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LETTER TO THE EDITOR

The shape of two-dimensional percolation and Ising clusters

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Abstract. We compute numerically the asphericity of (i) percolation clusters at the percolation concentration on a square lattice, and (ii) Ising clusters at the critical temperature of an Ising model, also on a square lattice. These results are compared with various analytical calculations. For the percolation problem, we also compute the distribution of asphericities among different clusters. Finally, we show that the lattice itself does not give rise to any anisotropy.

While the distribution of sizes of percolation clusters at the percolation concentration p_c has been studied for some time (Stauffer 1979, 1985), it has only recently been emphasised that the clusters are not spherical (Family *et al* 1985). A convenient measure of cluster shapes, known as the asphericity, has been given by Rudnick and Gaspari (1986) and Aronovitz and Nelson (1986). This is useful because it can be calculated analytically both for random walks (Rudnick and Gaspari 1986, Gaspari *et al* 1987, Aronovitz and Nelson 1986) and within an ε expansion, where $\varepsilon = 6 - d$ and d is the dimensionality, for the percolation problem (Aronovitz and Stephen 1987). While the pioneering work of Family *et al* (1985) showed that percolation clusters are not spherical, they did not explicitly calculate the asphericity parameter so one cannot directly compare their results with the ε expansion results of Aronovitz and Stephen (1987). We have therefore computed the asphericity for percolation clusters on a square lattice. Given the large extrapolation from $d = 6$ down to $d = 2$, our results compare well with the ε-expansion predictions. We also obtain the distribution of asphericities, finding that a spherical shape is the most probable one but that the distribution has a finite width even as the cluster size tends toward infinity. One can also discuss clusters in the two-dimensional Ising model (e.g. Cambier and Nauenberg 1986) which percolate at the critical temperature, T_c (Coniglio and Klein 1980). We have therefore looked at the asphericity of these Ising clusters and find that it is almost identical to our result for percolation clusters.

First of all, we define the asphericity parameter of Rudnick and Gaspari (1986) and Aronovitz and Nelson (1986). One computes the radius of gyration tensor R^2_{ij}, defined for a cluster of N sites by

$$R^2_{ij} = \frac{1}{N} \sum_{\alpha=1}^{N} (x_i^\alpha - \bar{x}_i)(x_j^\alpha - \bar{x}_j) \qquad (1)$$

where $\bar{x}_i$ is the ith coordinate of the centre of mass of the cluster, and $\alpha = 1, \ldots, N$ denotes a particular site in the cluster. The tensor R^2_{ij} is diagonalised to obtain its eigenvalues λ_i, $i = 1, \ldots, d$. For $d = 2$ to which we specialise from now on, the asphericity parameter $\bar{A}_2$, is defined to be (Rudnick and Gaspari 1986, Aronowitz and Nelson 1986)

$$\bar{A}_2 = \frac{\langle(\lambda_1 - \lambda_2)^2\rangle}{\langle(\lambda_1 + \lambda_2)^2\rangle}. \tag{2}$$

Note that this is called A_2 in Rudnick and Gaspari (1986). The averages in (2) are over different clusters. In practice, we looked at clusters in a range of sizes to eliminate corrections to scaling which occur for small clusters. At the percolation concentration there are arbitrarily large clusters in an infinite system. Obviously a simulation cannot contain very large sizes but we were able to study, without difficulty, a sufficiently large range of sizes where corrections to scaling are negligible. It is also of interest to consider the asphericity of a single cluster, i.e.

$$A_2 = \frac{(\lambda_1 - \lambda_2)^2}{(\lambda_1 + \lambda_2)^2} \tag{3}$$

from which the distribution $P(A_2)$ and average $\langle A_2\rangle$ are obtained by sampling many clusters. Obviously $A_2 = 0$ for a spherical (circular) cluster and $A_2 = 1$ for a cluster made of a single straight rod.

