape, we expect the excess number of

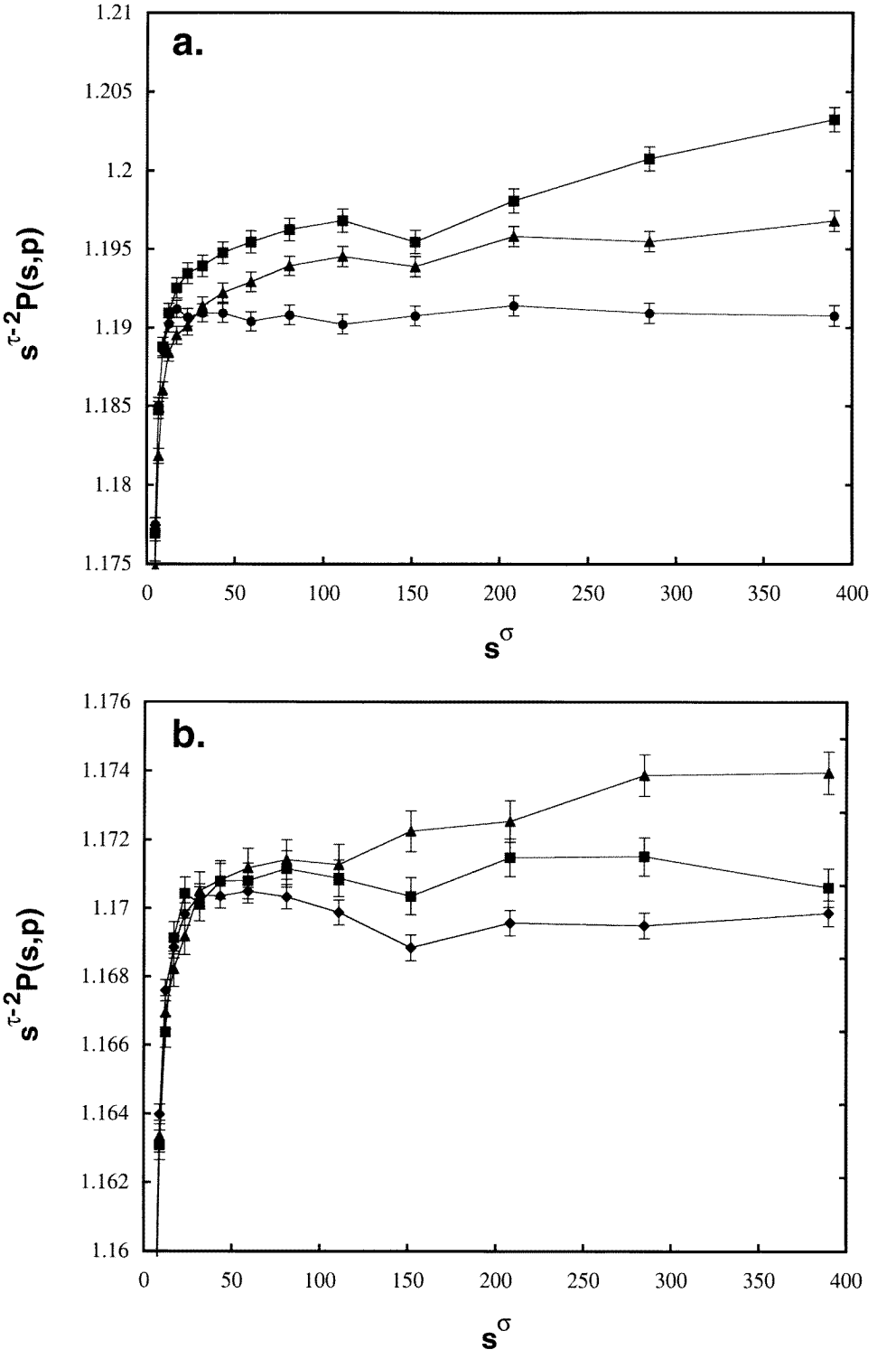

Figure 1. Plot of $s^{\tau-2}P(s, p)$ versus s^{σ} for (*a*) f.c.c. and (*b*) b.c.c. lattices using $\tau = 2.189$ and $\sigma = 0.445$. Each curve represents a different value of p, which are (from top to bottom) (*a*) 0.199 2375, 0.199 2365, and 0.199 2355, and (*b*) 0.245 9625, 0.245 9615, and 0.245 9605.

