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LETTER TO THE EDITOR

Accessible external perimeters of percolation clusters

Tal Grossman and Amnon Aharony

School of Physics and Astronomy, Raymond and Beverly Sackler Faculty of Exact Sciences,
Tel Aviv University, Tel Aviv 69978, Israel

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Abstract. We introduce a new definition of a cluster's accessible external perimeter, which is different from the usual definition of the 'hull'. This external perimeter can be measured by probing (adsorbent) particles coming from the cluster's exterior. The size of these particles determines which perimeter sites are accessible from the outside and hence one can define different 'external' or 'accessible' perimeters according to this size. Using a Monte Carlo simulation we measured the fractal dimensions of these accessible perimeters, D_e , for percolation clusters (at the threshold) on the square and the triangular lattices. The fractal dimension of the accessible perimeter is found to depend on the size of the probing particles. For several sizes which are larger than some (lattice-dependent) threshold we find $D_e = \frac{7}{4}$, which is significantly smaller than the 'hull dimension', $D_h = \frac{7}{4}$ (found with smaller probing particles).

The external perimeters of percolation clusters in two dimensions have recently received much attention. The 'hull', as defined and measured for percolation clusters (Reich and Leath 1978, Voss 1984), is usually considered as the external surface of the cluster. Like many other cluster properties at the percolation threshold, the hull has a fractal behaviour, i.e. its (average) mass, H , scales as a power of its linear size (or the cluster radius) L :

$$H \propto L^{D_h} \quad (1)$$

where D_h is its fractal dimension. Heuristic arguments (Sapoval *et al* 1985, Bunde and Gouyet 1985), as well as Monte Carlo simulations (Voss 1984, Ziff 1986, Grossman and Aharony 1986, Grassberger 1986) and an exact calculation (Saleur and Duplantier 1987) have established the value of the 'hull dimension' as $D_h = \frac{7}{4} = 1.75$.

One can define the hull of a cluster in two natural ways (see figure 1).

(i) All perimeter sites that are connected via empty sites to the cluster's exterior, i.e. the region around and away from the cluster, are external perimeter sites. This is the 'vacant hull'.

(ii) One can also define the cluster surface as those occupied cluster sites that are nearest neighbours of the external perimeter sites as defined above. These sites are the cluster's 'occupied hull'.

Ziff *et al* (1984) have shown that the vacant and occupied hulls are asymptotically proportional, and therefore they have the same fractal dimension D_h .

The percolation hull is also related to other problems such as diffusion fronts (Sapoval *et al* 1985), non-trapping self-avoiding walks (Ziff *et al* 1984, Weinrib and Trugman 1985, Kremer and Lyklema 1985a, b, Gunn and Ortuno 1985) and interacting polymer chains at the Θ point (Coniglio *et al* 1987). These relations have enabled several authors to obtain accurate values for the site percolation threshold on the square lattice (Rosso *et al* 1985, Ziff 1986, Ziff and Sapoval 1986).

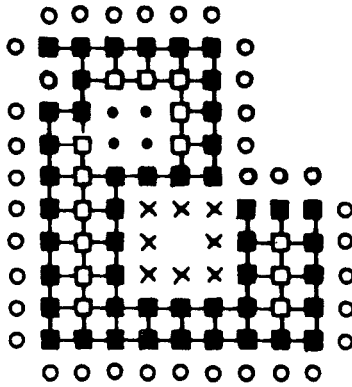


Figure 1. Different perimeters of a cluster on the square lattice. Occupied sites: ■, hull sites; □, internal sites. Perimeter (empty) sites: ●, internal perimeter; ○, accessible perimeter; ×, external perimeter according to NNN exterior connectivity, but not to NN connectivity (therefore these sites are considered as vacant hull sites but not as accessible perimeter).

