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Diffusion percolation: I. Infinite time limit and bootstrap percolation

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Abstract. Several models for the dynamic growth of percolation clusters, or 'diffusion percolation' (DP), are introduced and analysed. In these models a random walker (an 'ant') walks on percolation clusters (which are occupied with initial site concentration, p_i). The 'ant' is allowed to step off such clusters and add new sites to them if certain conditions are met. Some of these models are shown to have a one-to-one correspondence with models of bootstrap percolation (BP), in which sites which do not have a required number of neighbours are successively culled. (For concentrations p of occupied sites greater than some threshold p_c(BP) there will be an infinite cluster in the BP model.) The growth (shrinkage) continues until no more sites can be added (removed). The present paper concentrates on the infinite time limit ($t \to \infty$) of diffusion percolation, in the case where at least one 'ant' was initially on each cluster. There exists a threshold p_i^*(DP), so that at $t \to \infty$ there exists no infinite connected cluster if $p_i < p_i^*$ (DP). We show that $p_i^*(\text{DP}) \geqslant 1 - p_c(\text{BP})$ (for the corresponding BP-DP pair of models in two dimensions), with equality for self-matching lattices, such as the triangular lattice. For some systems p_i^*(DP) is extremely small, or even zero. The transition is found to be either second order, with the usual percolation exponents (within the error limits), or first order, with $1/\nu$ = dimension, where ν is the correlation length critical exponent. We have carried out extensive numerical simulations for several systems. In two and three dimensions, we fail to observe the expected crossover to $1/\nu$ = dimension. However, we see indications of this crossover in four dimensions. Two new percolation thresholds have been calculated for two diffusion percolation models on the square lattice. Both of these are larger than $[1 - p_c(\text{BP})] = 0.4073$ (for the corresponding bootstrap cases), in agreement with our inequality.

1. Introduction

Flow of fluids in porous media is clearly a subject of much scientific and technological significance (leading, e.g., to a better utilisation of oil from rocks). A full understanding of this flow involves first the study of the static geometry of the connected pores, and then the study of the dynamics of the flow on that geometry. In many cases, the geometry is also changing via a dynamic process, e.g., by fracture.

Much of the scientific understanding of flow in porous media has been based on percolation theory (Stauffer 1985, Aharony 1986). A typical percolation model places conducting and insulating bonds on a lattice, with random occupation concentrations p and $(1-p)$. For infinitely large samples, there is a sharp transition from an insulating to a conducting phase, at the percolation threshold p_c. At $p < p_c$ there exist only finite conducting clusters, with an average size that diverges as $p \to p_c^-$. At $p > p_c$ there also exists an infinite conducting cluster. The bonds can be used to model pores or cracks in rocks.

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Above p_c, fluid can pass through the entire rock and, when sufficient cracks are present in the rock sample, fragmentation can occur. The nature of the transition at the percolation threshold and of the geometry of these clusters for random occupation is now well understood, and significant progress has also been made towards the study of flow dynamics (see Aharony (1986) for general results and Englman and Jaeger (1986) for a review of percolation applications to the modelling of cracks in rocks).

There has, however, been relatively less progress in the study of percolation processes where the geometry is changing via a dynamic process. These models can either be viewed dynamically or sampled at some particular time frame and considered to be a correlated percolation process.

We have developed a new set of models for the dynamic growth of percolation clusters. These models are motivated by the need to model crack growth for the case where the nature of the growth depends on the local environment. We call these models 'diffusion percolation' (DP) and introduce them below by example.

The models are given the name DP because crack growth is generated via 'ant' motion. The 'ant' approach to the conductivity problem on percolation clusters was developed by de Gennes (1976). It is a locally definable alternative to the solution of Kirchhoff's equations which require knowledge of the entire system at each step. Here we propose it as a local alternative to the elucidation of crack development by the solution of equations that require input from the entire system. We believe that these models are a useful first step in an attempt to understand percolation processes where the geometry is changing via a dynamic process. Our models are developed in the language of site rather than bond percolation for ease of definition and study, but equivalent (if more clumsy) bond processes can easily be derived. A bond picture is, of course, more natural for crack visualisation.

Consider a square lattice, where each site is occupied with probability p_t, and parachute 'ants' (which can diffuse from one occupied site to a neighbouring occupied site) onto some fraction of the occupied sites. These ants are independent of each other. We may visualise them as being parachuted sequentially: each one moving until no further useful movement can be achieved.

Consider further the configuration of figure 1(a). If an ant at site i contemplates stepping onto the vacant site m, we may define rules that allow it to do so under certain conditions, for example if either of the sites j and k are occupied and it has tried, say, five times to step onto m. (These conditions are motivated by fluid flow in a cracked rock, where after some time has passed fluid succeeds in breaking through previously closed channels if there is a weakness in the surrounding rock.) Once an ant has

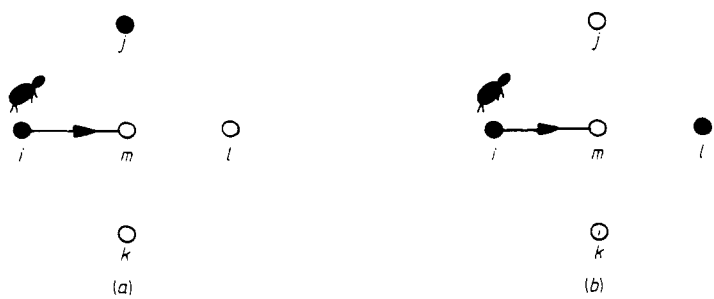

Figure 1. (a) Occupation of new sites in s2n DP. (b) Occupation of new sites in o2n DP. ●, occupied site; ○, vacant site.

stepped onto a site we treat this site as occupied and add it to the pre-existing clusters. In this process any site which has two neighbours that are second neighbours of each other will become occupied if an ant is parachuted onto the cluster containing one of these neighbours. We call this process s2n DP, where 2n stands for two neighbours needing to be occupied before the new site can be occupied and s stands for these two neighbours being on the same side of the site in question.

Alternatively (figure 1(*b*)), we could allow the ant to step onto m if site l is occupied (leading to occupied clusters that grow along the direction of the ant's travel, similar to crack development along weak lines of a rock). We call this o2n DP (o for opposite). This particular variant is probably the most relevant to crack development in real rocks. There is evidence (Englman and Jaeger 1986) that cracks develop further along weak lines of a rock and development along the direction of ant travel mimics this. Details of these and other DP models will be given in § 2, but we note here that in the s2n case any cluster onto which an ant has been parachuted will take a compact rectangular shape at $t=\infty$. In the o2n case clusters will not become compact. The necessity of several attempts prior to occupation is reminiscent of noise reduction in diffustion-limited aggregation (Nittmann and Stanley 1986). Noise reduction in DLA has the general effect of smoothing and leading to clusters that grow more slowly but more regularly. A similar phenomenon is expected here for short timescales. For longer times the noise reduction effect is less relevant for our model because returns to previously visited neighbourhoods near the origin of the motion are more likely than for DLA.

