Spanning Lengths of Percolation Clusters

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The spanning length of a percolation cluster is defined as the difference between the maximum and minimum coordinates of the cluster with respect to some chosen direction. It is statistically related to the number size of the cluster by an exponent that differs from the inverse dimension that would characterize a compact cluster. This exponent for large percolation clusters in simple cubic lattice sites was studied by the Monte Carlo technique, and results are presented. Previous theoretical treatments of this exponent and its relationship with other critical exponents are discussed.

KEY WORDS: Percolation; Monte Carlo; fractal dimension; clusters.

1. INTRODUCTION

The percolation cluster is a one-dimensional "skeleton" connecting points in a *d*-dimensional lattice, with a complex topology⁽¹⁾ for which such concepts such as "length," "volume," "surface," etc., are ambiguous without specific definition. By the *size* of a cluster we mean the *number* of occupied sites in that cluster.² We shall define the *spanning length* of a percolation cluster in a given direction to be the difference between the maximum and minimum coordinates or projections of the cluster in that direction.

In a previous publication ⁽²⁾ we have shown that the spanning length is a most useful concept in discussing percolation in finite volumes, since the existence of a percolation cluster connecting opposite faces of a finite volume provides the natural operational definition of percolation in that volume. In fact Levenshtein *et al.*⁽³⁾ have defined the critical percolation probability p_c for a finite lattice in terms of the peak in the probability distribution for spanning of that lattice. If one had complete statistical information on spanning lengths of clusters together with corresponding information on size distributions of

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² In the present paper we shall refer exclusively to the "site" percolation problem, and all our definitions will be within that context.

clusters, one would be able to reproduce for arbitrary size lattice the probability distribution curves of the sort described in Ref. 3. We have not done this in detail; however, we have previously⁽²⁾ used some simplifying assumptions to discuss the onset of spanning. We shall repeat this argument in the next section because of its relevance to the present work and for consistency with the present notation. In succeeding sections we shall present the results from Monte Carlo studies and discuss the relationship of the present work to that of others.

2. INEQUALITY FOR SPANNING CLUSTER

In Ref. 2 we have made the assumption that for large enough clusters the relationship between the mean spanning length l and the size of the cluster could be described by a power law,³

$$s = \text{const} \times [l(s)]^{d_f^{\dagger}} \tag{1}$$

We also assumed the power law distribution⁴ at percolation for the average number n_s of clusters of size s,

$$n_s = \text{const} \times s^{-\tau} \tag{2}$$

We then argued that the condition for critical percolation is equivalent to the condition for finite probability of spanning a box growing to infinity; namely that the probability for the existence of clusters of spanning length l or greater in a d-dimensional box of side l must not go to zero with large l. This probability is proportional to

$$\int_{s_{\rm span}(l)}^{\infty} n_s \, ds \tag{3}$$

The proportionality constant in Eq. (2) will be linear in S, the total number of lattice sites in the box, which in turn varies as l^d . The integral in (3) will therefore be proportional to

$$Ss(l)^{-\tau+1} \propto Sl^{-d_f^{\dagger}(\tau-1)} \propto l^{d-d_f^{\dagger}(\tau-1)}$$
(4)

The condition that the integral be nonzero for large l is then simply

$$d \ge d_f \dagger (\tau - 1) \tag{5a}$$

or

$$d_f^{\dagger} \leq d/(\tau - 1) \tag{5b}$$

Since τ is slightly greater than two, d_f^{\dagger} will be somewhat less than the dimensionality d.

³ The mnemonic for the notation d_f^{\dagger} for the exponent will be discussed in Section 4.

⁴ We shall also discuss this distribution at greater length in Section 4.