In a previous letter (Grossman and Aharony 1986), we introduced a new definition for the external perimeter of the cluster on the square lattice. The difference is in the connectivity of the cluster's exterior, being of next-nearest neighbours for the hull and of nearest neighbours for the new external perimeter (see figure 1). Using a Monte Carlo simulation, we found a significant change in the fractal dimension of the external perimeter (Grossman and Aharony 1986), which is about $\frac{4}{3}$, compared to $\frac{7}{4}$ for the hull.

Similar results were obtained by Shaw (1986), who measured the fractal dimension of the external perimeter of a drying front and found 1.39 ± 0.02 , and also by Meakin and Family (1986) for invasion percolation in a strip geometry. They measured the external (according to the new definition) perimeter of their upper surface and found a fractal dimension of 1.343 ± 0.002 .

Our new definition is based on the idea that the external perimeter can be measured by probing (adsorbent) particles coming from the cluster's exterior. We asked ourselves the following question: suppose each occupied site is a solid square of unit size, and each perimeter site represents a potential reaction (or adsorption) site for one adsorbent particle. How many adsorbing sites are available to the particles coming from the outside? In that case, adsorbent particles cannot penetrate through the 'narrow necks' between two occupied next-nearest neighbours. Thus, adsorption can take place only on those external perimeter sites that are connected to the exterior via nearest-neighbour vacant sites. We define these sites as the external or the accessible perimeter of the cluster and their number will be denoted by E_1 . On a triangular lattice, for example, there is no difference between this external perimeter and the (vacant) hull. However, on the square lattice there are many hull sites that are 'screened' or hidden out of reach from the adsorbent particles (see figure 1). Therefore, the accessible perimeter of clusters on the square lattice, at p_c , scales with a different exponent than that of the hull:

$$E_1 \propto L^{D_e} \quad (2)$$

where $D_e \approx \frac{4}{3}$ (Grossman and Aharony (1986) and this work) is the fractal dimension of the external perimeter.

In the present letter we generalise the definition of the accessible perimeter by considering adsorbent particles of various sizes. A particle of linear size slightly larger than unity cannot pass through an open space of width unity (see figure 2(b)). Therefore, the external perimeter available to these particles, E_2 , is a smaller subset of the external perimeter defined previously. An even smaller number of perimeter sites, E_3 , can be reached by particles of linear size slightly larger than $\sqrt{2}$ (see figure 2(c)), and so on.

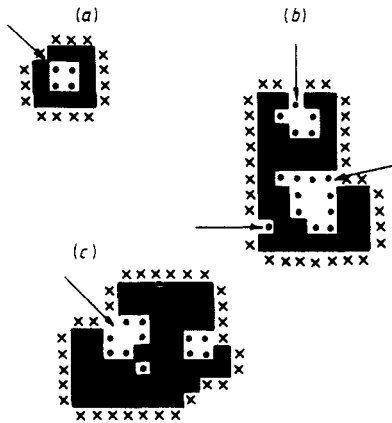


Figure 2. The accessible perimeters E_1 , E_2 and E_3 on the square lattice: ■, occupied site; ×, accessible perimeter site; ●, screened perimeter site. (a) The unpenetrable 'gate' from the external perimeter E_1 (×) into a screened hull (●). (b) The arrows point at the unpenetrable entrances for particles larger than unity. The E_2 sites are denoted by × and ● denotes a screened E_1 site. (c) The arrow shows the unpenetrable entrance for particles larger than $\sqrt{2}$. Of course, narrower entrances like the one on the right-hand side of the cluster also screen some perimeter sites. The accessible sites (×) for these particles are the E_3 perimeter.