We have studied the time development of clusters with these and other rules governing the ants' behaviour, but detailed considerations of the nature of the time development will be deferred to a second paper. In the present work we will mainly concern ourselves with the 'infinite time limit', and with the limit where sufficiently many ants are parachuted onto the sites, so that at least one falls on every cluster. There are two interesting aspects of these limits. One is the study of the models where the clusters become compact and analytic results can be developed. (This aspect does not concern the o2n case which is potentially more relevant to crack development. However, the knowledge gained from comparisons between numerical and analytic studies of the compact cases is extremely important for the development of simulation techniques for all DP models. The o2n model will receive further attention based on this knowledge in our second paper.) The second aspect is that in the above-mentioned limits we can obtain a one-to-one correspondence between certain DP and bootstrap percolation (BP) models (Kogut and Leath 1981). A summary of recent and new bootstrap percolation results is given in appendix 1. We suggest that the reader who has not previously encountered BP look at this appendix before reading § 2. In § 2 we introduce the various diffusion percolation models and present exact results concerning these systems and their relationship with bootstrap percolation. We show that many of the diffusion percolation models have first-order transitions, and in some of these cases we adapt Straley's BP (Kogut and Leath 1981) large void instability argument to show that $p_c=0$. For DP we call the equivalent cluster instability a Lifshitz–Griffiths–Straley (LGS) instability.

To complement our exact results we have carried out extensive numerical simulations of several DP and BP models. We have, in particular, studied those models where we expect first-order transitions to be present. We expect that $1/\nu=d$ in these cases, and develop exact results for BP on certain finite systems to justify this assumption in appendix 2. We observed $1/\nu=d$ in four dimensions only, probably because the

crossover at lower dimensions is very slow. The simulation results are presented in § 3. In addition to the study of the first-order transition, new p_i^* values for various DP models have been obtained. A discussion of the implications of these results is given in § 4. A summary of the different models discussed in this work is given in table 1, with cross reference to the definitions and correspondences.

Table 1. Summary of models discussed in this paper.

Diffusion percolation model†	Corresponding bootstrap case‡	Figure	p_i^*(DP)	p_c(BP)
Square lattice				
s2n		1(*a*)	0	1
o2n	Model of de Alcantara Bonfim and Engelsberg (1986)	1(*b*)	$0 < p_i^* < 0.338 \pm 0.004 < 1$	—
a1n	$m = 4$	—	0	1
a2n	$m = 3$	2-5	0	1
a3n	$m = 2$	7	0.423	0.5927
a4n	$m = 1$	7	0.551	0.5927
Triangular lattice				
a1n	$m = 6$	6	0	1
a2n	$m = 5$	6	0	1
a3n	$m = 4$	6	0	1
a4n	$m = 3$	6	0.628	0.372
a5n	$m = 2$	—	0.5	0.5
a6n	$m = 1$	—	0.5	0.5

† s = same side, o = opposite side, a = any, n = neighbours.
‡ m is the number of neighbours that must be occupied.

2. Exact results for diffusion percolation and its relation to bootstrap percolation

We assume that the reader who is unfamiliar with bootstrap percolation has taken a moment to glance at appendix 1 prior to reading this section. We also refer the reader to table 1 where a summary of the models discussed in the appendix and in this section is given. In this section we develop a one-to-one correspondence between BP and DP models, beginning for illustrative purposes with the case of $m = 3$ BP on the square lattice and a DP model on the square lattice that we call a2n DP. The a2n DP is a simple composite of the two cases introduced above. Consider (figure 1) the case where the ant at site i is allowed to step onto site m if any of i, k or l are occupied. In other words, at $t = \infty$, if at least one ant is parachuted to each cluster, all sites that have any two neighbours occupied will become occupied. The clusters will be compact, as in the s2n case, and this is strongly reminiscent of bootstrap percolation for $m \geqslant m_u$. For simplicity, let us allow ants to occupy new sites at their first attempt. Consider figures 2 and 3 for the illustration of the development of compact clusters in a2n DP: any occupied site i that has (figure 2) one or more of its neighbours p, q, r or s occupied (say p and q for example) will eventually become part of an occupied rectangle.

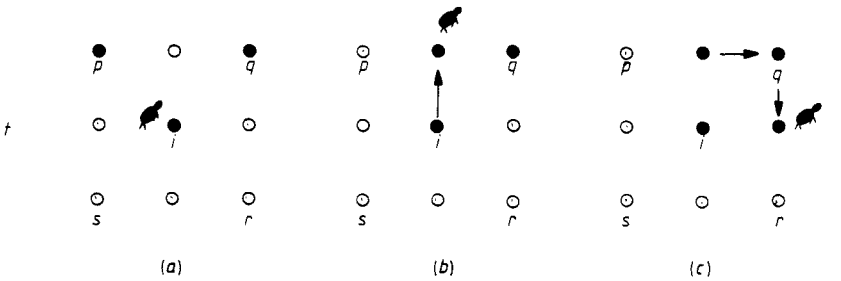

Figure 2. Occupation of new sites in s2n or a2n DP. If there is an ant at site i at $t=0$ (a) then at some time t' (b) it will reach site b and by $t=\infty$ (c) will have reached both b and c.

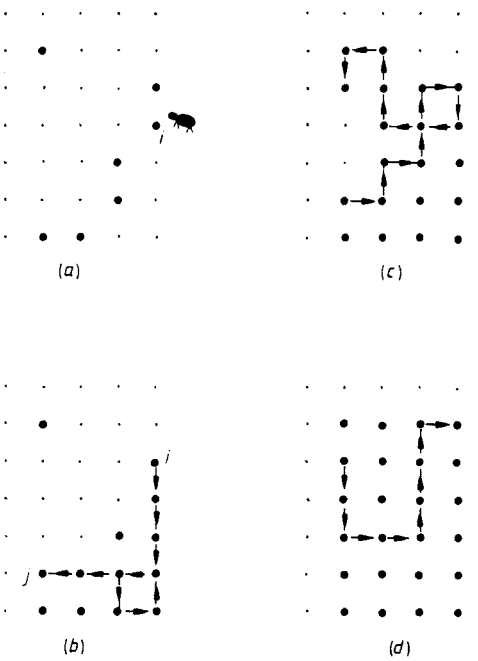

Figure 3. The joining of four distinct clusters to form one compact cluster in a2n DP. (a) $t=0$, (b) $t=t'$, (c) $t=t''$, (d) $t=\infty$.

Similarly, if there is an ant at site i at $t=0$, the configuration of figure 3, which initially consists of four distinct clusters, will consist of only two clusters at $t=t'$, when the ant has reached site j. At $t=t''$ there will be one cluster only, which will become compact at $t=\infty$. The paths indicated are just one possible choice; the actual path taken will probably double back on itself many times. In fact, in order for a $L\times M$ cluster that has an ant on it not to grow to engulf the entire lattice, it must have a border (figure 4) of $(4L+4M+4)$ vacant sites around it. (In the s2n case, a border of $(2L+2M+4)$ vacant sites is required.) This requirement for a cluster not to grow is identical with the requirement for a void not to grow in $m=3$ BP on the square lattice (see appendix 1, where we recall Straley's argument from Kogut and Leath (1981)). By the inverse of Straley's argument, as the cluster becomes larger, the probability for all $4L+4M+4(2L+2M+4)$ sites to be absent is vanishingly small.

