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Finite-Size Effects for Some Bootstrap Percolation Models

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The consequences of Schonmann's new proof that the critical threshold is unity for certain bootstrap percolation models are explored. It is shown that this proof provides an upper bound for the finite-size scaling in these systems. Comparison with data for one case demonstrates that this scaling appears to give the correct asymptotics. We show that the threshold for a finite system of size L scales as $O\{1/[\ln(\ln L)]\}$ for the isotropic model in three dimensions where sites that fail to have at least four neighbors are culled.

KEY WORDS: Bootstrap percolation; critical exponents; phase transition; finite-size scaling; simulation.

1. INTRODUCTION

In two recent papers Schonmann[1,2] has rigorously proven that the percolation threshold of an infinite system p_c is unity for two classes of bootstrap percolation[3] (BP) models.[4] In BP[5] one starts with a random distribution of occupied (with probability p) sites and then culls all those sites which do not fulfill a certain condition. This irreversible removal of sites is continued until either the whole lattice has become empty or until a stable configuration where no more sites can be removed is reached. For example, on a hypercubic d-dimensional lattice with $2d$ nearest neighbors we may remove all those sites which do not have at least m occupied neighbors. The condition may be anisotropic; for example, in directed BP models[6] on the square lattice, occupied neighbors are only counted in three directions. In the isotropic Schonmann model, $m \geq d+1$, and in the

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[4] Related systems have been studied in the context of cellular automata.[4]

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directed Schonmann model (DBP), $m=2$, $d=2$. The $p_c=1.0$ result was known for the isotropic case of $m \geqslant 2d-1$, but was somewhat unexpected for the other cases. The result was surprising because numerical data gave estimates below unity. These data had been analyzed with an incorrect assumption of the finite-size scaling form, and, as we shall explain below, this led to the incorrect result.

In the present paper we discuss the importance of using the correct form for the finite-size behavior of BP models in Section 2. A summary of numerical estimates of BP thresholds is given in Table I. A proposal for the correct forms for the two Schonmann cases is discussed in Section 3. Since the exact results only lead to upper bounds on the finite-size effects, we have made a numerical fit to existing data for both the isotropic and directed cases, in order to determine whether they provide the correct asymptotics. This fit and our conclusions are presented in Section 4.

2. THE IMPORTANCE OF THE CORRECT FINITE-SIZE SCALING

There are many variants of BP, and numerous independent routes to its discovery. A summary of early work prior to 1986 is given by Adler and Aharony,[5] who classified the different variants of the model according to the best information then available about the types of percolation transition that occur. Adler and Aharony present a mapping from bootstrap-percolation, with concentration p, to diffusion-percolation (DP), with concentration $1-p$, models. In the latter, sites become occupied if a certain configuration of neighboring sites is already occupied. The occupation processes terminate when no more sites can be added. We choose the BP language for this paper, and have translated all results originally given in DP language via the mapping from ref. 5.

In Table I we summarize the results of many different calculations of thresholds for BP models. In order to make numerical predictions for the infinite system threshold in a percolating system, some assumed form of size dependence for p_{50}^L must always be made. We define p_{50}^L to be the lowest concentration at which 50% of samples of linear size L percolate. If the correct form for the approach to $L=\infty$ has been chosen, then the extrapolated $p_{50}^{\infty}=p_c$. For second-order percolation transitions, the assumed behaviour is based on the same finite-size scaling that is used for second-order transitions in thermal systems. One assumes that

$$p_{50}^L - p_c \sim L^{-1/\nu} \tag{1}$$

where ν is the correlation length critical exponent. This assumption is well justified by the numerical agreement with exact and field-theoretic percolation results.[14] For one-dimensional percolation and $m=2d$ bootstrap in

Table I. Estimates for p_L^{50} BP Models Derived from Different Finite-Size Extrapolations

Dimension	Model	Extrapolation	Estimate
2	$m=3$ BP[a]	Eq. (2)	0.965 ± 0.005
2	$m=3$ BP[b]	Eq. (3)	0.998 ± 0.004
2	$s2n$ DP[a]	Eq. (2)	0.935 ± 0.015
2	$s2n$ DP[b]	Eq. (3)	0.998 ± 0.004
2	$c3n$ DP[c]	Eq. (3)	0.92
2	$m=2$ DBP[d]	Eq. (3)	0.966 ± 0.010
2	$m=2$ DBP[e]	Eq. (9)	0.996 ± 0.010
3	$m=4$ BP[a]	Eq. (2)	0.896 ± 0.010
3	$m=4$ BP[f]	Eq. (3)	0.937 ± 0.005
3	$m=4$ BP[e]	Eq. (6)	0.98 ± 0.02