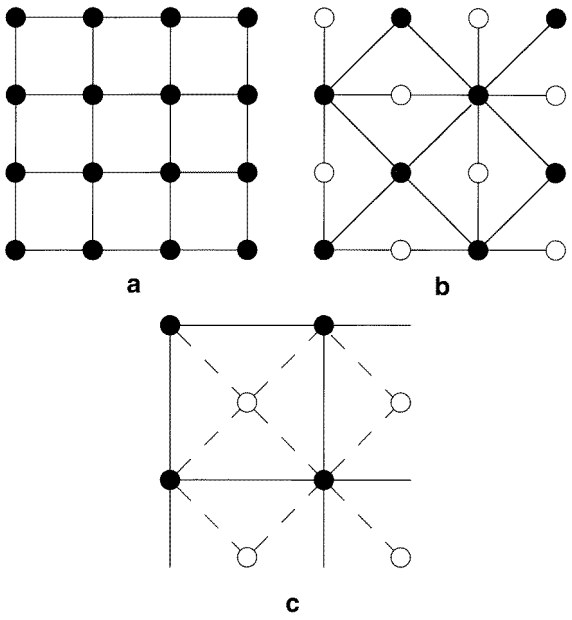

Figure 2. Representative 4×4 planes for the (*a*) s.c., (*b*) f.c.c., and (*c*) b.c.c. lattices. The full circles represent active sites in the plane and open circles represent active sites in the neighbouring planes. The full lines represent bonds in the plane and broken lines represent bonds which go to the neighbouring planes.

clusters per unit length $b/(L'/L)$ to be a constant $\tilde{b}$, i.e.

$$b \sim \tilde{b}L'/L \tag{4}$$

for $L' \gg L$. Then it follows from (3) that

$$n = n_c + \frac{\tilde{b}}{L^3} + \frac{\tilde{c}}{L^6} + \cdots. \tag{5}$$

Note that to obtain this form we wrote $c = \tilde{c}(L'/L)^2$. The justification for choosing this form for c is that it allows n to be independent of L' (necessary because (5) represents the limit $L' \gg L$) and this form is supported by numerical observations as shown below. While terms of fractional order in L may also appear in the series for L, we have not observed them numerically in this work.

In (5), both b and $\tilde{b}$ are functions of the system shape only and are universal quantities, but c and $\tilde{c}$ vary from system to system and are not universal. Equation (5) implies that n_c can be found from a plot of n versus $1/L^3$, as shown in figure 3 for our data from the b.c.c. lattice. The values of n_c, which are shown in units of number of clusters per unit volume as defined in figure 2 for the various lattices, are given in table 2. These values can be converted to units of number of clusters per site by taking into account that the s.c., f.c.c., and b.c.c. lattices have 1, $\frac{1}{2}$, and $\frac{1}{4}$ sites per unit volume, respectively.