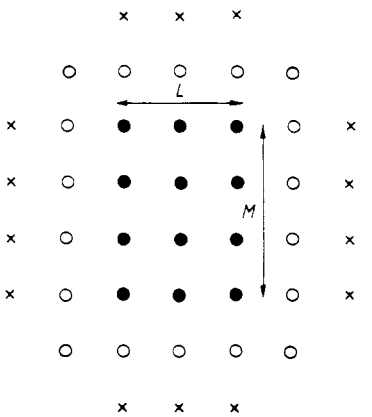

Figure 4. Illustration of conditions required to prevent growth of a large unstable cluster in a2n, o2n and s2n DP. ●, Occupied sites; ○, sites that must be vacant if s2n and a2n DP clusters cannot grow; ×, sites that must be vacant if a2n and o2n DP clusters cannot grow.

If ants are parachuted onto all clusters then, unless $p_i = 0$, the ants will eventually cover the entire lattice. We define the percolation threshold for this problem, p_i^*, as the value of p_i below which percolation will not occur at $t = \infty$ if ants are parachuted onto all clusters. By the above argument we see that $p_i^*(\text{a2n DP}) = p_i^*(\text{s2n DP}) = 0 = 1 - p_c(m = 3 \text{ BP})$†.

Thus we see that there is a connection between a2n DP and $m = 3$ BP on the square lattice. We now complete the identification by showing that a2n DP and $m = 3$ BP are dual to each other. Let us consider any particular realisation of an a2n DP process on a lattice with L^2 sites with some p_i and some initial configuration C of the $p_i L^2$ occupied sites. Let us make the transformation occupied $\leftrightarrow$ vacant, and consider the initial (before culling) configuration of a $m = 3$ bootstrap process, where, by the transformation, the initial concentration of occupied sites is given by p_i ($m = 3$ BP) $= 1 - p_i$(a2n DP). We shall motivate our general example by considering the transformed (figure 5) version of figure 3. We require in a $m = 3$ BP that each occupied site have three occupied neighbours in order to remain occupied. Therefore (see figure 5 ($t = 0$)) sites (3, 3), (4, 2), (2, 1) and (3, 0) will be unsatisfied and become vacant. Once these are vacant, at $t = t'''$, sites (3,4), (4, 1), (2, 2) and (1, 1) will be unsatisfied and become vacant. Finally, at $t = \infty$ all the sites with $x > 1$ and $y < 5$ will be vacant. Just as above, the condition for a void in a $m = 3$ bootstrap not to grow is identical with that for a cluster in DP. We can see that this bootstrap vacancy cluster is identical to the diffusion cluster that develops from the same starting configuration. In general, any vacancy cluster in the $m = 3$ bootstrap grows until all surrounding sites have three occupied neighbours and any occupied cluster in an a2n diffusion percolation that has an ant parachuted onto it grows until all surrounding sites have three vacant neighbours. Thus, for any initial configuration C of occupied/vacant sites, if ants are parachuted onto every cluster present at $t = 0$ in the diffusion process, the configuration of vacant sites in the

† We note that this argument does not apply for o2n DP, because the presence of a single site in the outer x collar would necessitate the occupany of only one additional o site and not an entire row, as in the a2n or s2n cases. Thus there is no engulfing of the lattice but merely some local change. We observe that p_i^*(o2n) is smaller than or equal to the critical concentration of the percolation problem where all nearest and third neighbours are connected. This value is 0.338 ± 0.040.

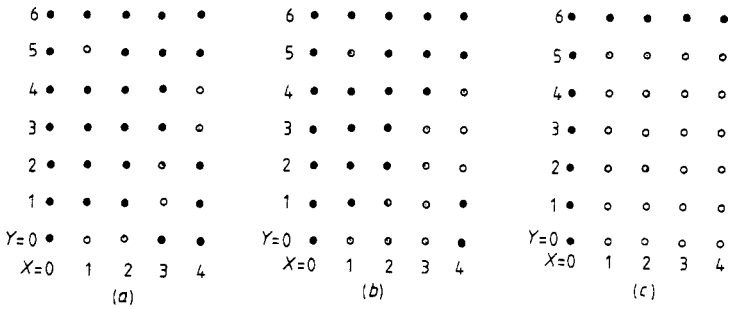

Figure 5. The joining of distinct holes in an occupied cluster to form a compact hole in $m = 3$ BP. Note that the initial configuration of vacant sites is the same as the initial configuration of occupied sites in figure 3 and likewise the final configuration of vacant sites is the same as the final configuration of occupied sites in figure 3. (*a*) $t = 0$; (*b*) $t = t'''$; (*c*) $t = \infty$.

$m = 3$ BP is identical to that of occupied sites in the a2n diffustion process. Therefore, there is a one-to-one correspondence between the two models.

The correspondence between $m = 3$ BP and a2n BP can be generalised for other BP and DP processes. For o2n DP, the corresponding BP is related to a model introduced by de Alcantara Bonfim and Engelsberg (1986). The s2n DP process on the square lattice does not seem to be related to any BP process previously studied. A similar DP process can be defined on the triangular lattice and is related to self-neighbour BP on the triangular lattice (Adler *et al* 1987). The diffusion percolation analogue of the $m = 4$ bootstrap on the square lattice is the rule that all neighbours of an occupied site become occupied (called a1n DP). The analogue of $m = 2$ BP on this lattice is that (figure 1) site m can become occupied only if any two of j, k and l are occupied (a3n DP), and the analogue of the $m = 1$ bootstrap is that m can become occupied only if j, k and l are occupied (a4n DP).

We may also consider the triangular lattice, figure 6. The case where any neighbour of an occupied site, i, will become occupied (a1n) is equivalent to the $m = 6$ bootstrap. The case where m can become occupied if any one of k, p, q, n, j are (a2n) is equivalent to the $m = 5$ bootstrap. When any two of k, p, q, n, j must be occupied we have a3n diffusion, which is equivalent to the $m = 4$ bootstrap. Just as for a2n on the square lattice, a1n, a2n and a3n (triangular) DP clusters will be compact. In order for these compact clusters not to grow, a large border of vacant sites around the cluster will be required. If ants are parachuted onto all clusters, $p_i^* = 0$, just as $p_i^* = 1$ for the corresponding bootstrap process.

We now come to the dual of $m = 3$ triangular BP. This is the (a4n) DP process, where the ant can move from i onto m if three of k, p, q, n and j are occupied. If

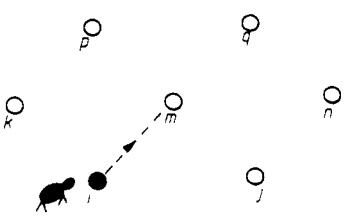

Figure 6. Occupation of new sites on the triangular lattice.

ants are placed on all clusters in this process, then at $t = \infty$ the only vacant sites will be those with three or more vacant neighbours; if there were less vacant neighbours there would be four or more occupied ones and the site would be occupied. There will therefore be percolation of vacant sites across the lattice if $q_i^* = (1 - p_i^*) \geq p_c(m = 3 \text{ BP})$. Since the triangular lattice is a planar graph with triangular faces, and therefore the site problem is self-matching (Essam 1972) on this lattice, there is always percolation of either occupied sites or vacancies. Therefore, if the vacancies do not percolate the sites must and therefore if $q_i^* \leq p_c(m = 3 \text{ BP})$ we have percolation and thus $p_i^* = 1 - p_c(m = 3 \text{ BP})$. An alternative demonstration of this result is by a consideration of the term by term graphical expansion of $k(p, L)$, the mean number of clusters per site for the $m = 3$ bootstrap, and $k(q, L^*)$ the mean number of clusters per site for the a3n diffusion problem†. These two expansions are identical in terms of p and q and thus $k(p, L) = k(q, L^*)$. If we assume that there is only one singularity in each case, and since $L = L^*$ for the triangular site (TS) lattice, we have $p_i^*(\text{a4n DP}) = 1 - p_c(m = 3 \text{ BP})$. A similar result holds for a5n and a6n diffusion (corresponding to $m = 2$ and $m = 1$ bootstraps). Here vacancies can percolate, if $q_i > p_c$ (TS percolation), since p_c ($m = 2$ and $m = 1$ bootstraps) $= p_c$ (TS percolation), and therefore occupied sites can percolate if $q_i < 0.5$ or if $1 - p_i < 0.5$ or $p_i^* = 0.5$.