[a] Ref. 5, where other early estimates for the BP values in which use of Eq. (2) is implicit are also quoted. These all fall below 0.96 for $d=2$, $m=3$ and 0.91 for $d=3$, $m=4$.
[b] Ref. 12, where estimates from refs. 8 and 9 that gave values of unity for related models with scaling of the Eq. (3) type are also quoted.
[c] Ref. 13
[d] Ref. 6
[e] This calculation.
[f] Ref. 15

other dimensions, Adler and Aharony showed analytically that a result analogous to that for thermal first-order transitions is found, i.e.,

$$p_{50}^L - p_c \sim L^{-1/\nu} \tag{2}$$

where $\nu = 1/d$. Numerical evidence from ref. 5 shows that p_{50}^L is equal to p_c for all this class of percolation first-order transitions.

The cases of $m=2d-1$ BP have long been known to be special; there are no stable finite clusters and the transitions are first order. Straley[7] argued that some of the rectangular voids that occur in the spanning ("infinite") clusters in these systems are unstable. One unstable void can grow to engulf the entire sample; this process leads to the threshold of unity for an infinite system. The result was independently obtained by others[8,9] and has been made rigorous by van Enter[10] with a simple contour argument. Aizenman and Lebowitz[11] showed that the p_{50}^L scales as

$$(1 - p_{50}^L)^{1/(d-1)} = \lambda/\ln L + \cdots \tag{3}$$

Bounds on the prefactor λ were estimated in ref. 11 and the λ for several systems were measured numerically by Adler *et al.*[12] In Table I we list results of extrapolation via Eq. (3) and compare these with some extrapolations via incorrect assumptions for this class. For the $m=2d-1$ class the numerical estimates for p_{50}^{∞} extrapolated according to Eq. (3) all include the exact 1.0, with the exception of the Frobose[13] model, where the crossover point to the asymptotic behavior has not been reached. As explained by

Adler *et al.*,[12] this model is the most difficult to vacate, so this is not surprising.

It is quite easy to see that there are also no finite clusters in the $m < 2d - 1$ Schonmann cases; this suggests that the percolation transition may also be first order. However, the voids in these models can have corrugated edges, and in an approximate analysis, this corrugation[7] implies a possibility of stability. If the voids are stable, then percolation could occur with a single "infinite" cluster at a threshold below unity. Numerical evidence (see Table I) based on several different extrapolations including Eq. (3) was consistent with this common wisdom. Prior to Schonmann's calculations no exact results were available for the $m < 2d - 1$ isotropic BP and $d = 2$, $m = 2$ DBP cases. Intuition suggested that if low-m bootstrap models had second-order transitions where p_{50}^L behaved as in Eq. (1) with the usual percolation ν value, the ($m = 2d$) cases had first-order ones with Eq. (2) and $\nu = 1/d$, and the $m = 2d - 1$ has a logarithmic L dependence as in Eq. (3), then the intermediate case of $m = d + 1$ would have some weaker form of $\ln L$ behavior. A serious attempt[15] to generate high-quality data for the $m = 4$, $d = 3$ bootstrap problem has recently been made. These data were analyzed with several trial behavior assumptions involving logarithms, but none was consistent with $p_c = 1.0$. The highest value measured was about 0.94. Similar large-system calculations by Duarte[6] for the directed case also gave a threshold of about 0.97, again below unity. The later sections of this paper will concern the reconciliation of the numerical data with Schonmann's exact result that $p_c = 1.0$ for these classes of BP models. This might be effected by obtaining the correct form for the finite-size scaling for both problems. Therefore, we conclude this section with a discussion of the importance of choosing the correct form.