Equation (5) can be rearranged as

$$(n - n_c)L^3 = \tilde{b} + \frac{\tilde{c}}{L^3} + \cdots. \tag{6}$$

Therefore, once n_c is determined, $\tilde{b}$ and $\tilde{c}$ can be found from a plot of $(n - n_c)L^3$ versus $1/L^3$. Figure 4 shows this plot for the systems that we studied. The resulting values of $\tilde{b}$

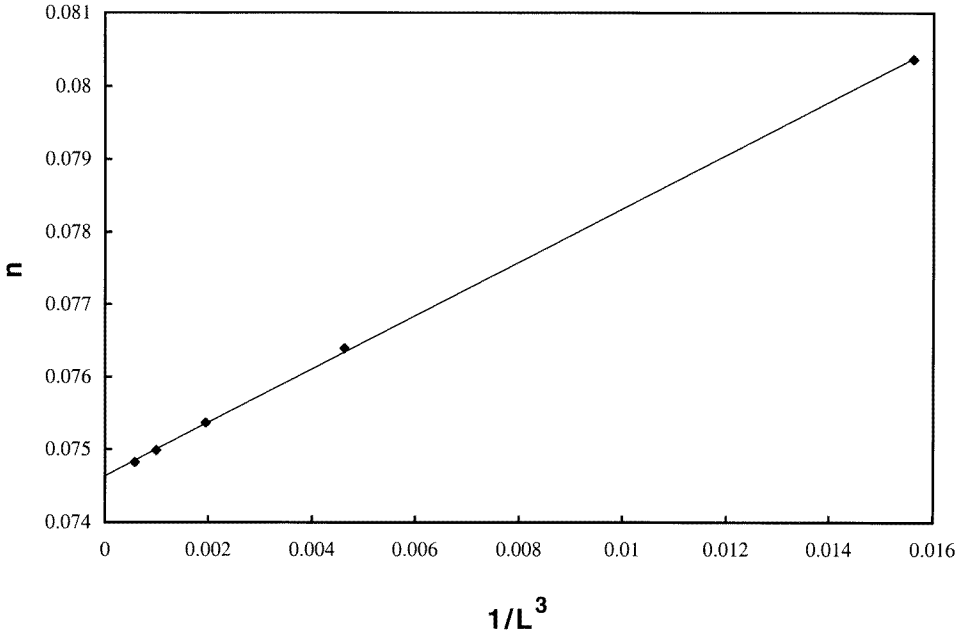

Figure 3. Plot of n versus $1/L^3$ for bond percolation on the b.c.c. lattice. The intercept of this plot yields n_c and the slope yields $\tilde{b}$ according to equation (5).

Table 2. Values of n_c (clusters per unit volume), $\tilde{b}$, and $\tilde{c}$ for the systems studied.

System	n_c	$\tilde{b}$	$\tilde{c}$
s.c. (bond)	0.272 9310(5)	0.414(3)	6.0(7)
f.c.c. (bond)	0.153 8440(5)	0.414(3)	−1.4(3)
f.c.c. (site)	0.013 2655(5)	0.409(3)	−1.8(3)
b.c.c. (bond)	0.074 5860(5)	0.409(3)	−5.5(7)

and $\tilde{c}$ for each of the systems are listed in table 2. A universal value of $\tilde{b} = 0.412 \pm 0.002$ is obtained from these results. Note that the linearity of the plot in figure 4 provides fairly good confirmation that the third term in (5) is indeed proportional to L^{-6}.

4. Critical crossing probability π_v

Our simulations for n_c could also be used to obtain π_v by comparing the distance from the growth plane to the maximum height plane. If this distance is greater than or equal to some fixed value L', then crossing will occur in an $L \times L \times L'$ system (with periodic boundary conditions in each $L \times L$ plane). In other words, we could determine $\pi_v(L, L, L')$ for all L' by keeping track of the distribution of distances between the growth plane and maximum height planes in our continuous simulations.