To be more systematic, the accessible perimeter for probing particles of a given size r is defined as all the perimeter sites that are connected to infinity by a channel (of empty sites) which has a minimal width larger than r . Thus, the surface of the cluster decreases when probed by particles of increasing size (when these are coming from outside). This definition can be applied now to other lattices, for different dimensionalities, and for any kind of clusters or structures (e.g. invasion percolation, DLA, etc). Figure 3 shows the three accessible perimeters E_1 , E_2 and E_3 on the triangular lattice. In this example, each occupied site is a solid hexagon. Therefore, particles with radius larger than $r = 1/\sqrt{3}$ cannot penetrate through gates like a in figure 3, and E_2 is the accessible perimeter for all particles of radii less than that r . Similarly, E_3 is accessible for particles smaller than unity, etc. Of course, the exact size, r , that distinguishes between particles which probe different perimeters depends on the shape and size of the 'occupied sites' of the cluster.

The concept of accessible perimeters is indeed relevant to the problem of adsorption on surfaces, chemical reactions on it, etc (Pfeifer *et al* 1984, 1985, Pfeifer 1986). 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.

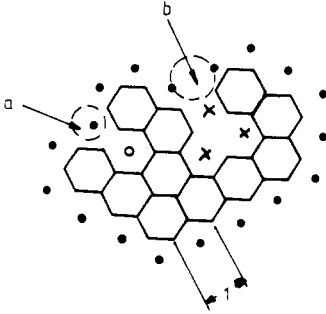


Figure 3. The accessible perimeters on the triangular lattice. The occupied cluster sites are solid hexagons (in the given cluster they are also hull sites). Particles of radius larger than unity cannot go through gates like a or b and therefore the accessible perimeter for such particles, E_3 , only includes those perimeter sites denoted by ●. Particles that are smaller than unity but larger than $1/\sqrt{3}$ can penetrate through b but not through a. Therefore the accessible perimeter E_2 also includes the perimeter sites that are denoted by x. The E_1 perimeter is the accessible perimeter for particles smaller than $1/\sqrt{3}$. It is identical with the vacant hull as defined on the triangular lattice. The site denoted by ○ belongs to this perimeter since it can be reached by these particles.

Another interesting application of the external perimeter was suggested recently by de Arcangelis *et al* (1986). They study the voltage distribution in conductor–superconductor mixtures, and find that, in this problem, the relevant superconductor surface is the external perimeter rather than the hull, since this is the part of the perimeter on which the voltage drop is not identically zero.

The question is: are we going to find a different dependence on the cluster size, i.e. a different fractal dimensionality, for each of the external perimeters E_1 , E_2 , E_3 , etc? A hierarchy of exponents is possible, i.e. $D_h \geq D_{e1} \geq D_{e2} \geq \dots \geq 1$ (Grossman and Aharony 1986). However, a simple heuristic argument suggests that all the accessible perimeters of two-dimensional percolation clusters (at p_c) scale with the same exponent, $D_e = \frac{4}{3}$ (Aharony 1986, Saleur and Duplantier 1987). This argument is based on the mapping between the two-dimensional percolation hull and a polymer chain at the Θ point (Coniglio *et al* 1987). The difference between the hull and the accessible perimeter can be regarded as adding a repulsive interaction between some of the chain monomers. Such an interaction should drive the polymer from the Θ point to the excluded-volume phase, in which the polymer behaves like a self-avoiding random walk and therefore has a fractal dimension of $\frac{4}{3}$ (Nienhuis 1984). Since different accessible perimeters differ only in the strength of this additional repulsion, one expects all of them to have the same behaviour, with $D_e = \frac{4}{3}$. Nevertheless, it must be emphasised that the above argument, although plausible, cannot be considered as an exact proof, for the following reasons.

(i) The difference between the ensemble of percolation hulls and the ensemble of accessible perimeters is not only in their statistical weight but also in the allowed configurations—any accessible perimeter can be a hull of a percolation cluster, but not vice versa. Therefore, the macroscopic restriction on the accessible perimeter cannot be simply interpreted as a finite-range interaction.

(ii) The mapping between the hull and a polymer chain relies on the equivalence between the percolation hull and the non-trapping self-avoiding walk (Ziff *et al* 1984, Weinrib and Trugman 1985). However, an equivalent walk for the accessible perimeter

has not been suggested (so far), and a mapping between the accessible perimeter and some kind of an interacting polymer is not established yet.