A simple way to generate percolation clusters was proposed by Alexandrowicz (1980). This was later modified by Grassberger (1983) and used in the work of Family *et al* (1985). One starts with a seed particle (occupied site) on the lattice. One of its nearest neighbours (perimeter sites) is chosen randomly. This site is occupied, and becomes part of the growing cluster, with probability p and otherwise is discarded and not considered again as a possible perimeter site. This process continues until either the number of perimeter sites becomes zero, in which case the radius of gyration tensor is computed, or the occupied sites go outside the bounds of the array used to store them, in which case this cluster is discarded. We generated 16 240 clusters of up to 4096 sites by this method at $p = p_c = 0.5928$. This took 26 h of computer time on a Sun 3/50 workstation. In this range no clusters had to be discarded. For each factor of two in size we computed $\langle A_2\rangle$, $\bar{A}_2$ and $\sigma(A_2)$, the standard deviation of A_2. The results are shown in figure 1 for sites N between 5 and 4096. Apart from very small sizes, the results are independent of size and give, for $256 < N < 4096$,

$$\begin{aligned} &\langle A_2\rangle = 0.258 \pm 0.006 \qquad \text{(percolation)} \\ &\bar{A}_2 = 0.325 \pm 0.006. \end{aligned} \tag{4}$$

The distribution $P(A_2)$, obtained by averaging over 8892 clusters of sizes between 129 and 4096 sites, is shown in figure 2. Because the mean and standard deviation appear to have settled down to their asymptotic values for $N \to \infty$, as shown in figure 1, we expect the whole distribution to be unchanged from figure 2 in the thermodynamic limit. Notice that the most probable result is $A_2 = 0$, corresponding to a spherical shape, but that the distribution has a finite width as $N \to \infty$.

For $d = 2$, Aronowitz and Stephen (1987) find $\bar{A}_2 = 0.286$, to zeroth order in ε and 0.374 to first order. Our result lies in between these two values, which is reasonable considering that the ε expansion generally oscillates (Lipatov 1977, Brézin *et al* 1977). It would be interesting to see how the ε-expansion results are approached in higher dimensions.

We have also studied the shapes of Ising clusters on a square lattice at the critical temperature. A standard Monte Carlo simulation (see, e.g., Binder 1984) was performed

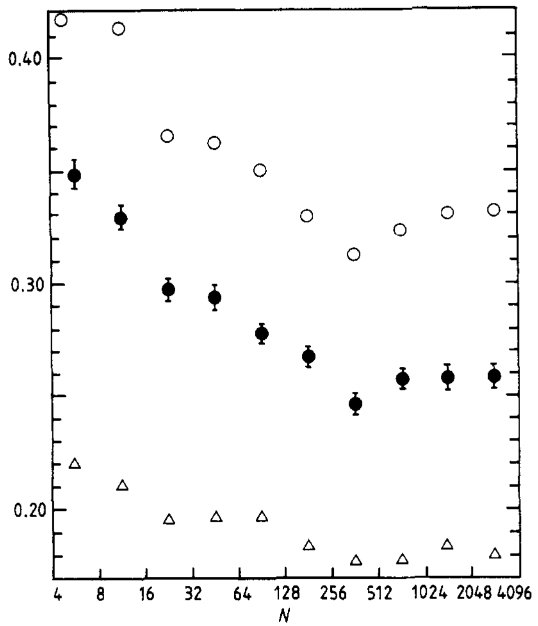

Figure 1. A plot of $\langle A_2 \rangle$ (●), $\bar{A}_2$ (○) and $\sigma(A_2)$ (△) for $5 \leq N \leq 4096$ for the percolation problem on a square lattice at concentration $p = p_c = 0.5928$. Results for each factor of two in size (e.g. $5 \leq N \leq 8$, $9 \leq N \leq 16$, etc) are lumped together.