In two dimensions, the probability of crossing a system of aspect ratio r = height/width in the vertical direction, with periodic boundary conditions in the horizontal direction, is

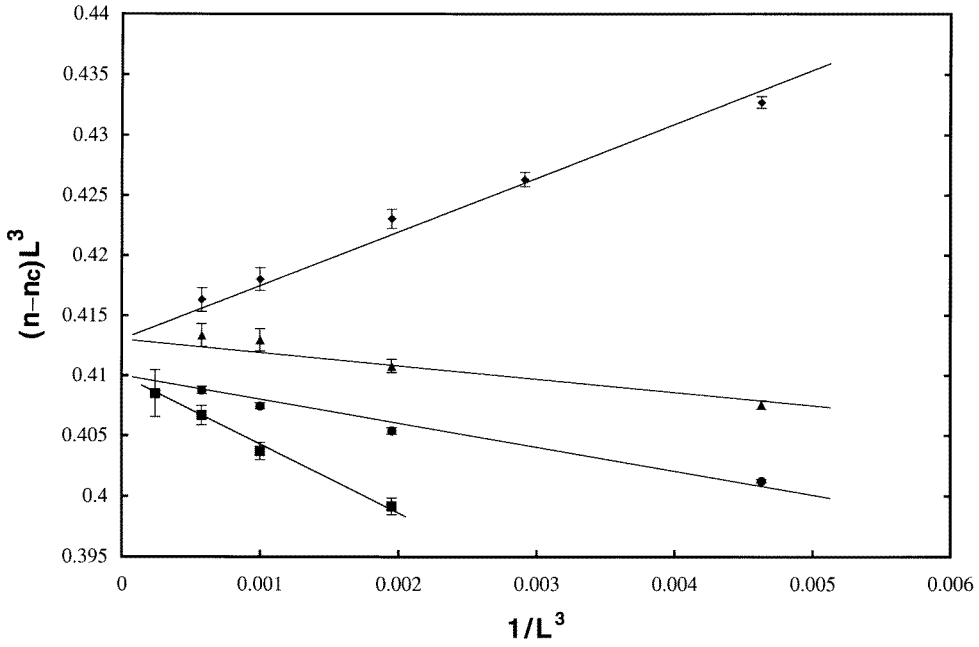

Figure 4. Plot of $(n - n_c)L^3$ versus $1/L^3$ for the b.c.c. (bond), f.c.c. (bond), f.c.c. (site), and s.c. (bond) (from top to bottom) systems at p_c. In these plots, the intercept represents the value of $\tilde{b}$ and the slope is the second correction term $\tilde{c}$. The values of $\tilde{b}$ and $\tilde{c}$ are listed in table 2.

given by [13, 29]

$$\pi_v(r) \sim \mathrm{e}^{-2\pi r(2-D)} = \mathrm{e}^{-\frac{5}{24}\pi r} \tag{7}$$

for large r, where $D = \frac{91}{48}$ is the 2D fractal dimension. Equation (7) follows from a conformal transformation from an annulus to a rectangle, using that the probability a cluster extends beyond a radial distance R scales as R^{D-d}. We have separately verified that equation (7) holds accurately for all r somewhat greater than 1.

For 3D systems, while it is still true that the radial probability scales as R^{D-d}, we cannot connect it to π_v of the $L \times L \times L'$ system, because we cannot make a conformal transformation between the concentric spheres and a rectangular solid. However, we still expect an exponential dependence upon $r = L'/L$, because that term represents the smallest eigenvalue of the transfer matrix. We thus hypothesize

$$\pi_v \sim K\mathrm{e}^{-mr} \tag{8}$$

for large r. To check this, we plot $\ln \pi_v$ versus r in figure 5, which contains the results from all four systems studied, for $L = 8$, 10, and 12. To get the best data collapse, we defined $r = (L' + \ell)/L$, which allows for a lattice finite-size effect or boundary extrapolation length in the L' direction, in which the effective location of the free boundary is not uniquely defined [22]. (Such an ambiguity in size does not occur in the L directions, because of the periodic boundary conditions.) In fact, the data for all three bond percolation systems collapsed nicely with $\ell = -1.3$, while the data for site percolation on the f.c.c. lattice required a constant of $\ell = 1.36$ to fall on the same curve. Figure 6 shows the effect of ℓ by comparing an enlarged portion of our data from the s.c. (bond) lattice when $\ell = 0$