In this letter we investigate the behaviour of the hull and the accessible perimeters E_1 , E_2 , E_3 of percolation clusters, at p_c , on the two-dimensional square and triangular lattices. We found that, on the square lattice, the three external perimeters have practically the same fractal dimension, $D_e = \frac{4}{3}$, which differs significantly from the hull dimension, $D_h = 1.75$. Similar results were obtained for the triangular lattice, on which the E_1 accessible perimeter scales with the hull dimension (since it is the vacant hull of the cluster), but the E_2 and E_3 perimeters scale with the accessible perimeter dimension D_e . Our numerical results thus support the heuristic argument, yielding $D_e = \frac{4}{3}$ for all accessible perimeters.

A Monte Carlo simulation was used to study the fractal behaviour of the different perimeters. In this simulation, finite clusters were grown one at a time around a 'seed' (by a method that was used by Pike and Stanley (1981) and Grossman and Aharony (1986)). The clusters were grown on a two-dimensional array of $M \times M$ sites, with periodic boundary conditions. The linear size of the cluster is defined as $L = \max(L_x, L_y)$, where $L_x(L_y)$ is the $x(y)$ component of the cluster's 'length'. By rejecting the clusters that grew to be larger than $L > M - 3$, we ensured that, up to this upper cutoff, the ensemble of clusters is unbiased by any boundary effect. More than 10 000 clusters were created on the square lattice at $p_c = 0.59277$ (Gebele 1984), with linear size $7 < L < 700$, and about 4000 on the triangular lattice, at $p_c = 0.5$ (see, e.g., Stauffer 1985).

For each cluster, the perimeters were measured by 'walk' algorithms. Such algorithms were used by Ziff *et al* (1984) to create the percolation hulls, and by Grossman and Aharony (1986) to measure various cluster properties. In our simulation, the program traces the external perimeter by 'walking' around the cluster on perimeter sites and checking the nearest and next-nearest neighbours to avoid getting into the 'forbidden gates' (shown in figures 2 and 3). A more detailed description of the algorithms and of the analysis procedure that follows is given in Grossman (1987).

The clusters are grouped in bins according to their size. Each bin contains all the clusters with linear size in a certain interval $[L, L + \Delta L]$ (with $\Delta L = 0.28L$), and their properties are averaged in each bin. When plotting the bin averages of H , E_1 , E_2 and E_3 against L on a double logarithmic scale, we find a linear behaviour which is consistent with (1) and (2) (figures 4(a) and 5(a)). The slope of such a log-log plot should give the fractal dimension. However, because of corrections to scaling, this slope slowly changes, reaching its asymptotic value at the limit $L \rightarrow \infty$. Since we are interested in the large- L limit (where (1) and (2) are valid), we calculate the local slopes $D(L)$ (using groups of successive 8-bins) for each of the perimeters, and plot them against $1/L$. By extrapolating $D(L)$ to the limit $1/L \rightarrow 0$, we estimate the asymptotic exponents (see figures 4(b) and 5(b)). Such a linear extrapolation with $1/L$ assumes a leading correction-to-scaling term proportional to L^{D-1} . Assuming a more general form of the first correction term, i.e. $L^{D-\omega}$, one should extrapolate $D(L)$ with $L^{-\omega}$. Trying several values of ω we found that the variations in D_h and D_e are quite small. These variations give reasonable estimates for the errors in the exponents (see, e.g., Stauffer 1985, Grossman 1987).