3. MONTE CARLO RESULTS

Using the same Monte Carlo techniques described earlier,^(1,2) we determined the size distribution of percolation clusters for the simple cubic lattice with nearest neighbor sites (SC-1) as a function of concentration. In addition, we recorded the spanning length for each cluster in *one* of the three principal cubic directions.⁵ Figure 1 shows a log-log plot of spanning length vs. cluster size. The figure shows considerable scatter, because of the fact that we have not plotted the *mean* spanning length for each size, because of insufficient data at each individual size; Fig. 2 shows a plot of the same data where partial averaging has been done by averaging data in size groups. The slope of the line in Fig. 1 is 2.66 ± 0.13 , where the error represents that based upon a least squares fit, weighting all clusters of size 512 and above equally. Inclusion of smaller clusters would somewhat lower the estimated exponent, and in fact such considerations make the error estimate a lower limit. The inequality (5) with $d_r^{\dagger} = 2.66 \pm 0.13$ leads to the corresponding inequality $\tau \le 2.13 \pm$ 0.005. The size distribution data we have obtained for the SC-1 site problem

⁵ It would have been of interest to record this length in several directions to obtain quantitative data on anisotropy. This was not convenient with the current computer program. We have, however, measured the spanning lengths in the [10] and [01] of 45-site clusters (40 < s < 650) on the SQ-1 lattice by graphical methods. This limited sample indicates that any anisotropy is small, i.e., the ratio of the spanning lengths in the two directions is comparable to that arising from a random distribution of ellipses whose major/minor axis ratio is 1.5.



Fig. 1. Spanning length of percolation clusters vs. size for longer clusters ($s \ge 512$) on SC-1 lattices of size (86)³. Data are for p = 0.311 and from seven trials each with an independent random number starter.



Fig. 2. The same data as in Fig. 1, but with data for the smaller clusters ($512 \le s \le 5792$) divided into seven groups by size and the average spanning length in each group plotted vs. the geometric mean of the size group. The width of the size groups increases geometrically by a factor of $\sqrt{2}$. The line drawn is that from Fig. 1.



Fig. 3. Size distribution of percolation clusters on SC-1 lattices of size $(86)^3$ for p = 0.311. Data averaged over eight independent trials. Open squares indicate size intervals in which fewer than ten clusters were observed.

is plotted in Fig. 3. In the plot we have grouped the data according to the method we have used previously.^(1,2) τ is determined from the slope of the straight line fit to the size data in this figure. Again there is a certain amount of judgement to be used in deciding which points should be excluded from the least squares fit, and in fact what weighting factors should be used. The data for the smaller size groupings have the least statistical error, because of the larger numbers of clusters in these groups; however, by definition τ represents the asymptotic slope for large clusters, and the smaller clusters should be discounted. The largest size groups not only suffer from the largest fluctuations, but are influenced more by the finite size of the simulated lattice and by the uncertainties in p_c for the SC-1 lattice. Thus a least squares fit to the data for $8 \le n_s < 4096$ yields $\tau = 2.13 \pm 0.007$. On the other hand, for $64 \le n_s < 4096$ we obtain $\tau = 2.18 \pm 0.024$. Weighting the data for $16 \le n_s < 1024$ more heavily, we judge the most probable value of τ to be 2.15 ± 0.03 . We deduce⁶ from Gaunt's work the value $\tau = 2.20 \pm 0.05$.

Thus we find no inconsistency between the inequality (5) and the present results or even the possibility that (5) is an exact equality. We have only preliminary Monte Carlo results of d_f [†] and τ in two dimensions, but if we assume that the radius of gyration that was recorded in Leath's work⁽⁶⁾ is proportional to the spanning length,⁷ then we can use his results for the SQ-1 site lattice. For clusters in the size range 100–1000 he measures the exponent as 1.634 and 1.764 at p = 0.50 and 0.55, respectively. Extrapolating linearly to $p_c = 0.59$ suggests d_f [†] = 1.87 there.⁸ If we assume a value of τ from Gaunt and Sykes,⁽⁴⁾ then $d/(\tau - 1) = 1.89$, again consistent with either the equality or inequality.