For the square lattice analogues of the $m = 2$ and $m = 1$ bootstraps we do not find $p_i^* = 1 - p_c$ (square site (SS) percolation). We have vacancies percolating for $q_i \geq p_c$ (SS percolation) but since the lattice is not self-matching, absence of vacancy percolation does not imply percolation of occupied sites. All we can say is that for some $q_i \geq 0.5927$ (Rappaport 1985) we have percolation (i.e. for some $1 - p_i \leq 0.5927$) and thus $p_i^* \geq 0.4073$. It is quite obvious that in the square case $p_c(\text{a3n}) \neq p_c(\text{a4n})$, even though the p_c of their bootstrap analogues are identical. This is because while the lack of dangling bonds and isolated clusters in the $m = 2$ and $m = 1$ bootstraps does not affect the connectivity of the lattice, the presence or absence of isolated vacancies or dangling rows of vacancies does affect the connectivity of a square lattice. In an a3n diffusion process, site i (figure 7) would be occupied if an ant was placed at the lower right corner but in an a4n process it would not, and therefore $p_i^*(\text{a3n}) < p_i^*(\text{a4n})$. Similarly,

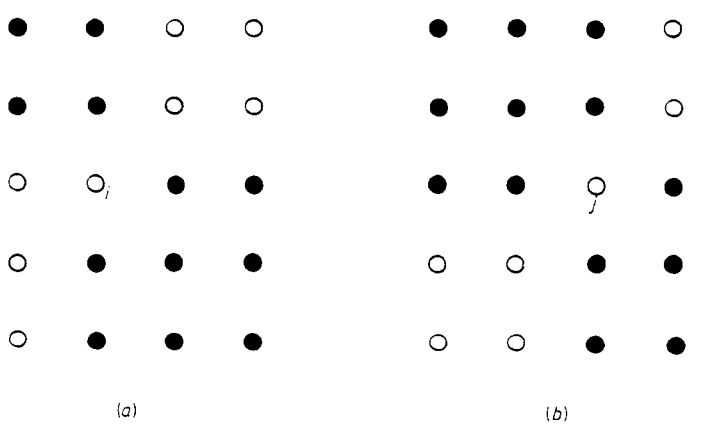

Figure 7. (*a*) Configuration where site i could become occupied in a3n DP but not in a4n DP. (*b*) Configuration where site j could become occupied in a4n DP but not in usual percolation.

† L^* is the matching lattice to the lattice L, on which the bootstrap problem was defined.

in an a4n process site j would be occupied but in usual percolation it would not and hence $p_i^*(\text{a4n}) < p_i^*(\text{ss})$. We will present numerical estimates of $p_i^*(\text{a4n})$ and $p_i^*(\text{a3n})$ for the square lattice and evidence to support the claims of $p_i^* = 0$ in the following section.

The numerical estimates will be obtained via a study of $P(p, L)$, the probability that a site on a lattice of linear size L, if occupied, belongs to the infinite cluster. For BP we calculate $P(p, L)$ by filling sites with probability p_i and then successively culling those that did not have the required m neighbours. For s2n DP (square lattice) we filled sites with probability p_i and then achieved the same result that we would get by parachuting ants onto each cluster and allowing them to move until they could go no further ($t = \infty$), by 'completing the rectangle'. The 'completing the rectangle' algorithm simply means that we identify all clusters of nearest- and second-neighbour sites, and then if these sites have coordinates (x_i, y_i) we find maximum and minimum values of x_i and y_i ($x^{\max}$, $x^{\min}$, $y^{\max}$ and $y^{\min}$) for the cluster and occupy all the sites with $x^{\min} \leq x \leq x^{\max}$, $y^{\min} \leq y \leq y^{\max}$, compact rectangles. This algorithm is also iterative, since two completed rectangles may overlap or have two sites that are second neighbours. Therefore, the process is repeated until no further sites are added. The sites thus occupied are exactly equivalent to all the sites that ants parachuted onto all the clusters could reach by $t = \infty$. For other DP cases we made use of the duality relationship with the corresponding BP model to grow the clusters.

We complete this section with a discussion of the similarities and differences between the percolation free energy $k(p)$ (mean number of clusters), percolation probability $P(p)$ and mean cluster size $S(p)$ for BP and DP, for cases where there are no finite clusters (BP) and holes (DP). A schematic illustration of the correspondence between these cases is given in figure 8. This class includes all bootstrap models for which $m > m_1$ and their corresponding diffusion percolation cases. By observation, $S(p)$ and $k(p)$ are zero for all the bootstrap models, the former because there are no finite clusters anywhere and the latter because there is only one infinite cluster and therefore the mean number of clusters tends to zero as system size tends to ∞. For diffusion percolation, however, there are finite clusters for $p < p_i^*$ (and for at least one non-trivial case, a3n on the simple cubic lattice $p_i^* > 0$) and thus $k(p)$, $S(p) \neq 0$ for $p < p_c$. This result indicates an asymmetry in the bootstrap-diffusion correspondence due to the fact that holes and clusters are not equivalent.

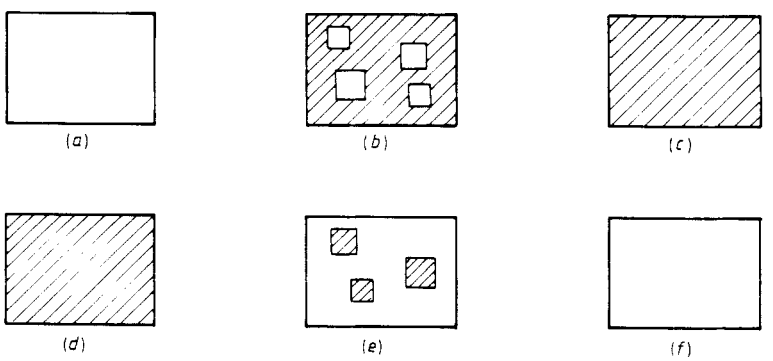

Figure 8. Schematic correspondence between BP and DP for cases of first-order transitions. (*a*) BP, $p < p_c$; (*b*) BP, $p > p_c$ ($p_c < 1$); (*c*) BP, $p = p_c = 1$; (*d*) DP, $p > p_i^*$; (*e*) DP, $p < p_i^*$ ($p_i^* > 0$); (*f*) DP, $p = p_i^* = 0$.

3. Numerical simulations

In this section we present the results of simulations where either first- or second-order transitions are expected. Both cases are analysed with finite-size scaling which is discussed in detail in appendix 2. In the appendix we review the results for finite-size scaling for a second-order percolation transition and show that these are exact for $d = 1$, $m = 1$ BP and for BP in the case where $m = z$, the coordination number of the lattice. Both $d = 1$ percolation and $m = z$ BP have first-order phase transitions and we may thus expect that the finite-size scaling analysis will hold for other first-order BP and DP transitions. In order to carry out the finite-size scaling, we evaluate $P(p, L)$, the percolation probability for a lattice of size L for different values of L, and measure the width, $W(L)$, of this curve. Details of the method by which ν and p_c are deduced from these data are given in appendix 2.