The results for the extrapolated exponents (fractal dimensionalities) are as follows. For clusters on the square lattice, we found that the change in the exterior connectivity from NNN to NN results in a very large change in the fractal dimensionality: from 1.75 of the hull to 1.35 ± 0.02 of the external perimeter E_1 . A further increase of the

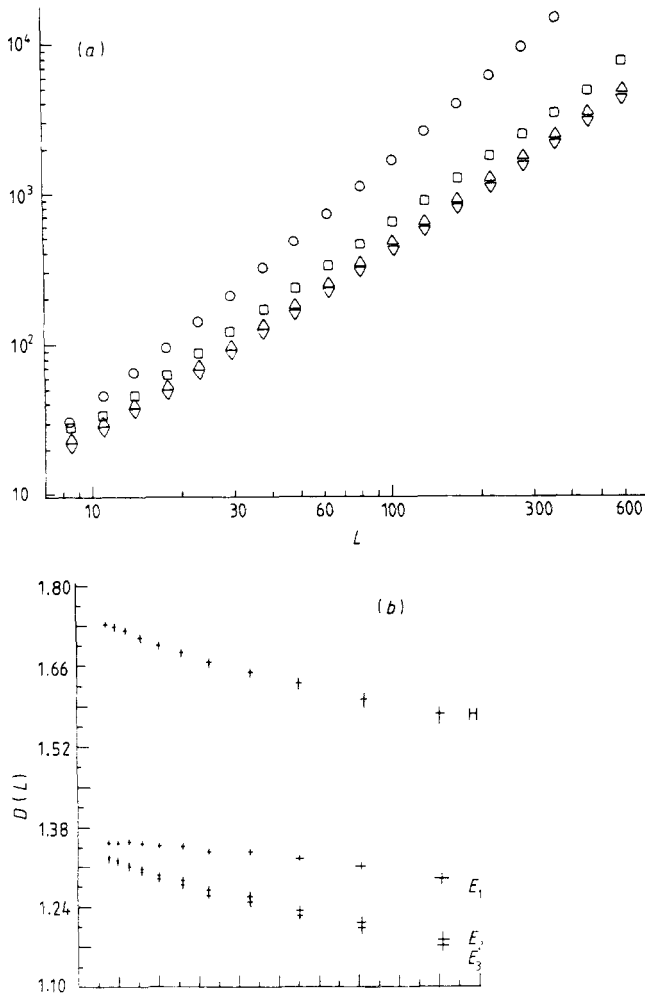


Figure 4. Square lattice. (a) The log-log plot of the hull (○) and of the accessible perimeters E_1 (□), E_2 (△) and E_3 (▽) against L . (The size of the symbols is about three times larger than the actual error bars.) (b) The local exponents $D(L)$ of the hull and the accessible perimeters E_1 , E_2 and E_3 extrapolated with $1/L$.

adsorbent particle size does not cause a significant change in the fractal dimensionality: E_2 and E_3 both scale with the exponent 1.34 ± 0.03 , as seen in figure 4(b), which shows the effective exponents $D(L)$ of the hull and the three accessible perimeters E_1 , E_2 and E_3 , extrapolated with $1/L$.

The results for the triangular lattice are shown in figure 5. As expected, the occupied hull and the E_1 perimeter (the vacant hull) are asymptotically identical. At $p_c = 0.5$, their ratio should indeed approach the limit (Ziff *et al* 1984):

$$\frac{\text{vacant hull}}{\text{occupied hull}} \rightarrow \frac{1 - p_c}{p_c} = 1.$$

However, the E_2 and E_3 perimeters clearly exhibit the new accessible perimeter behaviour. The extrapolation results for the exponents are (see figure 5(b)) $D_h = 1.76 \pm 0.02$ for the hull and the E_1 perimeters, and $D_e = 1.34 \pm 0.02$ for E_2 and E_3 . An