Simulation of percolation systems is not the only area in which assumptions need to be made about the correct form of the critical behavior. An incorrect assumption for the nature of the critical behavior in second-order phase transitions can lead to incorrect "effective" exponents and erroneous critical temperature and threshold estimates. This effect has been observed (far too frequently) in the analysis of both experiments[16] and series expansions.[14,17–19] It is not always easy to see that estimates derived from incorrect assumptions are in error, since the "effective" exponents may satisfy scaling relations. Numerical tests of convergence, such as scatter in simulation or experiment, or variation in different Padé approximants in series analysis, do not always discount the incorrect estimates *a priori*. Signatures of trouble are more likely to be violation of hyperscaling relations[14,17] or disagreement with exact or field-theoretic results.[19] Examples of this kind of problem occurred in some early series analyses of the 3D Ising model[17,18] and 2D percolation,[14,19] when corrections to scaling were neglected. Field-theoretic analyses do not suffer from the possibility of neglect of corrections to scaling since these often arise from irrelevant operators which are taken care of in the field theory. Another trouble signature is violation of relations between the critical amplitudes. For example, Ahlers[16] observed that although on initial analysis the specific heat exponent of superfluid helium appeared to be zero, the critical amplitude ratio was not unity as expected for a logarithmic divergence. More careful analysis using a correction to scaling term showed that the exponent was slightly negative and that the experimental amplitude ratio agreed with the field-theoretic value.

The need for a correct assumption about the critical behavior as a function of temperature or threshold for an analysis of experimental or series expansion data is paralleled by the need for a correct assumption about the nature of the finite-size dependence for the analysis of simulation data. One example of the application of an incorrect assumption of the functional form for finite-size behavior for a first-order transition within bootstrap percolation is the assumption[12] of L^{-d} behavior for some models in the $m=2d-1$ bootstrap family. This assumption, once used in the absence of better information, is now known to be erroneous.[11] Its application to the $m=2d-1$ models leads to effective critical exponents similar to the second-order percolation ones and estimates of ~ 0.96 for p_{50}^{∞}. As noted above, the correct behavior for these systems is that of Eq. (1) and later reanalysis of the same data using the correct logarithmic law for these systems gave prefactors within the exact range and the correct threshold of unity.

The correct forms for critical behavior in thermal systems are usually based on scaling arguments which are, in turn, based on thermodynamic results. For second-order percolation transitions, the forms have been based on analogies with magnetic systems and field-theoretic results in high dimensions and can today be justified by Kesten's[20] exact proof of hyperscaling in two dimensions. In the absence of a thermodynamic scaling or a field theory for bootstrap percolation, the only reliable guides for the correct finite-size scaling are exact results. These exact results, mathematically speaking, often give upper bounds on the finite-size effects. Thus it is important in *principle* to make simulations in order to check if this bound describes the true behavior. It is of *practical* interest to determine what size system is needed to observe this behavior.

One distinction between the cases cited in refs. 16–19, and the scaling forms proposed *to date* for BP systems, is that the scaling forms used in the cited references all include a dominant divergence with some kind of correction term. This correction term, which is a manifestation of irrelevant operators, is well motivated by the physics of the thermal system or of the percolation field theory. There is no reason why similar corrections cannot be present in BP systems. If this is the case, then the correct scaling form for BP systems might be made up of two or more competing terms; one could dominate near the infinite system limit, and the second for smaller sample sizes. In fact, for very small DP systems,[12] a different slope is seen in a graph of $1 - p_c$ as a function of $1/\ln L$. Just as thermal systems cross over to a different type of behavior far from the critical point, BP models could have different behaviors in different size regimes. For example, for very small DP systems,[12] a different slope is seen in a graph of $1 - p_c$ as a function of $1/\ln L$, to that observed in the larger samples and modeled by Eq. 3. To the best of our knowledge no scaling form that models such a crossover has yet been proposed for this DP model or for any other BP system. We will propose a crossover scaling form for the DBP case below.

3. DERIVATION OF THE FINITE-SIZE SCALING

We begin our derivation of the finite-size scaling form with a discussion of the $m=4$, $d=3$ BP model. The main observation in Schonmann's proof[1] is that an empty cube of size N^3 becomes unstable if its side squares become internally spanned by a vacant cluster (i.e., emptied out by growth of a rectangular void) in the $d=2$, $m=3$ BP model. According to Aizenman and Lebowitz,[11] this happens if $p \simeq O(1/\ln N)$ or $N \sim \exp O(1/p)$. In this case the cube keeps growing with high probability. The probability that such a large cube is empty is

$$p^{N^3} = p^{\{\exp[O(1/p)]\}^3} = p^{\exp[O(1/p)]} \tag{4}$$

because $[\exp(1/p)]^3 = \exp(3/p) \simeq \exp[O(1/p)]$.