We begin with a study of $P(p, L)$ for those cases where a first-order transition is expected. The cases considered are s2n DP on the square lattice (400^2 sites) and $m = 3$ ($d = 2$, 500^2 sites), $m = 4$, 5 ($d = 3$, 50^3 sites) and $m = 7$ ($d = 4$, 12^4 sites) BP on hypercubic lattices. With the exception of $m = 4$ ($d = 3$) BP those systems are all expected to exhibit large void/cluster instabilities in the infinite system. It is unclear how large samples must be to exhibit these, but they should probably be considerably larger than the simulations usually made, since to obtain $p_c = 1.000$ one would need a large void instability to occur in every sample. Since experimental crack systems to which we wish to apply diffusion percolation are not infinite, we turn our attention to evaluating p_l^* for those systems which do not exhibit large void instabilities and to evaluating p_{50}^{∞} for those that do. We note that in the cases studied in appendix 2 there certainly are large void instabilities present, but in these cases they are so dominating that they are seen on all sample sizes and thus p_c can be easily calculated. The problematic cases are those where samples must be very large for the void instabilities to manifest themselves. We also wish to see if we can observe indications of the expected first-order transitions from the Monte Carlo data for the models we study. We used periodic boundary conditions in all cases, in order to speed convergence, and averaged over 50–100 lattice realisations.

We present data from several simulations in figures 9–11. The data include graphs of the percolation probability $P(p, L)$ for different system sizes L and various graphs describing the analysis of $P(p)$. A discussion of the type of analysis used is given in appendix 2.

Figure 9 contains the data for the two-dimensional models with expected first-order transitions. In figure 9(a) we present $P(p, L)$ curves for s2n DP and in figure 9(b) we present graphs of the width $W(L)$ against system size on a log-log scale for s2n DP and $m = 3$ BP. Comparison slopes with $\nu = \frac{4}{3}$ ($d = 2$, second-order transition) and $\nu = \frac{1}{2}$ (to be expected for a first-order one) are given for clarity of interpretation. We observe that $\nu = \frac{4}{3}$ appears to be consistent with the data, and we shall discuss this further in the next section. There is no conclusive evidence of a crossover to a slope of $\nu = \frac{1}{2}$, although preliminary data do suggest such a crossover for $L > 100$ (Adler and Aharony 1986); the preliminary data were taken on the same 50 lattices for each p_c value whereas in the final data a different set of 100 lattices was used for each point. We note with satisfaction the strong similarity between the $m = 3$ BP and s2n DP, confirming that they are in the same universality class as expected. Figure 9(c) contains plots of p_{50}^{L} against $W(L)$ for different L values. Again the DP and BP curves appear similar. We extrapolate $p_{50}^{\infty} = 0.965 \pm 0.003$ for $m = 3$ BP and $p_{50}^{\infty} = 0.065 \pm 0.015$ for s2n DP for large L values.

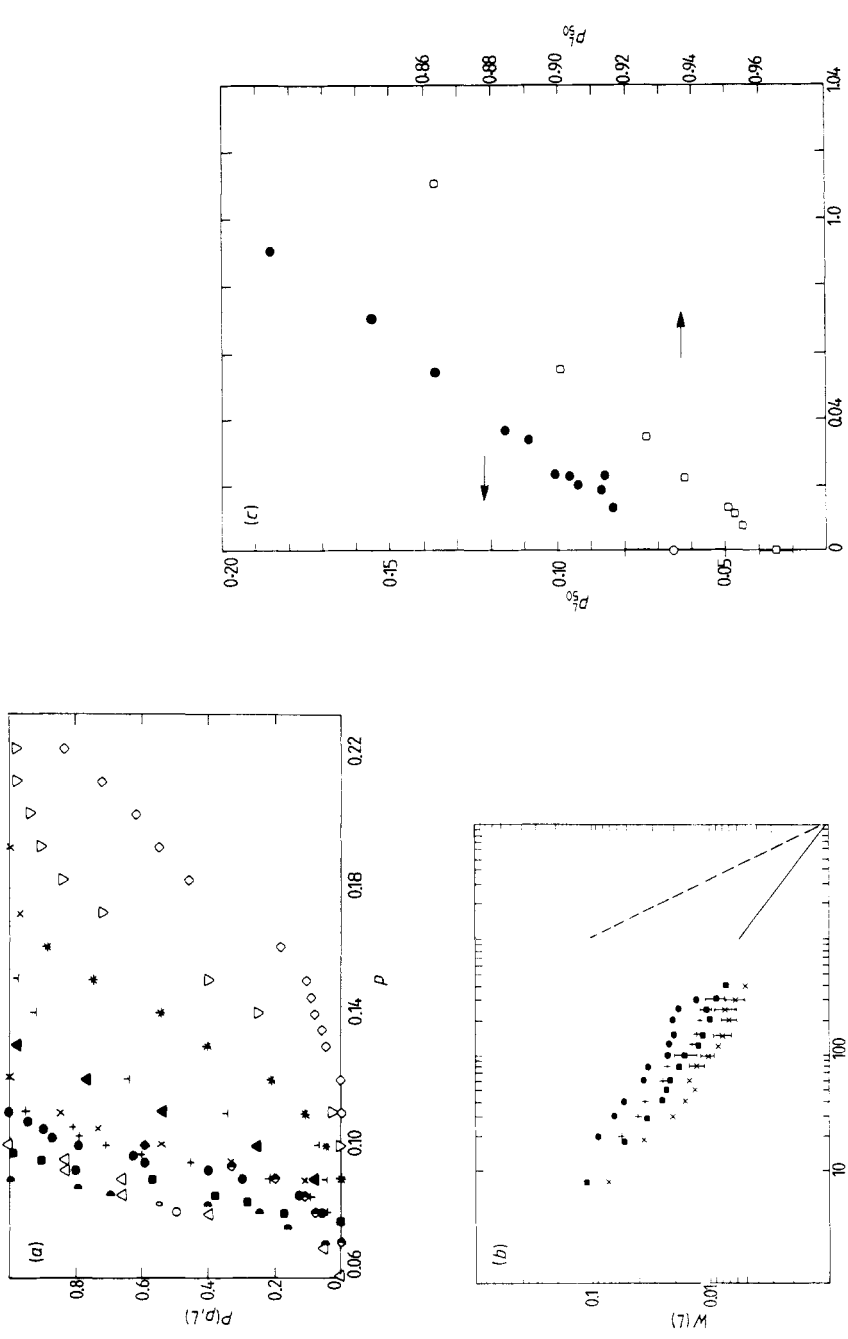

Figure 9. Data for $d = 2$ first-order transitions on the square lattice. (*a*) $P(p, L)$ for s2n DP ($L = 20(\diamond)$, $30(\triangledown)$, $40(*)$, $60(\perp)$, $80(\blacktriangle)$, $100(\times)$, $110(\blacklozenge)$, $125(+)$, $150(\bullet)$, $200(\triangle)$, $250(\blacksquare)$, $300(\blacktriangleright)$, $350(\circ)$, $400(\bigcirc)$); (*b*) $W(L)$ for s2n DP ($\bullet$, $p_{90} - p_{10}$; $+$, $p_{80} - p_{20}$) and $m = 3$ DP ($\blacksquare$, $p_{90} - p_{10}$; $\times$, $p_{80} - p_{20}$); comparison slopes: $\nu = \frac{4}{3}(-)$, $\frac{1}{2}(- - -)$; (*c*) p_{50}^{L} for s2n DP ($\square$, $p_{90} - p_{10}$) and $m = 3$ BP ($\bullet$, $p_{90} - p_{10}$).