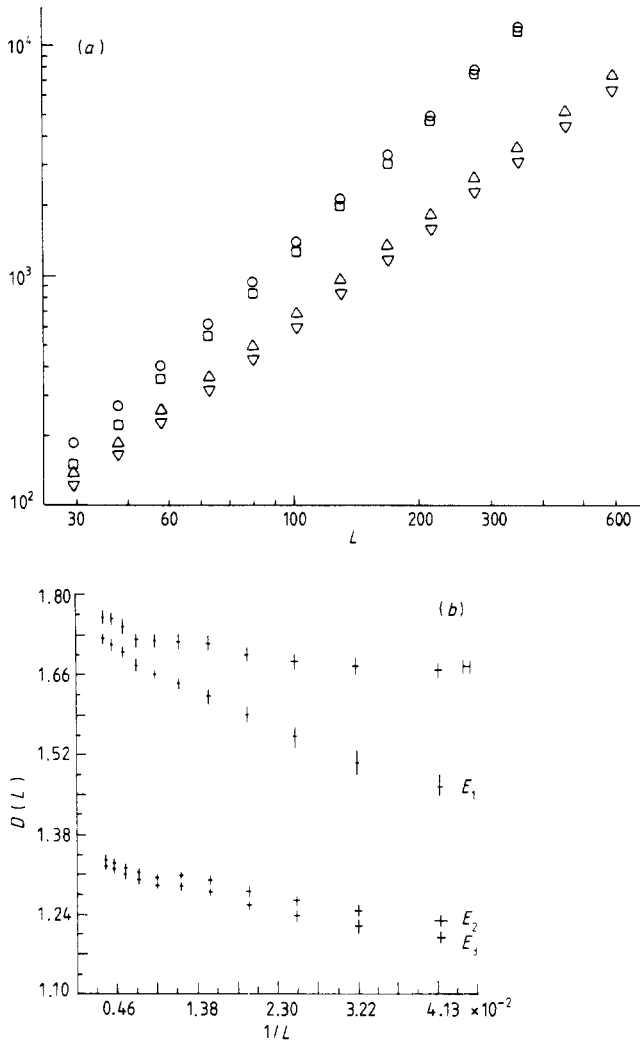


Figure 5. Triangular lattice. (a) The log-log plot of the hull (\circ) and of the accessible perimeters E_1 (\square), E_2 (\triangle) and E_3 (∇) against L . (The size of the symbols is about three times larger than the actual error bars.) (b) The local exponents $D(L)$ of the hull and the accessible perimeters E_1 , E_2 and E_3 extrapolated with $1/L$.

impressive qualitative illustration of this 'jump' from the hull dimension to the accessible perimeter dimension is given by figure 6, which shows the hull, the E_1 perimeter and also the E_2 , E_3 perimeters of a large cluster on the triangular lattice. The occupied hull and the vacant hull (the E_1 perimeter) are certainly covering most of the cluster's area, while the external perimeters E_2 and E_3 really look like an external surface. Furthermore, one can hardly notice the small differences between the E_2 and E_3 perimeters.

Within the error bars, our results agree with the possibility that all the accessible perimeters do scale with the same exponent $D_e = \frac{4}{3}$. It would be preferable, then, to have a better analytic calculation of the accessible perimeters' exponents. More implications of these results are as follows.