4. CLUSTER SIZE DISTRIBUTION AND MOMENT RELATIONS

The asymptotic form of the size distribution function n_s , the probable number of percolation clusters of size s, that we have used has been discussed extensively in the literature. Quinn *et al.*^(1,2) discussed the numerical evidence

- ⁶ If we identify $(\tau 2)^{-1}$ with the exponent δ_p for which Gaunt and Sykes⁽⁴⁾ and Gaunt⁽⁵⁾ have the two- and three-dimensional series results $\delta_p = 18.0 \pm 0.75$ and $\delta_p = 5.0 \pm 0.8$, respectively, this yields $\tau = 2.056 \pm 0.002$ (2D) and $\tau = 2.205 \pm 0.053$ (3D).
- ⁷ For both random walks and self-avoiding walks the ratio of mean square radius of gyration to mean square length approaches a constant value (albeit different for the two cases) with large numbers of steps.⁽⁷⁾ The spanning length (diameter) of a cluster produced by a random or self-avoiding walk would likely be on the average twice the mean square radius.
- ⁸ While Leath does not give probable errors for these data, we guess that the probable error on the extrapolated result is at least ± 0.03 .

for this form in various lattices and give estimates of the value of τ that is numerically somewhat larger than 2. The distribution function for percolation clusters has also been discussed by others,^(8,9) and quite extensively by Stauffer.⁽¹⁰⁻¹³⁾ Away from p_c there is a very sharp fall-off of n_s from the power law form above some dominant value of s, call it s_{dom} , depending strongly upon $|p_c - p|$. Although the form of this falling off has received considerable attention,^(12,13) we shall, for simplicity and without affecting our final results, assume that n_s falls abruptly to zero at s_{dom} . The concentration dependence of s_{dom} can then be expressed in terms of the critical exponent γ governing the cluster size distribution near critical⁹

$$s_{\rm av} \propto |p_c - p|^{-\gamma} \tag{6}$$

$$s_{\rm av} \propto \int^{s_{\rm dom}} n_s s^2 \, ds \propto s_{\rm dom}^{(3-\tau)} \tag{7}$$

Relations (6) and (7) give the combination of critical exponents for s_{dom} ,

$$s_{\rm dom} \propto |p_c - p|^{-\gamma/(3-\tau)} \tag{8}$$

Stauffer⁽¹²⁾ has previously discussed the critical exponents in terms of a "typical" cluster size s_{ζ} with

$$s_{\zeta} \propto |p_c - p|^{-1/\sigma} \tag{9}$$

The identification of s_{ζ} with s_{dom} gives $\sigma \equiv (3 - \tau)/\gamma$.

The quantity s_{av} defining the average cluster size may be regarded as the zeroth moment of a correlation length, where the *m*th moment of this length is given⁽¹⁴⁾ in terms of the critical exponents γ and ν by

$$\mu_m \propto |p_c - p|^{-\gamma - m\nu} \tag{10}$$

These moments of the correlation function would be expected below p_c

⁹ In our previous work⁽²⁾ we had pointed out that, "for p in the immediate vicinity of p_c the distribution curves are very nearly parallel to the canonical distribution up to quite large cluster sizes." In a footnote on that same page we referred to the fall-off of these curves above some cluster size as being consistent with the exponential increase of average cluster size near p_c . That is, we estimated the exponent $\gamma = 1.7$ from our results on average cluster size vs. p, while when we examined the "fall-off point" vs. p using the distribution data in Fig. 2 of Ref. 2 together with additional unplotted data, we obtained a value 2.05 for $\gamma/(3 - \tau)$, consistent with our relation (8). We have also examined our size distribution data for the simple cubic lattice for $p < p_c$ and this also shows the same behavior as with the bcc results. Our simplified distribution function may be described in terms of the form given in the literature cited, namely $n_s \sim s^{-1}f(x)$, where $x = s^{\sigma} |p_c - p|$. Our form is equivalent to the assumption that $f(x) = \text{ const for } x < x_0$ and f(x) = 0 for $x > x_0$. The normalization conditions on f(x) are not satisfied by this choice; however, this produces only higher order corrections to our results.