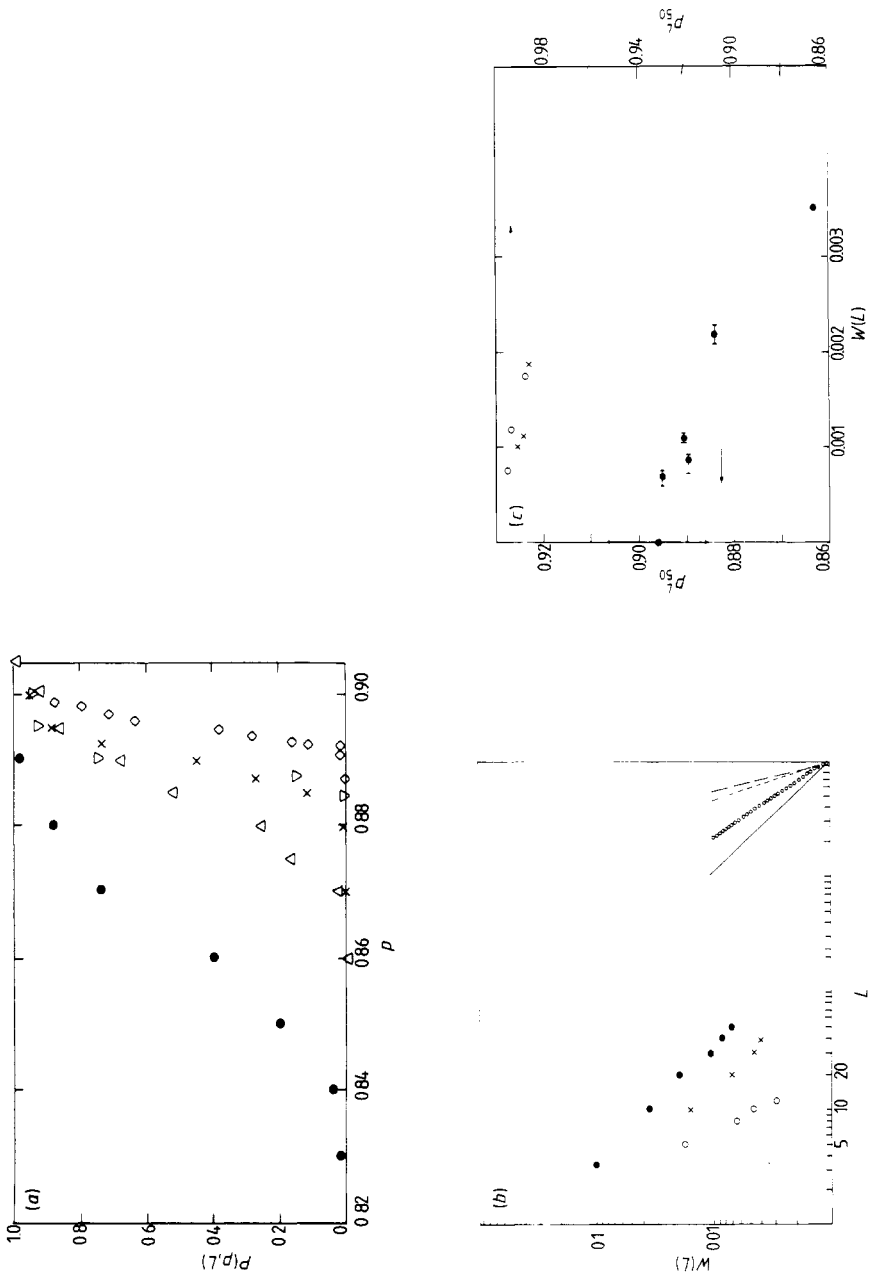

Figure 10. Data for $d = 3$, 4 first-order transitions, hypercubic lattices. (*a*) $P(p)$ for $m = 4$, $d = 3$ BP ($L = 10$ (●), 20 (△), 30 (×), 40 (▽), 50 (◇)); (*b*) $W(L)$ for $m = 4$, ($d = 3$) BP (●, $p_{90} - p_{10}$), $m = 5$, ($d = 3$) BP (×, $p_{90} - p_{10}$) and $m = 7$, ($d = 4$) BP (○, $p_{90} - p_{10}$) comparison slopes: $\nu = 0.88$(—), 0.67(. . . .), $\frac{1}{3}$(– – –), $\frac{1}{4}$(— —). (*c*) p_{50}^{L} for $m = 4$ (○) and 5 (×), ($d = 3$) BP and $m = 4$ (●), ($d = 4$) BP.

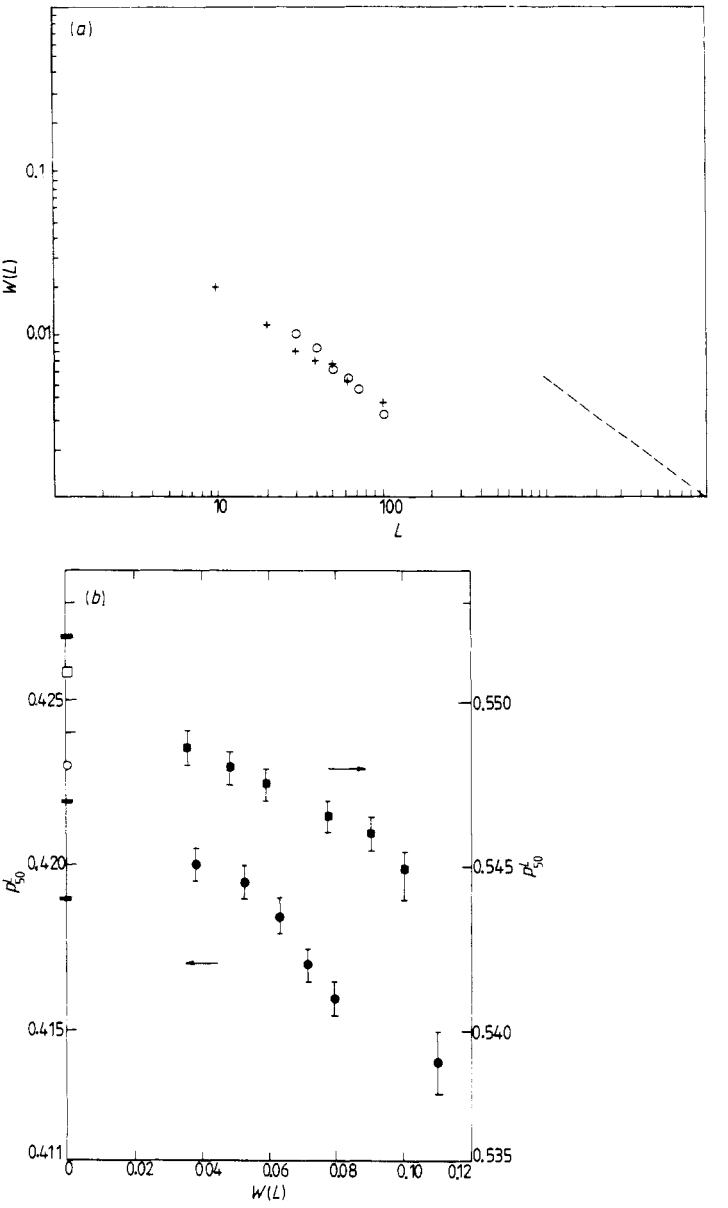

Figure 11. Data for $d = 2$ DP with second-order transitions on the square lattice. (*a*) $W(L)$ for a3n (+) and a4n(○) DP; comparison slope: $\nu = \frac{4}{3}$; (*b*) p_t^* estimates for a3n (●) and a4n (■) DP.

