LETTER TO THE EDITOR

Structure and perimeters of percolation clusters

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Abstract. Site percolation clusters are simulated at the percolation threshold on the square lattice. An algorithm for walks around each cluster is used to obtain information on its fractal geometry. The fractal dimensionality of the external perimeter is found to depend on the size of adsorbent particles used to measure it: if the vacant perimeter sites have only nearest-neighbour connectivity then the perimeter has dimension $D_e = 1.37 \pm 0.03$, instead of that of the hull ($D_h = 1.75$). We also measured the mass of internal dangling sites (surrounded by the backbone's 'blobs'), singly and doubly connected sites, the number of 'blobs' and the average linear distance between entry into and exit from a 'blob'.

Many dilute physical systems are modelled by site percolation, in which a random fraction p of the sites on a lattice are occupied, and the remaining sites are vacant (e.g. Stauffer 1985). An infinite cluster of connected sites appears above the percolation threshold, p_c, with a density $P_\infty \sim (p - p_c)^\beta$. The average distance between sites on connected finite clusters diverges as $\xi \sim |p - p_c|^{-\nu}$. It has been realised for some time (Stanley 1977, Mandelbrot 1982) that these clusters have a fractal geometry. The number of sites s on a cluster of linear size L behaves as $s \sim L^D$, with the fractal dimensionality $D = d - \beta/\nu$, where d is the Euclidean dimensionality (Kirkpatrick 1979, Kapitulnik *et al* 1983 and references therein). It was later realised that various physical properties are determined by various *subgroups* of sites on the cluster, and that the number of sites in these may scale with different powers of L, i.e. with different fractal dimensionalities (Pike and Stanley 1981, Stanley 1984). The present letter presents the results of computer simulations of site percolation clusters on the square lattice, which concentrated on several new subgroups of sites, relevant to several physical problems, and measured their fractal dimensionalities.

Our first results concern the *external perimeters* of the clusters. Voss (1984) defined the hull of a cluster as the occupied sites on it, which neighbour 'external' vacant sites, the latter being connected to the outside of the cluster via either nearest or next-nearest unoccupied neighbours (on the square lattice). He found that the average number of sites on the 'hull' of clusters of linear size L scales as

$$H \sim L^{D_h} \tag{1}$$

with $D_h = 1.74 \pm 0.02$. Similar results were obtained for the vacant neighbouring sites by Ziff *et al* (1984), who generated the 'hull' by a special self-avoiding random walk

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(see also Weinrib and Trugman 1985). The 'hull' was also related to the number of particles on a diffusion front by Sapoval *et al* (1985), who conjectured that $D_h = (1 + \nu)/\nu (= 1.75$ at $d = 2)$.

One possible application of the hull concept may relate to surface energy. Other applications may involve the adsorption of particles on the surface, chemical reactions on it, etc (e.g. Pfeifer *et al* 1984). In these applications, the size of the adsorbent particles is very important. In fact, particles of different sizes were used by Pfeifer *et al* to measure the fractal dimensionality of fractal surfaces. Our first result shows that the fractal dimensionality of the external perimeter of percolation clusters is not independent of the adsorbent particle size. In particular, if this size is larger than the 'open space' (distance) between next-nearest-neighbour occupied sites, these particles will not be able to enter regions connected to the outside via next-nearest (vacant) neighbours. In the example shown in figure 1(*a*), this will exclude the vacant sites denoted by × from the external perimeter, and leave only those denoted by ○, which are connected to the outside only via nearest-neighbour vacant sites. Denoting the average number of these by E, we find that

$$E \sim L^{D_e} \tag{2}$$

with $D_e = 1.37 \pm 0.03$. This fractal dimensionality is very different from D_h, showing that there are large impenetrable regions. The perimeter of these regions thus dominates the hull.