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to be proportional to the moments of the spanning length, which we may define as

$$\mu_m \propto \int l^m s^2 n_s \, ds \tag{11a}$$

$$\propto \int s^{m/d_f^{\dagger}} s^2 n_s \, ds \tag{11b}$$

where Eqs. (1) and (2) have been used in (11b). The identification of moments of spanning length with moments of correlation length reflects the fact that there is only intracluster correlation over the distance comparable to a spanning length and no intercluster correlation.

We have used our Monte Carlo data on spanning length and size for the SC-1 lattice to plot the moments $\mu_m = \sum l^m s^2$ at various concentrations. From (10) the slope of the curves when $\log \mu_m$ is plotted against $\log |p_c - p|$ will yield $\gamma + m\nu$. Figure 4 shows these curves with the choice $p_c = 0.3115$.

Figure 5 shows these slopes vs. *m*. From this we determine the values $\gamma = 1.65 \pm 0.04$ and $\nu = 0.77 \pm 0.03$ ($p_c = 0.3115$). The curves in Fig. 2 and hence their least-square-fitted slopes depend upon the value chosen for p_c and we can write $\gamma = 1.65 \pm 0.50(p_c - 0.3115)$, $\nu = 0.77 \pm 80(p_c - 0.3115)$. On the other hand, the same data show that the dependence on the assumed value for p_c nearly vanishes for the ratio γ/ν which is equal to 2.13 \pm 0.10.



Fig. 4. Log of the spanning length moments vs. $\log|0.3115 - p|$ for percolation clusters on SC-1 lattices of size (86)³. The moments are defined as $\mu_m(p) = \sum l^m s^2$, with the summation over all clusters.



Fig. 5. Plot of $\gamma + m\nu$ vs. m. The quantity $\gamma + m\nu$ is determined from the least square slopes of the log $\mu_m(p)$ vs. log|0.3115 - p| plots in Fig. 4.

Sur et al.⁽¹⁵⁾ obtained 0.3115 \pm 0.0005 as the most probable value of p_c for the simple cubic lattice consistent with their data, using a simple scaling relationship to reduce data corresponding to different lattice sizes. It should be noted, however, that they assumed p_c to be independent of the lattice size in their scaling. There is evidence, however, that p_c for the simple cubic lattice is a slowly decreasing function of lattice size⁽³⁾ and therefore a suitably modified scaling law might have reduced their estimate of p_c . Kirkpatrick⁽¹⁶⁾ has obtained 0.312 \pm 0.001, while Dean and Bird,^(17,18) using a different criterion for p_c , suggested 0.320 \pm 0.001. We may also note that a rough estimate based upon our data on cluster spanning length at p = 0.311indicates the probability for spanning is 59%, consistent with this being near the peak in the probability distribution, which is p_c as defined in Ref. 3.¹⁰ This reference also shows that the distribution will have a standard deviation denoted by W, which will vary as the linear dimension of the lattice to the power $-1/\nu$. For a lattice of size (86)³, W is about 0.0033. We tried plotting our data from our Monte Carlo computation for a lattice of size (86)³, plotting the quantities that are usually assumed to diverge as $\log |p_c - p|$, using instead the abscissa $\log[(p_c - p)^2 + W^2]^{1/2}$. This is shown, for example, in Fig. 6. For this choice we found a definite improvement in linearity for the

¹⁰ The 59% figure would indicate that p_c is about 0.23 standard deviation lower. However, our probability estimate is at present much too crude (±20%) to say any more than that it does not rule out most suggested values of p_c .



Fig. 6. Plots of $\mu_0 = \sum s^2$ vs. $\log[(0.3115 - p)^2 + W^2]^{1/2}$. (a) W = 0, least squares slope = 1.63 ± 0.07 ; (b) W = 0.0033, least squares slope = 1.80 ± 0.08 .

points having values of p near p_c . Whether this fact will prove to have fundamental significance remains to be seen. In any case it would seem preferable to base the definition of p_c for a finite lattice upon data relating to the expected approach to a singularity.