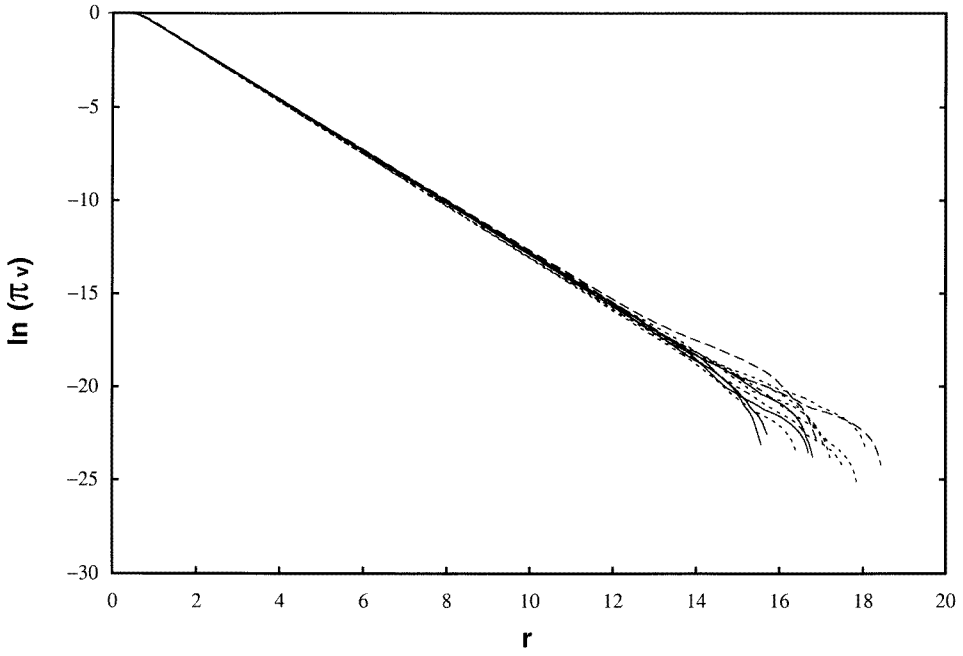

Figure 5. Plot of $\ln \pi_v$ versus $r = (L' + \ell)/L$ for the b.c.c. (bond) (broken curves), f.c.c. (bond) (dotted curves), f.c.c. (site) (also dotted curves), and s.c. (bond) (full curves) lattices of size $L \times L \times L'$ with $L = 8$, 10, and 12 at p_c. In these plots, the intercept represents the value of $\ln K$ and the slope is m. The values of $\ln K$ and m are 0.75 ± 0.05 and 1.37 ± 0.01.

and $\ell = -1.3$. The corresponding values of m and $\ln K$ are 1.37 ± 0.01 and 0.75 ± 0.05, respectively.

The exponential form of (8) can be understood as follows. For each additional cube added to a $L \times L \times L'$ system, (8) states that π_v decreases by a factor of $e^{-m} \approx 0.254$. For large L', these factors are statistically independent, implying the exponential form. However, for small L' the probability will be affected by the complete occupation of the first plane, which is reflected in the coefficient K as well as higher-order terms not included in (8).

5. Discussion of results

Our values for the critical thresholds of site percolation on the f.c.c. and b.c.c. lattices are listed in table 1. Along with the other results which are summarized in that table, the thresholds of all three 3D systems, for both site and bond percolation, are now known to a very high accuracy.

Table 2 lists n_c, $\tilde{b}$ and $\tilde{c}$ for the four systems studied. Our simulations confirm that $\tilde{b}$ is universal in three dimensions as in two dimensions [2], with a value $\tilde{b} \approx 0.412$. In two dimensions, the corresponding value is $\tilde{b} = (5\sqrt{3})/24 = 0.360\,844\ldots$ [8].

The average density of clusters per site, n_c, varies from system to system, as expected. The values for n_c in table 2 show that the simple cubic is the most dense system, according to the convention we used to define the unit volume of the system.