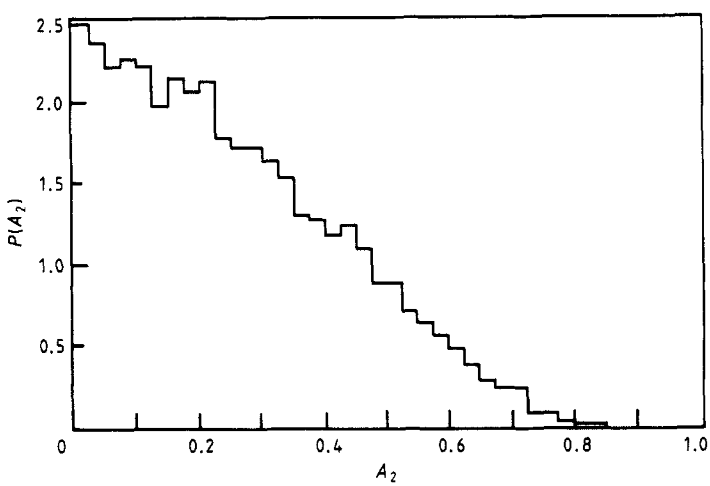

Figure 2. The probability distribution $P(A_2)$ for percolation clusters on a square lattice ($\langle A_2 \rangle = 0.258$). 8892 clusters of size $129 < N < 4096$ have been averaged over.

for $L \times L$ lattices of sizes $L = 60$ and 120, with periodic boundary conditions at the critical temperature T_c, which is 2.269 in units of the nearest-neighbour interaction. A cluster is a set of sites containing up spins, such that one can go from any site in the cluster to any other site by nearest-neighbour steps, staying always on up-spin sites. Because the model is symmetrical between up and down spins, one could equally well define the clusters in terms of down spins. Clusters were identified by the algorithm of Hoshen and Kopelman (1976). To obtain good statistics it was necessary to run the simulation for many times the longest relaxation time. Because of critical slowing down, relaxation times are very long at T_c and diverge for an infinite system. We ran the simulation for 120 000 steps per spin after an equilibrium period of 20 000 steps.

Results for $\bar{A}_2$ and $\langle A_2 \rangle$ for $5 < N < 4096$ are shown in figure 3. Apart from small sizes (and also very large sizes comparable with the system size where finite-size effects play a role) the results do not depend much on size and we find

$$\begin{aligned} \langle A_2 \rangle &= 0.264 \pm 0.002 \qquad \text{(Ising)} \\ \bar{A}_2 &= 0.328 \pm 0.002. \end{aligned} \tag{5}$$

These results are almost the same as those of the percolation problem given in (4). Within our errors they could be identical but there is no reason to expect this since the percolation and Ising problems are in different universality classes. We are not aware of any ε-expansion calculations for the shape of Ising clusters. It is noticeable that corrections to the infinite-N results at small size are larger for the percolation problem than for the Ising model.

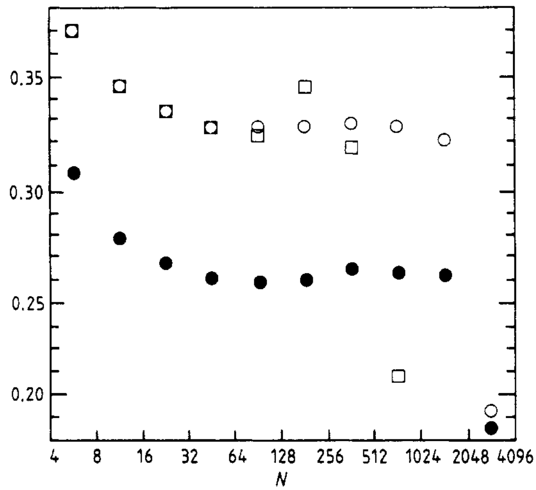

Figure 3. A plot of $\langle A_2 \rangle$ (●) and $\bar{A}_2$ (○) for $5 < N < 4096$ for an $L \times L$ Ising lattice with $L = 120$. Also shown in $\bar{A}_2$ for an $L = 60$ lattice (□). The reduction in $\bar{A}_2$ which occurs for large sizes is clearly a finite-size effect; for the $L = 120$ lattice it happens at about four times the cluster size where it occurs for the $L = 60$ lattice, as expected.