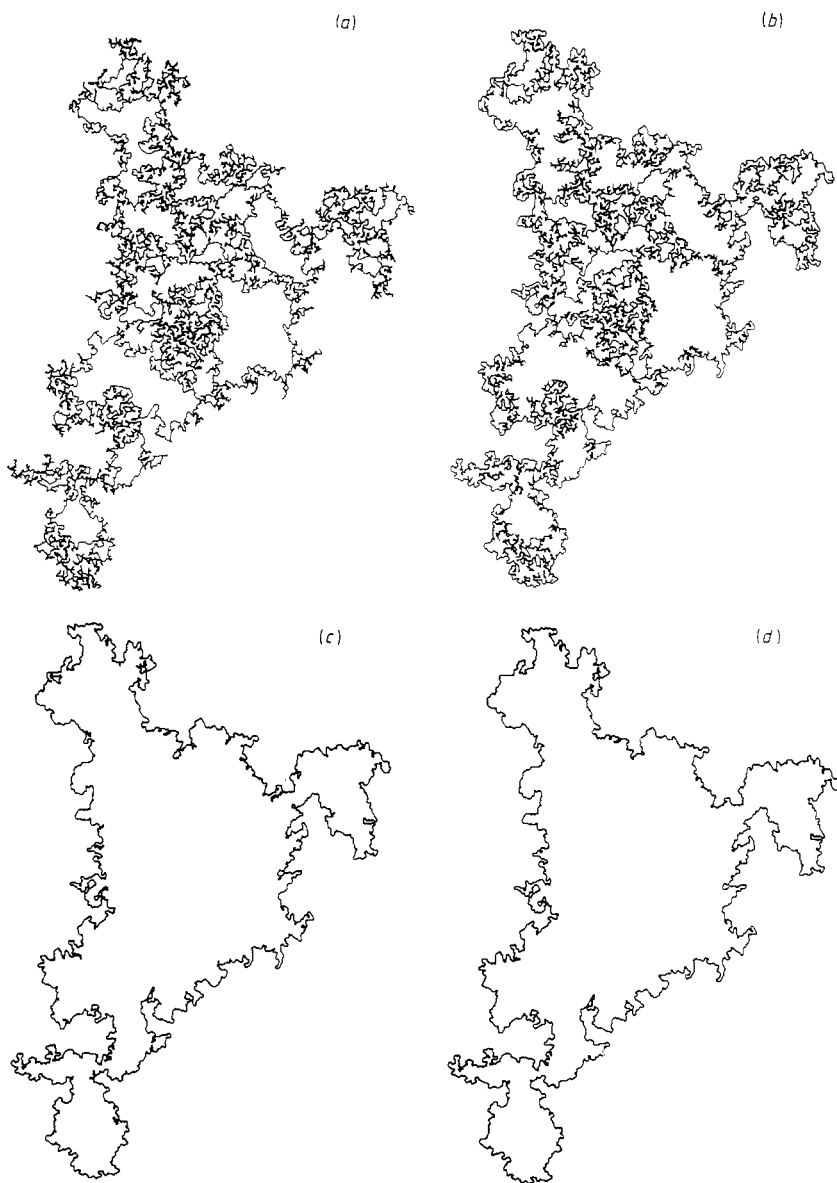


Figure 6. The hull and the accessible perimeters of a large cluster on the square lattice: (a) the hull (10 734 sites); (b) the E_1 perimeter (the vacant hull) (10 932 sites); (c) the E_2 perimeter (3560 sites); (d) the E_3 perimeter (3284 sites).

(i) The fractal dimension of a surface, measured by adsorption of particles on its exterior, can be particle-size dependent. Similar results (for different problems) were found by Van Damme *et al* (1986) and Pfeifer (1986).

(ii) As a consequence, it is evident that the adsorption method is not equivalent to the caliper or 'yardstick' method (Mandelbrot 1982) of measuring the fractal dimensionality of a surface. In the caliper method, one traces the surface and puts on it 'yardsticks' of a given size b . Measuring a surface in three dimensions is done

in a similar way, by using two-dimensional plaquettes of a given size. The number N of these yardsticks (or plaquettes), which measures the length (or the area) of the surface, depends on their size b with the power law

$$N(b) \propto b^{-D} \quad (3)$$

The experiments in which one measures the fractal dimension of a surface by adsorption (Pfeifer *et al* 1984, 1985) are based on this idea. In these experiments, a monolayer of adsorbent particles of a known size is created on the measured surface. The experiment is repeated with particles of different linear sizes b and the number of adsorbed particles $N(b)$ is recorded. The fractal dimension of the surface can then be calculated from (3). However, unlike the idealised caliper method (in which one can trace the whole surface), the probing particles in the adsorption experiments come from the outside, and therefore parts of the surface can be screened, as explained above. What they measure is the accessible surface, which is the generalisation of the accessible perimeter presented in this work to three dimensions. It is not clear, though, whether such a change in the fractal dimensionality occurs in three dimensions or can be observed in real systems.

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