Our simulations have also shown that π_v is universal as shown in figure 5, and

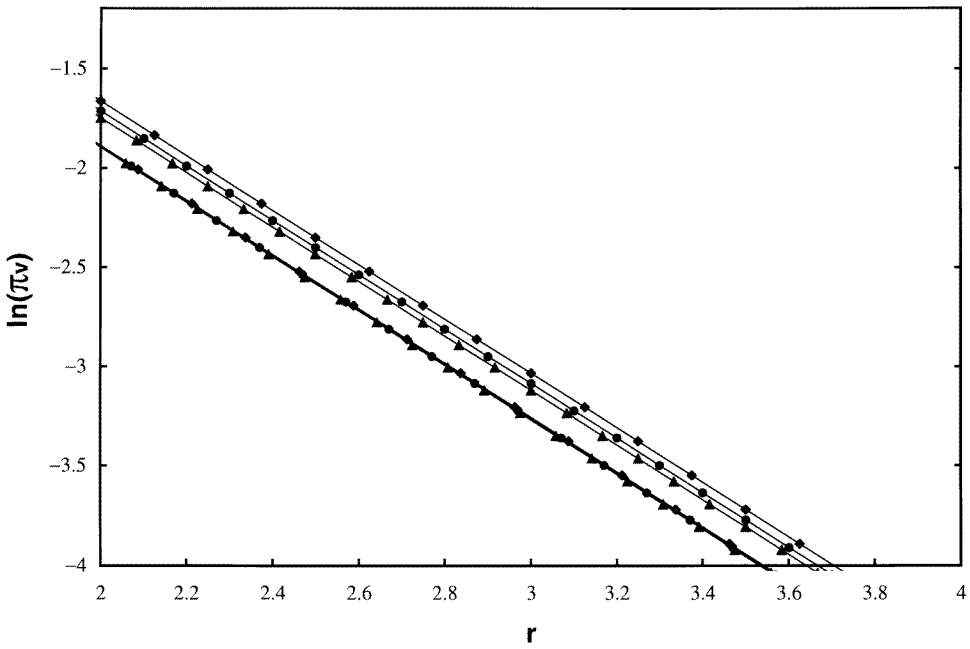

Figure 6. Plot of $\ln \pi_v$ versus $r = (L' + \ell)/L$ for an enlarged portion of the data from the s.c. (bond) lattice of size $L \times L \times L'$ with $L = 8$ (square), 10 (circle), and 12 (triangle) at p_c. The upper three curves show the data plotted with $\ell = 0$, and the bottom curve shows the data collapse when $\ell = -1.3$ is used.

possesses an exponential decay (8) with $m = 1.37 \pm 0.01$, compared with a value of $5\pi/24 = 0.654\,498\ldots$ in two dimensions. For a cubical system ($L \times L \times L$ or $r = 1$), equation (8) implies a value of $\pi_v = 0.54 \pm 0.04$, while a direct analysis of our data at that point yields the more precise value $\pi_v = 0.573 \pm 0.005$. The latter value is somewhat higher than the result 0.513 ± 0.005 recently reported by Acharyya and Stauffer [21] for a system with helical boundary conditions in the plane, which are similar to periodic boundary conditions but with the rows shifted by one. We believe that in the limit of large L these two boundary conditions should be equivalent, although this belief is not supported by the discrepancy in the values seen above.

Many additional questions are raised for 3D systems. What is $b(r', r'')$ where $r' = L'/L$ and $r'' = L''/L$ for an $L \times L' \times L''$ system (with periodic boundary conditions in all directions)? What is the effect of helicity or a twist of the order L in the periodic boundary conditions? Is $\tilde{b}$ related to the number of 'percolating' clusters per unit length (however precisely that may be defined)? Finally, can one devise a system that conformally transforms to concentric spheres, so that the crossing probability across that system will be given by a formula analogous to (7)?

Acknowledgments

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