The necessary system size L^3 to find such a critical droplet (generalized Straley void) is the inverse quantity

$$L^3 = (1/p)^{\exp[O(1/p)]} \tag{5}$$

Inverting Eq. (5), we find $\ln(\ln L)$ is of $O(1/p)$ or

$$p = O\left(\frac{1}{\ln(\ln L)}\right) \tag{6}$$

If such a cube is empty, then it will continue to grow and therefore the entire L^3 lattice will become vacant. Thus, p_c^L scales as $O[1/\ln(\ln L)]$. This is an upper bound on the scaling because there is a possibility that the void will grow even if its sides are not internally spanned. For higher-dimensional hypercubic lattices with $m = d+1$ there is an extra ln factor in the denominator of the rhs of Eq. (6) for each additional dimension.

For the $d=2$, $m=2$ directed model Schonmann considers critical wedges consisting of a sequence of increasing squares. These play the role of the rectangular voids. The probability that a particular point is at the end of such a critical wedge is [Schonmann, Eq. (0.2)]

$$\alpha(p) = \prod_{k=1}^{\infty} [1 - (1-p)^k]^{k+1} \tag{7}$$

Hence,

$$\begin{aligned}\ln \alpha(p) &= \sum_{k=1}^{\infty} (k+1)\ln[1-(1-p)^k] \\ &\simeq \sum_{k=1}^{[1/p]} (k+1)\ln[1-(1-p)^k] - \sum_{k=[1/p]}^{\infty} (k+1)(1-p)^k \\ &\simeq \sum_{k=1}^{[1/p]} (k+1)\ln(pk) - O\left(\frac{1}{p^2}\right) \\ &\simeq -O\left(\frac{1}{p^2}\right)\end{aligned} \tag{8}$$

We invert Eq. (8) to obtain the system size $L^2 \sim 1/\alpha(p)$ that is needed to contain the edge of at least one critical wedge of the Schonmann form. This gives

$$p \sim O[(\ln L)^{-1/2}] \tag{9}$$

to have a chance of obtaining a critical wedge in the system. With periodic boundary conditions, such a wedge will imply growth of the void and a p_c of unity. The scaling is $O[(\ln L)^{-1/2}]$. The generalization of both exact results and a scaling form for the directed problem in higher dimensions is an open problem, to the best of our knowledge.

After we completed the derivations of the above forms and submitted an earlier version of this paper, Schonmann[21] informed us that after reading our paper he has now been able to improve the arguments for the directed model. The improved arguments are based on a different geometry, of a wedge growing from empty vertical segments of length $N(p)$, rather than wedge segments that grow from a point. They result in a modification of Eq. 8, which becomes

$$\ln \alpha(p) \simeq N(p)\ln(p) + \frac{d}{dp}\left(\frac{\exp-(pN(p))}{p}\right) \tag{10}$$

and Schonmann[21] proposes taking $N(p) = p^{-(1+c)}$, where c is small, or $N(p) = \ln(1/p)/p$. This means that the first term in Eq. 10 now gives the asymptotics (rather than both terms contributing similarly as in Eq. 8 on which the old asymptotics was based) and that the correct scaling is $1/\ln L$, with possible additional logarithmic corrections.

4. NUMERICAL FIT AND CONCLUSIONS

We have tested both the forms by reanalyzing the simulation data of refs. 6 and 15. The plot for the directed problem[6] is given in Fig. 1. The data were obtained for lattices of linear size between 5 and 15,360. Both the extrapolation as a function of $1/(\ln L)^{1/2}$ (large triangles) and the extrapolation as a function of $1/(\ln L)$ (small stars) are given. A simple extrapolation by placing a ruler on the final points of this plot gives