Returning to our discussion of (11b) with the upper limit in the integral taken as s_{dom} , we have

$$\mu_m \propto s_{\rm dom} (3 - \tau + m/d_f^{\dagger}) \tag{12}$$

With (8) this yields the relationship

$$\mu_m \propto |p_c - p|^{-\gamma(3 - \tau + m/d_f^{\dagger})/(3 - \tau)}$$
(13)

Consistency between (10) and (13) yields

$$\nu = \gamma / [d_f \dagger (3 - \tau)] \tag{14}$$

or

$$d_{f}^{\dagger} = (\gamma/\nu)(3 - \tau)^{-1}$$
(15)

We note that Stanley *et al.*⁽¹⁸⁾ have defined a fractal dimension d_f for the percolation problem as equal to the ratio of the critical exponents γ and ν , which respectively describe the *average* cluster size¹¹ s_{av} and the average correlation length ξ . Our mnemonic d_f^{\dagger} is to suggest that one can make the same kind of argument to regard d_f^{\dagger} as a fractal dimension.

It may be noted that Leath⁽⁶⁾ has also applied the concept of fractal dimension to the relation between the number of open sites bordering the cluster and the size of the cluster. This work has been discussed by Stauffer⁽¹³⁾ and Domb.⁽²³⁾ Stauffer⁽¹³⁾ makes a distinction between the numerous internal surfaces defined by open sites within the cluster and the external bounding surface of the cluster. He discusses the volume enclosed by this bounding surface and how it varies as a function of cluster size. Although it seems difficult to make a precise definition of this volume, we might identify it with a mean spanning volume of a cluster defined as one proportional to the dth power of the mean spanning length. Stauffer suggests there will be three regimes of variation-for small, intermediate, and large sizes, such that the spanning volume will be linear with size (i.e., $\langle l \rangle^d \propto s$) for both large and small sizes. Our data on the largest clusters we sampled were all consistent with a nonlinear relation between spanning volume and size, $\langle l \rangle^d \propto s^{(d/d_f^{\dagger})}$. characteristic of the intermediate range. If the equality in (5) holds [see discussion after (18)], then the exponent d/d_t is identical with the exponent

¹¹ $s_{av} \equiv \sum (all clusters) s^2 / \sum (all clusters) s$. In integral form this would be

$$s_{\rm av}\equiv\int s^2n_s\,ds\Big/\int sn_s\,ds.$$

The denominator is the total number of occupied sites.

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 $1 + 1/\delta$ given by Stauffer⁽¹³⁾ in his Eq. (5b). Because our observations were made below and in the neighborhood of p_c , Stauffer's hypothesis on the upper linear region remains untested.¹² It is also interesting to note that Stauffer's hypothesis on the behavior of percolation clusters is based very closely upon the analogy with the theory of droplets in the critical region as proposed by Fisher,⁽¹⁹⁾ with many of the equations of the present paper relating critical exponents and d_f [†] having been anticipated in pursuit of this analogy.^{(20),13}

5. OTHER CRITICAL CONSTANT RELATIONSHIPS

By arguments similar to those presented above, Stauffer^(12,13) related σ and τ to the critical exponents α and β by

$$2 - \alpha = (\tau - 1)/\sigma = \gamma(\tau - 1)/(3 - \tau)$$
(16)

$$\beta = (\tau - 2)/\sigma = \gamma(\tau - 2)/(3 - \tau)$$
(17)

leading to the scaling law $\gamma + 2\beta = 2 - \alpha$. Using Eqs. (15) and (16), the inequality (5) becomes

$$2 - \alpha \leqslant \nu d \tag{18}$$

Dunn et al.⁽¹⁴⁾ discussed the inequality (18) following their Eq. (67) describing the two-exponent equality, arguing that the inequality is related to the interpenetration of clusters, which perhaps is more likely in three than in two dimensions. Equation (17) is equivalent to the scaling law $\delta = (\gamma/\beta) + 1$, providing $\tau - 2$ is identified with $1/\delta$.