Consider now two endpoints on a cluster, e.g. the points with the largest (smallest) y coordinate and—among these—with the largest (smallest) x coordinate. The Euclidean distance between these is denoted by L, and serves as a measure for the linear size of the cluster. The structure of the cluster between these endpoints is described by the 'links and blobs' picture (Stanley 1977, Coniglio 1981, 1982, Pike and Stanley 1981, Herrmann and Stanley 1984 and references therein): if one applies a voltage between the two terminals, current will flow only through the 'backbone', which
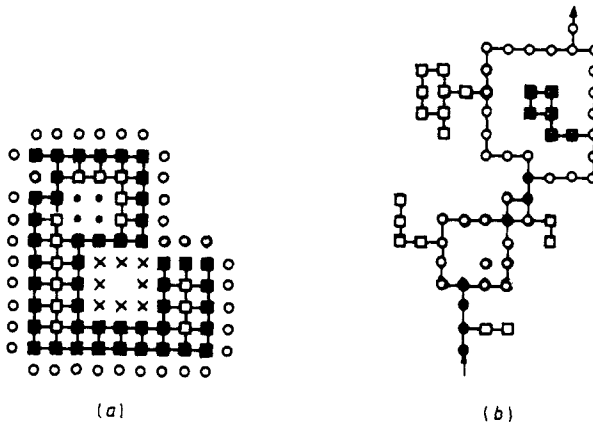

(*a*)   (*b*)

Figure 1 Examples of clusters. (*a*) Occupied sites divide into hull sites (full squares) and internal sites (open squares). Perimeter sites divide into the external perimeter with nearest-neighbour connectivity (open circles), additional external sites with next-nearest-neighbour connectivity (×) and internal perimeter sites (full circles). (*b*) Backbone sites are divided into singly connected sites (⊗) and blobs (○). Dangling sites include external (□) and internal (⊠) ones.

contains $L_1(L)$ *singly connected sites* (carrying the full current) and 'blobs' of various sizes. In addition, there exist many dangling sites, which do not carry current (each group of these is connected to the backbone via a single backbone site). A schematic picture is shown in figure 1(*b*). We measured the following new properties.

(a) Dangling sites are divided into 'external' ones, which are almost surrounded by external perimeter vacant sites, and 'internal' ones, which 'hang' inside the 'blobs' and do not touch any external perimeter site. As might be expected, most of the mass of the cluster consists of external dangling sites. Indeed, we find that their 'mass' scales with the fractal dimensionality $D \simeq 1.9$. We measured the sum of the 'mass' of the internal dangling sites, s_i, and that of the backbone s_B (total mass minus external dangling sites), and found that it scales as L^{D_i}, with

$$D_i = 1.77 \pm 0.04. \tag{3}$$

(b) It has been proved by Coniglio (1981, 1982) that $L_1(L) \sim L^{1/\nu}(\nu = \frac{4}{3}$ at $d = 2)$. The singly connected bonds are dominant in determining the elasticity of clusters (Kantor and Webman 1984, Kantor 1984), the conductivity of non-linear resistor networks, with $V \sim I^\alpha$ and large α (Blumenfeld and Aharony 1985), the magnetic correlations of Ising spin systems (Coniglio 1981, Aharony *et al* 1984, 1986), etc. In many of these cases, the next important term involves pairs of *doubly connected sites*, such that the elimination of the two sites in a pair breaks the cluster in two. Coniglio's proof can be generalised to show that the average number of these pairs, $L_2(L)$, scales as $L^{2/\nu}$. We measured both $L_1(L)$ and $L_2(L)$, and confirmed that indeed $L_2 \sim L_1^2 \sim L^{2/\nu}$. In addition, we counted the *number of blobs* between the endpoints, N_B, and found that it also scales as $L^{1/\nu}$, confirming Herrmann and Stanley's (1984) conclusion that the 'strings' of singly connected bonds have a finite average length.

(c) The minimal path L_{min} between the endpoints consists of the singly connected sites and the sum of minimal paths between entry and exit into the blobs. This path is known to scale as $L^{d_{min}}$, with $d_{min} \simeq 1.13$ at $d = 2$ (e.g. Havlin and Nossal 1984, Hong and Stanley 1983a, b). Since $d_{min} > 1/\nu$, it is clear that L_{min} is dominated by the sum of minimal paths through the blobs. Having identified the entry and exit point of each blob, we measured the Euclidean distances between them, and found that their sum scales as L^{d_x}, with $d_x = 1.10 \pm 0.07$. The minimal path between the endpoints is dominated by the sum of the minimal paths between entry and exit of the blobs (plus L_1, which is negligible). Since d_x is very close to d_{min}, the minimal path inside each blob seems to be practically proportional to the Euclidean distance between entry into and exit from the blob. The average of this distance scales as $L^{d_x - 1/\nu}$, and $d_x - 1/\nu = 0.35 \pm 0.07$.