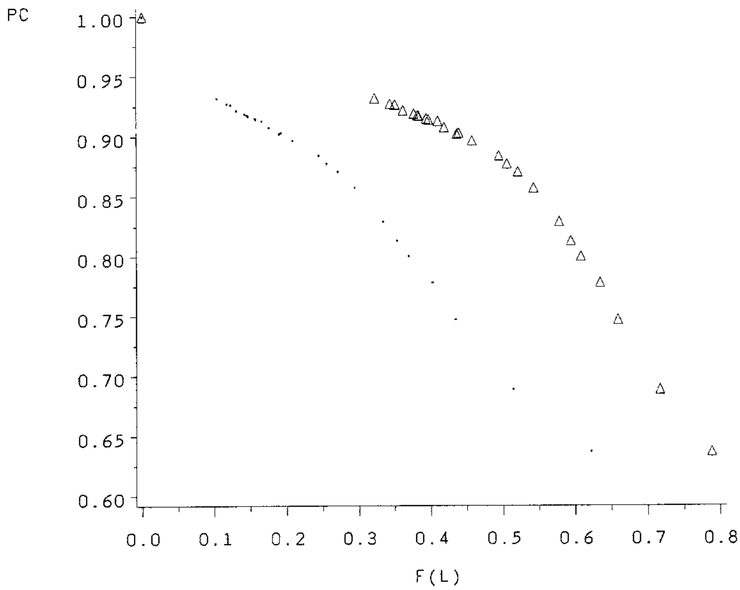

Fig. 1. Graph of p_{50}^{L} as a function of $1/(\ln L)^{1/2}$ and as a function of $1/(\ln L)$ for the $m=2$, $d=2$ directed BP model. The data are taken from ref. 6. ($\triangle$) Square root scaled points; ($*$) logarithmic points. The asymptotic result of $L=\infty$ and $p_c=1.0$ is indicated by a superposition of both symbols.

$p_c=1.0\pm 0.05$ for the square root scaling, to be compared with $p_c=0.966\pm 0.010$ for the inverse logarithmic one.[6] A more detailed analysis has also been made using 3, 4, 5, and 6 consecutive points to fit the form of Eq. (9). This will be presented in more detail in a forthcoming paper on the dynamics of this model.[21] This analysis shows that the square root scaling is only applicable to lattice sizes above $L=300$, but for samples above this size it gives an extrapolated threshold in good agreement with the exact value of $p_c=1.0$.

It is clear that the numerical data favors the square root scaling based on Eq. 8, rather than the now-believed-correct form from the first term in Eq. 10. One possible explanation is that the wedge type geometry dominates in the size range of these simulations leading to the square root behavior, and that still larger samples are needed to see the true asymptotic behavior. It is also possible that neither the square root nor the logarithmic behavior is the correct form and that the square root is an effective behavior in intermediate sizes. Larger simulations of the DBP system, and/or an analysis of the type of void structures that actually occur in the samples in different size ranges, will be needed to resolve this question.

The plot for the isotropic problem is given in Fig. 2. The data have been obtained[15] for samples of linear dimension $\leqslant 704$. Both the

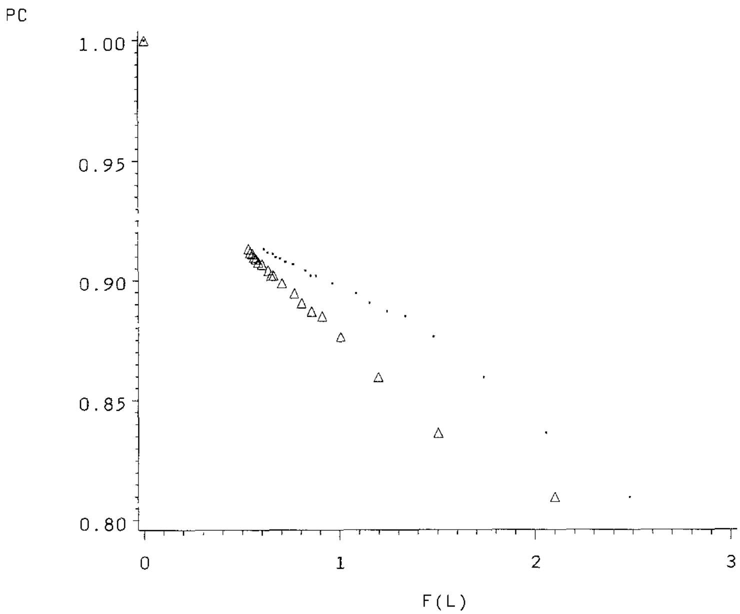

Fig. 2. Graph of p_{50}^{L} as a function of $4/\ln L$ and as a function of $1/\ln(\ln L)$ for the $m=4$, $d=3$ isotropic BP model. The data are taken from ref. 15. (△) Double logarithmically scaled points; (∗) logarithmic points. The asymptotic result of $L=\infty$ and $p_c=1.0$ is indicated by a superposition of both symbols.