We note that p_{50}^{∞} for a2n DP would be expected to be greater than $1 - 0.965 \pm 0.005 = 0.035 \pm 0.015$ which is much less than 0.065 ± 0.015 as expected, since s2n diffusion clusters grow more slowly than a2n ones. We may compare the $m = 3$ BP numbers with the results of the renormalisation group study of Branco *et al* (1986). They work with small cells (thus their calculation cannot include the effects of the large void instabilities), and obtain $p_c(m = 3 \text{ BP}) = 0.956$, 0.931, 0.918, 0.834 or 0.873 for different scale factors. Their first value is in good agreement with our $p_{50}^{\infty} = 0.965$ as would be expected.

The data for the three- and four-dimensional models with expected first-order transitions are given in figure 10. In figure 10(a) we present $P(p, L)$ curves for $m=4$ ($d=3$) BP, where there are no large void instabilities and thus $p_c<1$. In figure 10(b) we plot $W(L)$ against L for $m=4(d=3)$ BP, $m=5(d=3)$BP and $m=7(d=4)$ BP. For the $d=3$ cases $W(L)\,L^{-1/\nu}$ with ν taking the second-order transition value, 0.88. Plots of p_{50}^L against $W(L)$ are presented in figure 10(c) and for $m=4(d=3)$ we find $p_{50}^{\infty}=p_c=0.896\pm0.010$, just at the bottom of Kogut and Leath's (1981) range of $p_c=0.902^{+0.007}_{-0.006}$. For the $m=7(d=4)$ BP graph of figure 10(b) we observe that the slope measured over all four points is $1/\nu=2.0+0.5$, but if we consider the last two we find $1/\nu=3.4+0.18$ and the first three alone give $1/\nu=1.6\pm0.5$. These values are compatible with a crossover from the second-order value of 1.49 (de Alcantara Bonfim *et al* 1981) to the first-order value of $1/\nu=4.0$.

Results for DP systems on the square lattice with second-order transitions are given in figure 11. The statistics here are only 60 lattices per point, as one expected better convergence. In figure 11(a) $W(L)$ is plotted against L for a3n and a4n DP. The slope gives $\nu=1.1+0.2$ for a4n DP and $\nu=1.3+0.2$ for a3n DP. Figure 11(b) contains extrapolations of p_{50}^L against W results to give the first p_i^* estimates for these two systems. We find

$$p_i^*=0.551\pm0.004 \text{ (a4n DP)}$$

$$p_i^*=0.423\pm0.004 \text{ (a3n DP)}.$$

In § 2 we deduced that both these p_i^* values must be greater than $1-p_c$ (usual percolation) $=0.4073$ (Rappaport 1985) for this lattice, and this inequality is clearly satisfied here.

4. Discussion

We have introduced a new percolation process, diffusion percolation (DP), and established the connection between DP and bootstrap percolation (BP). We note that this connection is similar to that between invasion percolation (Wilkinson 1983) and invasion percolation with trapping (Newman 1986 private communciation). A similar duality connection does not seem to exist between DLA and anti-DLA (Paterson 1987). Exact results for both DP and BP have been developed. Numerical simulations of several different cases have been made, which confirm that the corresponding DP and BP have the same critical behaviour. We have confirmed our prediction of $\nu=1/d$ in four dimensions, for first-order transitions, but failed to see clear evidence of any crossover to this behaviour in $d=2$ or $d=3$. This presumably means that we have not considered sufficiently large lattices. We hope to remedy this in the future. For the second-order DP processes in two dimensions we found new p_c values and ν values that are consistent with the usual percolation value. This is to be expected from the BP-DP correspondence and the observation that ν in percolation depends on the geometry of the infinite cluster, which is the same for $m=0$, 1 and 2 BP.

A summary of the correspondence between DP and BP with p_c and p_i^* estimates is given in figure 12.

Acknowledgments

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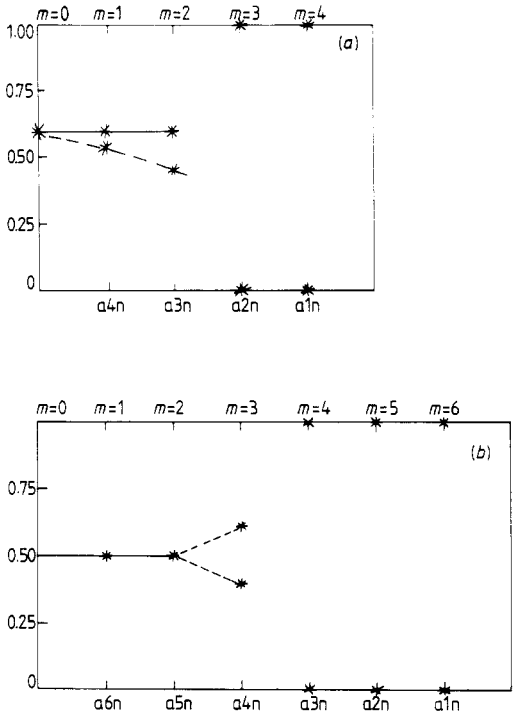

Figure 12. Graphs of p_c for BP and p_i^* for DP on the (a) square lattice, (b) triangular lattice.

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Appendix 1. Bootstrap percolation

Bootstrap percolation (Chalupa *et al* 1981, Kogut and Leath 1981, Branco *et al* 1986, Khan *et al* 1985 and references therein) is a percolation model wherein all sites with less than m neighbours are successively culled from the lattice. For $m = 0$, we have usual percolation. For $m = 1$ or 2 we have the same p_c as for usual percolation, although the cluster statistics will vary since in both cases isolated sites, and in the $m = 2$ case sites connected to dangling bonds, will be removed. For $m = z$ (the coordination number of the lattice), on the other hand, $p_c = 1.0$ since any absent site will mean that its neighbours do not have z neighbours and thus unless the lattice is completely full no sites will survive the culling. In this case the transition is first order, as in $d = 1$ percolation. For intermediate m values, there are two possibilities: if $m > m_u$ then by Straley's argument (described in Kogut and Leath (1981) and rigorised by van Enter (1987)), of large void instabilities, $p_c = 1$. For $2 < m < m_u$ there will be a transition at some $p_c < p_c(m) < 1$. If $m_u > m > m_1$ there will be no finite clusters and the transition will be first order. We define m_u as the smallest m for which $p_c = 1$ and m_1 as the smallest m for which the transition is first order.