Our numerical algorithm combines the methods of Leath (1976a, b), Pike and Stanley (1981) and Ziff *et al* (1984). Beginning with an initial occupied site at the origin, we use a pseudo-random number generator to decide whether each of its nearest neighbours is occupied (with probability p) or vacant. The procedure continues for the (untested) neighbours of the connected occupied sites, until all of these are found to be vacant. The connected sites and the total perimeter (all vacant neighbours) are counted during growth. Using a frame of size 740×740, we rejected all the clusters with $L > 370$. At $p = p_c = 0.592\,77$ (Gebele 1984), this left a population of about 17 000 clusters, with sizes $s \leqslant 20\,000$.

On each cluster, we identified the two endpoints and then applied a biased walk around it. Beginning at the lower endpoint, the walker attempts to move to its nearest neighbour on the left. If that site is vacant, it will try moving forward (up). If vacant,

it will move to the right. The procedure is now repeated iteratively, and the walker is forced to move backwards only if all the other alternatives are vacant. As the procedure is continued, the walker reaches the other endpoint.

Figure 2(a) shows an example of a cluster, with the numbers indicating the steps of the left-turning walker. Note that after step number 17 the walker finds itself again on site number 10. It is thus clear that all the sites between 10 and 17, and all the sites connected to them, are *external dangling sites*. The next step back to 9 verifies that 10 is also a dangling site. The same is true for site 24.

The procedure is then repeated with a right-turning walker. The steps of this walker are denoted by letters on figure 2(a). The total number of sites visited by the two walkers is the *hull*. Sites visited by both walkers, e.g. 1, 6, 7, 8, 9, 18, 19, 20, 21, 27, 28 and 29 in figure 2(a), are *singly connected*.

The *external perimeter* is identified by a similar procedure that walks on nearest-neighbour vacant sites around the external surface of the cluster and counts every perimeter site. (Around the corners the walk steps on non-perimeter sites to keep the n–n connectivity but these are not counted; see figure 1(a)).

To find L_2, the left-turning walker is sent again into each blob, beginning after one step to the right (see figure 2(b)). This forces the walker to cover the smallest loop including its starting step. Some of the sites on this loop will have already been marked as left or right hull sites. The others are internal dangling sites or 'cross links'. The
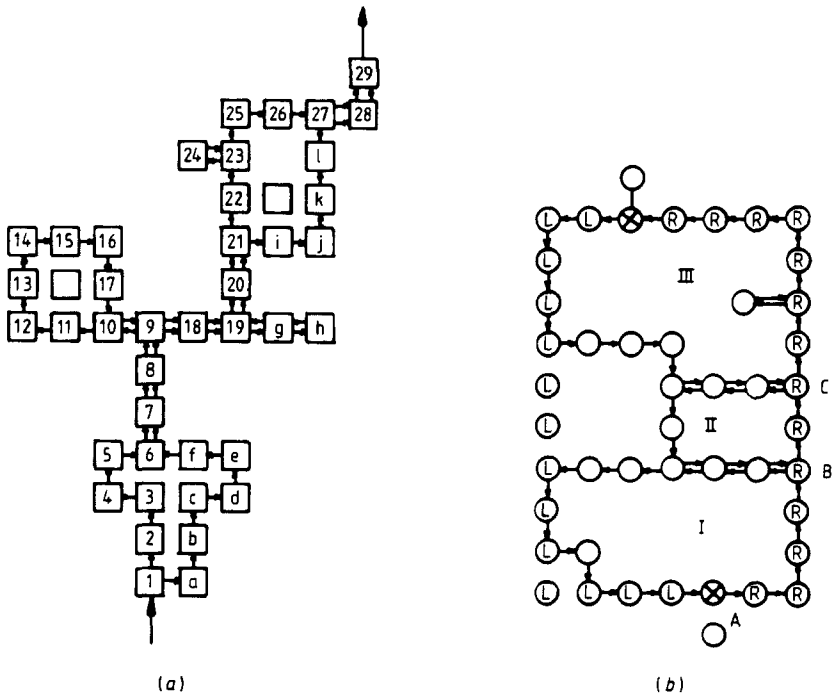

(a)   (b)

Figure 2 (*a*) Example of left- (numbers) and right-turning (letters) walks, covering the hull sites. (*b*) Procedure of identifying pairs of doubly connected sites: left-turning walk starts at A, and covers loop I with five right (R) and six left (L) hull sites. Walker next starts loop II at B, counting three right sites and zero left sites, and then loop III with eight right and five left sites.

contribution of this loop to L_2 will be the product of the numbers of left and right hull sites on it. The procedure is now repeated from the place where the walker left the right hull (B, C in figure 2(b)), and the contributions to L_2 are collected until the other endpoint is reached.