6. SUMMARY AND CONCLUSIONS

Analysis of Monte Carlo computations on size and spanning length distributions of percolation clusters have qualitatively confirmed theoretical concepts and relationships among critical exponents. It is anticipated that further computations on larger lattices and with increased statistical sampling will make possible more precise tests of these relationships, while comparisons of results on different lattice geometries will similarly test universality hypotheses. There still remains the problem of deciding how best to analyze the results of such computations to extract the optimum values of the relevant coefficients. Scaling methods such as those used by Sur *et al.*⁽¹⁵⁾ are a step in

¹² From Leath's observations⁽⁶⁾ the exponent relating size and radius of gyration increased with p. The data are consistent with it approaching d_f^{\dagger} as $p \rightarrow p_c$ and approaching d as $p \rightarrow 1$.

¹³ Domb⁽²¹⁾ has also commented on the relation of the Fisher droplet model to percolation cluster geometry. Coniglio *et al.*⁽²²⁾ have recently discussed the relationship between percolation and condensation of physical clusters.

the right direction, but do not answer the question of how to properly weight or even reject data describing small clusters or small lattices or concentrations too far away from p_c and which therefore have not reached the proper asymptotic region where scaling applies. Extrapolation methods similar to the series methods that utilize information on the smaller size clusters without necessarily assuming they are in the complete asymptotic range are needed to make the most efficient use of the Monte Carlo data.

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REFERENCES

- 1. G. D. Quinn, G. H. Bishop, and R. J. Harrison, Nuclear Metallurgy 20:1215 (1976).
- 2. G. D. Quinn, G. H. Bishop, and R. J. Harrison, J. Phys. A: Math. Gen. 9:L9 (1976).
- M. E. Levenshtein, B. I. Shklovskii, M. S. Shur, and A. L. Éfros, Sov. Phys.—JETP 42:197 (1976).
- 4. D. S. Gaunt and M. F. Sykes, J. Phys. A: Math. Gen. 9:1109 (1976).
- 5. D. S. Gaunt, J. Phys. A: Math. Gen. 10:807 (1977).
- 6. P. Leath, Phys. Rev. B 14: 5046 (1976).
- 7. C. Domb, Adv. Chem. Phys. 15:229 (1969).
- 8. C. Domb and E. Stoll, J. Phys. A: Math. Gen. 10:1141 (1977).
- 9. H. Müller-Krumbhaar and E. P. Stoll, J. Chem. Phys. 65:4294 (1976).
- 10. D. Stauffer, Phys. Rev. Lett. 35:394 (1975).
- 11. D. Stauffer, Z. Physik B 22:161 (1975).
- 12. D. Stauffer, J. Chem. Soc. Faraday II 72:1354 (1976).
- 13. D. Stauffer, Z. Physik B 25: 391 (1976).
- 14. A. G. Dunn, J. W. Essam, and J. W. Loveluck, J. Phys. C 8:743 (1975).
- A. Sur, J. L. Lebowitz, J. Marro, M. H. Kalos, and S. Kirkpatrick, J. Stat. Phys. 15:345 (1976).
- 16. S. Kirkpatrick, Phys. Rev. Lett. 36:69 (1976).
- P. Dean and N. F. Bird, Mathematics Division Report Ma61 (1966), National Physical Laboratory, Teddington, Middlesex, England; Proc. Camb. Phil. Soc. 63:477 (1967).
- 18. H. E. Stanley, R. J. Birgenau, P. J. Reynolds, and J. F. Nicoll, J. Phys. C: Solid State Phys. 9: L553 (1976).
- 19. M. E. Fisher, Physics 3:255 (1967).
- 20. D. Stauffer, C. S. Kiang, and G. H. Walker, J. Stat. Phys. 3:323 (1971).
- 21. C. Domb, J. Phys. A: Math. Gen. 9:283 (1976).
- 22. A. Coniglio, U. DeAngelis, and A. Forlani, J. Phys. A: Math. Gen. 10:1123 (1977).
- 23. C. Domb, J. Phys. A: Math. Gen. 9: L141 (1976).