Table 2. p_c estimates.

		m								
		0	1	2	3	4	5		6	
$D=1$	$p_c=$	1	1	1						
$D=2$										
Square										
$m_l=3$	$p_c=$	0.5927[a]	0.5927[a]	0.5927[a]	1[b]	1[b]				
$m_u=3$					0.83 0.96[c]					
	$p_{50}^{\infty}=$				0.965 ± 0.005[d]					
Triangular										
$m_l=?$[e]	$p_c=$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		0.606[b]				
$m_u=4$					0.60 0.76[c]					
					0.628 ± 0.02[f]					
	$p_{50}^{\infty}=$						0.81	0.89[c]	0.96	1.0[c]
$D=3$										
Simple cubic										
$m_l=4$	$p_c=$	0.3116[g]	0.3116[g]	0.3116[g]	0.568[b]	0.902[b]	1			
$m_u=5$	$p_c=$					0.896 ± 010[d]				

[a] Rappaport (1985).
[b] Kogut and Leath (1981); error bars are ~0.005.
[c] Branco *et al* (1986).
[d] This work.
[e] m_l is probably 4 but there is no proof that the $m=3$ transition is second order.
[f] Khan *et al* (1985).
[g] Stauffer and Zabolitzky (1986).

A summary of m_l, m_u and p_c values from previous and parallel studies is given in table 2 for bootstrap percolation on several common lattices. In the case $m > m_u$, small samples fail to show any sign of the large void instabilities. It is therefore possible to define a quantity p_{50}^L which is the concentration at which 50% of lattices of size L percolate. In the thermodynamic limit $L\to\infty$, p_{50}^L would tend to p_c and by the large void instability argument $P_{50}^L\to 1$ if $m > m_u$. However, for a finite system the behaviour of P_{50}^L for large L is a useful measurement and by arguments given in § 3 some systems of interest are not believed to have the $L=\infty$ behaviour. We call the large L value of p_{50}^L, p_{50}^{∞}. This quantity is equal to p_c in the case of second-order transitions, first-order transitions without large void instabilites and the cases discussed in appendix 2. It is also possible to consider variants of bootstrap percolation, for example percolation where the neighbours of a site must be neighbours of each other (Adler *et al* 1987).

We note that the behaviour of p_{50}^L as $L\to\infty$ has been considered by Lenormand and Zarcone (1984) for another model with large cluster instabilities. They estimated that $p_l^* = K/\log L$ for asymptotically large L, and found $K=0.33$ from numerical simulations.

Appendix 2. Exact results

We consider below some exact results in the infinite time limit for BP/DP $m=z$ and/or $d=1$. For a first-order transition one expects (Nienhuis and Nauenberg 1975, Fisher

and Berker 1982) $\nu = 1/d$. For the usual second-order percolation transition (Stauffer 1985), we know that the width, $W(L)$, of the percolation probability $P(p, L)$ (defined as the probability that if a given site is occupied it is part of the incipient infinite cluster in a system of linear dimension L) scales as $L^{-1/\nu}$ and so does $p_{50}^L - p_c$ where p_x^L is the concentration at which $x\%$ of the samples of size L are connected in all directions. We measure $W(L)$ by either $p_{90}^L - p_{10}^L$ or $p_{80}^L - p_{20}^L$.

These various quantities are illustrated schematically in figure 13. We may use the fact that $W(L)$ and $p_{50}^L - p_c$ both have the same ν dependence as a function of L to deduce p_c from the intercept of a plot of p_{50}^L against $W(L)$. We have no rigorous proof that the same finite-size scaling will work for a first-order transition, but we show below that $W(L) \sim L^{-1/\nu}$ for first-order transitions in $d = 1$ and when $m = z$.

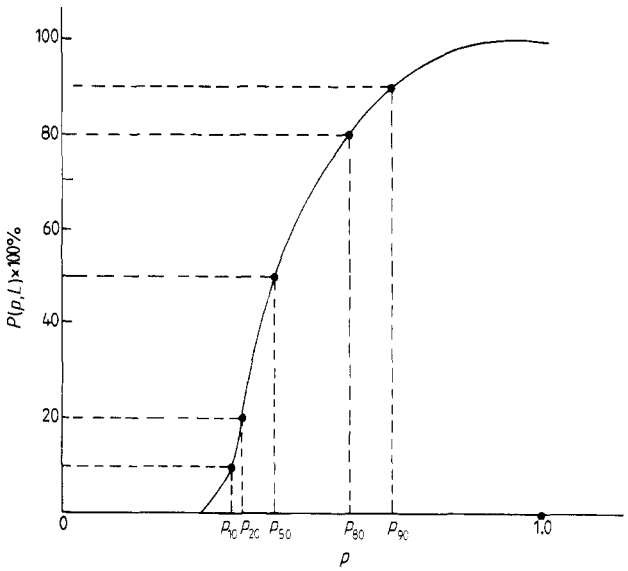

Figure 13. $P(p, L)$, the percolation probability, for a system of size L (schematic diagram).

We note that it will become necessary in certain cases to distinguish between the true p_c or p_i^* of a system and the result of the extrapolation of p_{50}^L to very large sample sizes. In these cases we have called the numerical extrapolation of p_{50}^L, p_{50}^∞. It should also be noted that a real-space RG study would estimate p_{50}^∞ and not the true p_c in these cases.

We begin with a consideration of $d = 1$. For $m = 1$ BP and its corresponding model a2n DP we have no single site clusters (or single vacant sites if ants are parachuted onto all clusters) but otherwise the transition and cluster distribution are not very different from usual 1D percolation. For $m = 2$ BP and a1n DP, the cluster size distributions are quite different. There are no finite clusters in the BP case for $p < p_c = 1$ and if ants are parachuted onto all clusters in the a1n diffusion then every lattice site is occupied for $p > 0$. All these transitions are first order and $p_c = 0$ or 1.0.

For $m = 2$ BP we now look at a set of imaginary simulations of samples of different lengths L. There will be pL occupied sites, all of which will be part of the infinite cluster. If $pL < 1$ or $p < 1/L$, then $P(p, L) = 0$. The probability that $P(p, L) = 1$ is p^L,

therefore $P(p, L) = p^L$ or $p = P(p, L)^{L/2}$. Thus

$$W(L) = p_{90}^L - p_{10}^L = 0.9^{1/L} - 0.1^{1/L}$$
$$= \exp^{(1/L \ln 0.9)} - \exp^{(1/L \ln 0.1)}$$
$$= 1/L \ln(0.9/0.1)$$
$$= 1/L \ln 9 \sim L^{-1}$$

and $p_{50}^L = 0.5^{1/L}$. We know that $p_c = 1$, thus $p_{50}^L - p_c \sim 1/L = \ln 0.5 \sim L^{-1}$. These results imply that $\nu = 1$, as expected for a first-order transition in one dimension, and suggest that we may use a graph of $W(L)$ against p_{50}^L on a linear scale to determine p_c, exactly as for a second-order transition. The extrapolation may or may not be linear.

These results can be extended to general dimension, for the case where m is equal to the coordination number of the lattice, z, and $p_c = 1$. Here $P(p, L) = 1$ with probability p^{L^d} and therefore

$$W(L) = p_{90}^L - p_{10}^L = (0.9)^{1/L^d} - (0.1)^{1/L^d}$$
$$= 1/L^d \ln 9 \sim L^{-d}$$

and $p_{50}^L - p_c \sim L^{-d}$. This implies $1/\nu = d$ as expected.

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