The properties of all clusters with linear size (distance between endpoints) in the bin $[L, L+\Delta L)$, with $\Delta L = 0.28L$, were averaged, and the results were plotted on a log–log scale. Although the curves look almost straight on this scale, their slopes vary slowly with L. Graphs of the local slopes (calculated for groups of eight points each) against $1/L$ are shown in figure 3. All these curves are very close to straight lines, indicating a leading correction-to-scaling term of order $1/L$. Least-square fits to straight lines yield the asymptotic extrapolated values at $L \to \infty$. Parabolic fits give very close values, and the differences are included in our quoted error bars. An exception involves
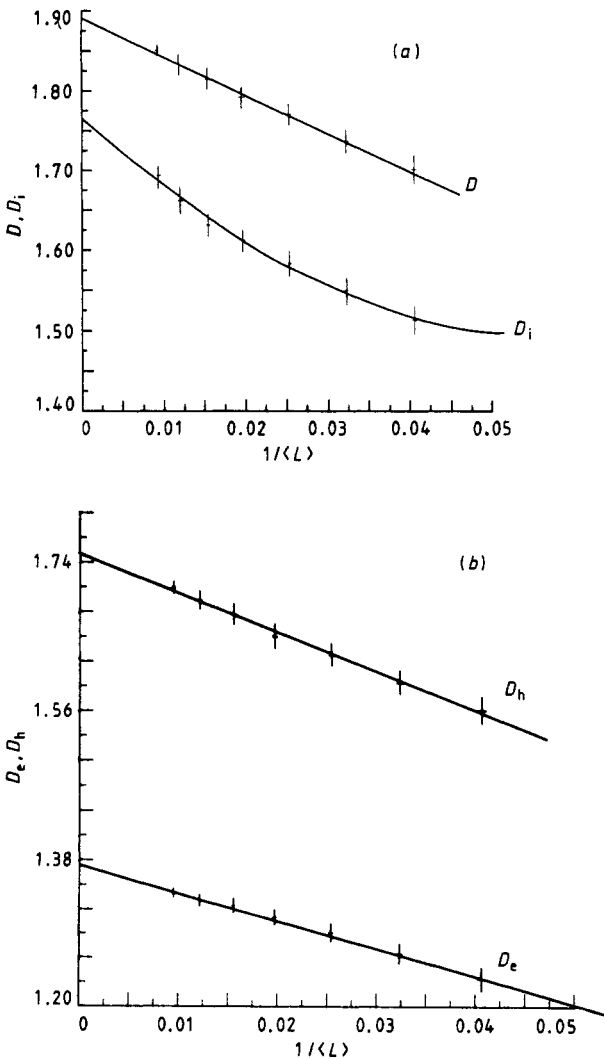

Figure 3 Local values of $D(=d \log s/d \log L)$, D_i, D_h and D_e. Full lines represent linear (for D, D_h, D_e) and parabolic (for D_i) fits.

D_i, where our final value, equation (3), is based on the much better parabolic extrapolation (shown in figure 3(a)). In addition to the results already quoted, we also note the following: (a) the ratio $L_1/(N_B+1)$, which is the average number of sites in a continuous 'string' of L_1 sites, is practically independent of L, and is equal to 4.7 ± 0.5. This value is (expectedly) higher than that found by Herrmann and Stanley (1984), because (unlike them) we consider the two sites and the ends of each 'string' (e.g. 6 and 21 in figure 2(a)) and single sites which connect two 'blobs' as singly connected; (b) the same analysing procedure was applied with the cluster's mass, s, as the basic parameter instead of L. The results were consistent in the sense that L^x is replaced (within the error bars) by $s^{x/D}$; and (c) the linearity in $1/L$ indicates that the leading secondary dimensionality, after D, is $(D-1)$, as discussed by Aharony *et al* (1985).

In conclusion, we emphasise again our main result: the fractal dimensionality measured using adsorbent particles, which approach the cluster from the outside, is *not* equivalent to that measured by different yardsticks between points on the hull. There probably exists a hierarchy of external perimeters, depending on the minimum size of the adsorbent particles, with a decreasing set of fractal dimensionalities $D_h > D_e > \cdots > 1$.

Note added. After we finished the present study we were informed by Meakin and Family of their recent study of invasion percolation in a strip geometry. They measured the analogue of our external perimeter of their upper surface, and found $D_e = 1.343 \pm 0.002$, in close agreement with our results. We thank Meakin and Family for this communication.

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