Finally, we compare our results with calculations on random walks. For closed walks, which are more appropriate than open walks for comparison with Ising or percolation clusters, Gaspari *et al* (1987) find

$$\bar{A}_2 = 0.333 \tag{6a}$$

which is remarkably close to ur values given in (4) and (5). They can only calculate $\langle A_2 \rangle$ in a $1/d$ expansion where d is the dimension, with the result

$$\langle A_2 \rangle = \begin{cases} 0.291 \\ (0.200). \end{cases} \qquad \text{(closed walks)} \tag{6b}$$

The first figure is obtained by including the $1/d$ correction while the figure in brackets is the zeroth-order approximation. The numerical results of Bishop and Saltiel (1986) are $\bar{A}_2 = 0.321 \pm 0.035$.

After this work was completed we received a preprint from Straley and Stephen (1987) who evaluated $\bar{A}_2$ for percolation by high-temperature series expansions for clusters of up to fifteen sites, obtaining $\bar{A}_2 = 0.38 \pm 0.01$, substantially higher than our value of 0.325 ± 0.006. In fact, Straley and Stephen (1987) note that their estimate may be too high, because it is based on small cluster sizes. Our results for $N \simeq 15$ are indeed consistent with their value (see figure 1) but give our lower value for larger clusters.

Finally, for the percolation problem, we have examined whether the square lattice itself gives rise to anisotropy. Since the lattice has fourfold, rather than fully isotropic, symmetry, we looked for a measure of fourfold anisotropy. For cluster of N sites we computed

$$A_4 = \sum_{\alpha=1}^{N} r_\alpha^4 \cos 4\theta_\alpha \left(\sum_{\alpha=1}^{N} r_\alpha^4 \right)^{-1} \tag{7}$$

where

$$\begin{aligned} r_\alpha &= (x_\alpha - \bar{x})^2 + (y_\alpha - \bar{y})^2 \\ r_\alpha \cos \theta_\alpha &= x_\alpha - \bar{x} \\ r_\alpha \sin \theta_\alpha &= y_\alpha - \bar{y} \end{aligned} \tag{8}$$

and averaged this over many clusters to obtain $\langle A_4 \rangle$. Clearly $-1 \leqslant \langle A_4 \rangle \leqslant 1$ and $\langle A_4 \rangle = 0$ if there is no fourfold anisotropy. Figure 4 shows our results for 3200 clusters of size between $N = 5$ and 4096. Apart from the smallest sizes which appear to show a minor effect just outside the error bars we find that $\langle A_4 \rangle$ is clearly zero. Hence large clusters, are, on average, isotropic, as expected, at the critical point.

We conclude that all closed fractal clusters studied in two dimensions have very similar sphericity with $\bar{A}_2 \simeq 0.33$ and $\langle A_2 \rangle \simeq 0.26$.

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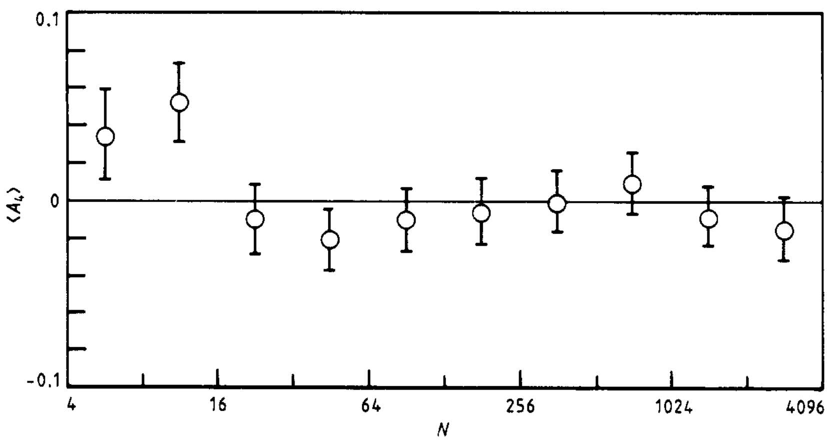

Figure 4. A plot of $\langle A_4 \rangle$ for $5 \leqslant N \leqslant 4096$ for the percolation problem on a square lattice at $p = p_c$.

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