extrapolation as a function of $1/[\ln(\ln L)]$ (large triangles) and the extrapolation as a function of $1/(\ln L)$ (small stars) are given. [Note a normalization by a factor of 4 in the $1/(\ln L)$ data in order to fit both sets of data onto the same plot.] The data for the double logarithm have curvature up toward $p_c=1.0$, whereas the data plotted as a function of $1/(\ln L)$ curve in the downward direction or fall on a straight line that extrapolates to $p_c=0.937\pm0.005$ according to the authors of ref. 15. This suggests that the double logarithm is a better fit, although the 704^3 sample may not yet be in the truly asymptotic regime. If we force a straight line through the double logarithmic plot, we find $p_c=0.98\pm0.02$.

We conclude that the $m=4$, $d=3$, BP model we have been able to deduce an asymptotic scaling form for extrapolation that gives the correct threshold of unity.

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REFERENCES

1. R. H. Schonmann, On the behavior of some cellular automata related to bootstrap percolation, Preprint.
2. R. H. Schonmann, Critical points of two dimensional bootstrap percolation like cellular automata, *J. Stat. Phys.* **58**:1239 (1990).
3. J. Chalupa, P. L. Leath, and G. R. Reich, *J. Phys. C* **12**:L31 (1981); see also M. Pollak and I. Riess, *Phys. Stat. Sol. b* **69**:K15 (1975).
4. D. Griffeath, *Notices AMS* **35**:1472 (1988); G. Vichniac, *Physica* **10D**:96 (1988); G. Vichniac, in *Disordered Systems and Biological Organization*, E. Bienenstock, F. Fogelman-Soulié, and G. Weisbuch, eds. (Springer, Heidelberg, 1986).
5. J. Adler and A. Aharony, in *STATPHYS 16*, Abstracts (Boston, Massachusetts, 1986); J. Adler and A. Aharony, *J. Phys. A* **21**:1387 (1988).
6. J. A. M. S. Duarte, *Physica A* **157**:1075 (1989).
7. J. Straley, unpublished, cited in ref. 3.
8. H. Nakanishi and H. Takano, *Phys. Lett. A* **115**:187 (1986).
9. R. Lenormand and C. Zarcone, in *Kinetics of Aggregation and Gelation*, F. Family and D. P. Landau, eds. (Elsevier, Amsterdam, 1984), p. 177.
10. A. C. D. van Enter, *J. Stat. Phys.* **48**:943 (1988).
11. M. Aizenman and J. L. Lebowitz, *J. Phys. A* **21**:3801 (1988).
12. J. Adler, D. Stauffer, and A. Aharony, *J. Phys. A* **22**:L297 (1989).
13. W. Ertel, K. Frobose, and J. Jackle, *J. Chem. Phys.* **88**:5027 (1988); Frobose, K. *J. Stat. Phys.* **55**:1285 (1989).
14. J. Adler, A. Aharony, Y. Meir, and A. B. Harris, Series study of percolation moments in general dimension, *Phys. Rev. B*, to appear.
15. S. S. Manna, D. Stauffer, and D. W. Heermann, *Physica A* **162**:20 (1990).
16. G. Ahlers, *Rev. Mod. Phys.* **52**:489 (1980).
17. J.-H. Chen, M. E. Fisher, and B. G. Nickel, *Phys. Rev. Lett.* **48**:630; A. J. Liu and M. E. Fisher, *Physica A* **156**:35 (1989).
18. J. Adler, *J. Phys. A* **16**:3835 (1983).
19. J. Adler, M. Moshe, and V. Privman, in *Percolation Structures and Processes*, G. Deutscher, R. Zallen, and J. Adler, eds. (Adam Hilger, London, 1983).
20. H. Kesten, *Commun. Math. Phys.* **109**:109 (1987).
21. R. Schonmann, private communication.
22. J. A. M. S. Duarte, in preparation.