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Percolation cluster shapes in two and three dimensions

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Abstract. The asymmetry and prolateness of site percolation clusters and lattice animals are determined for two and three dimensions, with agreement with ϵ expansion results.

Recently the shapes of polymers, clusters in percolation-type lattice models and lattice animals (related to branched polymers in solution) have been investigated [1-3]. Such shapes are of interest for polymers in solutions where they affect the rotational relaxation and flow properties. Family *et al* [1] have performed Monte Carlo sampling to study the shapes of bond percolation clusters and lattice animals at the percolation threshold. Universal amplitude ratios measuring the asymmetry and degree of prolateness were introduced for polymers by Aronovitz and Nelson [2] and calculated in ϵ expansion near four dimensions. Similar amplitude ratios were introduced by Aronovitz and Stephen [3] for lattice percolation clusters and lattice animals and were calculated in ϵ expansion near six and eight dimensions respectively. The ϵ expansion is not expected to be reliable in two or three dimensions.

We have studied the asymptotic shape of site percolation clusters and lattice animals in two and three dimensions by exact enumeration of all clusters of K sites (with $K \leq 15$ in 2D and $K \leq 11$ in 3D) on the square and cubic lattices. For each cluster we determined:

- (i) the perimeter P of the cluster, which is the number of sites in contact with the cluster that do not belong to it,
- (ii) the moment of mass tensor

$$M_{\alpha\beta} = \sum_i (r_{i\alpha} - \bar{r}_\alpha)(r_{i\beta} - \bar{r}_\beta) \quad (1)$$

- (iii) the traceless tensor $Q = M - \lambda I$, where $\lambda = (1/D) \text{Tr } M$ is the average eigenvalue of M .

From these terms, several cluster anisotropy quantifiers were formed. These anisotropy quantifiers were accumulated for each value of K and P ; the sums were used to construct generating functions corresponding to each quantifier F :

$$\{F\}_p = \sum_{\text{clusters}} FKx^{K-1}(1-x)^P \quad (2)$$

for the percolation problem, and

$$\{F\}_a = \sum_{\text{clusters}} FKx^{K-1} \quad (3)$$

for the animals problem.

In the percolation context we may readily interpret x as being the density of sites, and $\{F\}_p$ the average value of F : in particular if F is a constant, $\{F\}_p = F$ for any $x < x_c$. The interpretation of $\{F\}_a$ is not so simple; even $\{1\}_a$ depends on x and is singular for some sufficiently large x_c . However, we find that for the anisotropy quantifiers to be studied, the functions $\{F\}_a/\{1\}_a$ are non-singular and can be used to determine the asymptotic shape of a cluster.

Since we can only enumerate small clusters, we only know the small x behaviour of $\{F\}$. To extrapolate the behaviour to x_c , we wrote these functions as power series in x , expanding the $(1-x)^p$ factor in $\{F\}_p$. These series, and series resulting by synthetically dividing one series by another, were extrapolated to x_c by means of Padé approximants. The cluster shape calipers we studied are not singular at x_c , and the Padé approximants generally had no poles near x_c . As a check on the accuracy of the method we also studied the logarithmic derivative of $\{K\}$, which should have a pole at x_c ; in this case the approximants had poles reasonably close to the x_c values found by others (table 1).

The asphericity of a cluster is measured by the quantity

$$\Delta_D = \frac{D}{D-1} \frac{\{\text{Tr } Q^2\}}{\{(\text{Tr } M)^2\}}. \tag{4}$$

Written in terms of the eigenvalues λ_i of M , this becomes

$$\Delta_D = \frac{\{(\lambda_1 - \lambda_2)^2\}}{\{(\lambda_1 + \lambda_2)^2\}} \tag{5}$$

in two dimensions. This quantity would be small if the most common clusters were isotropic.

Table 1. Anisotropy quantifiers as determined here and in other work. The numerical uncertainties quoted reflect the variability in different Padé approximants to the series; the systematic errors inherent in using a short series might be ten times larger.

	2D percolation	2D animals	3D percolation	3D animals
x_c				
(from our series)	0.58 ± 0.01	0.246 ± 0.001	0.31 ± 0.01	0.120 ± 0.001
(from literature)	0.592 74 ^a	0.246 15 ^a	0.3117 ^b	0.120 ^c
$\{\text{Tr } (Q^2)\}/\{\text{Tr } (M^2)\}$	0.280 ± 0.005	0.318 ± 0.001	0.37 ± 0.03	0.440 ± 0.002
Δ_D				
(from series)	0.38 ± 0.01	0.466 ± 0.002	0.30 ± 0.03	0.390 ± 0.003
(ϵ expansion $O(\epsilon^1)$)	0.376	0.385	0.312	0.326
$\langle \text{Tr } (Q^2) \rangle / \langle \text{Tr } (M^2) \rangle$	0.141 ± 0.001	0.192 ± 0.002	0.191 ± 0.005	0.24 ± 0.01
$(\lambda_{\min}/\lambda_{\max})$				
(from series)	0.346 ± 0.006	0.280 ± 0.003	not determined	
(from [1])	0.40 ± 0.01	0.29 ± 0.01	not determined	
$\{\text{Tr } (Q^3)\}/\{\text{Tr } (M^3)\}$	0	0	0.12 ± 0.01	0.132 ± 0.001
$S_3 = \frac{3}{2}\{\text{Tr } Q^3\}/\{(\text{Tr } M)^3\}$				
(from series)	0	0	0.23 ± 0.02	0.27 ± 0.01
(ϵ expansion $O(\epsilon^0)$)	0	0	0.164	0.164

^a From [5].

^b From [6].

^c [7] gives $1/x_c = 8.35 \pm 0.04$.

Family *et al* [1] study a different quantity

$$R = \{\lambda_{\min}/\lambda_{\max}\}/\{1\} \quad (6)$$

and, for the purposes of comparison, we constructed this quantity in two dimensions.

In two dimensions $\{\text{Tr } Q^3\}/\{(\text{Tr } M)^3\}$ is identically zero; in three dimensions we can define

$$S_3 = \frac{9}{2} \frac{\{\text{Tr } Q^3\}}{\{(\text{Tr } M)^3\}} = \frac{\{(\lambda_1 - \lambda)(\lambda_2 - \lambda)(\lambda_3 - \lambda)\}}{2\{\lambda^3\}}. \quad (7)$$

This quantity will be positive if the clusters are prolate in shape, and negative if they are oblate.

Family *et al* analyse their data in a different way. They add together $\lambda_{\min}/\lambda_{\max}$ for all clusters of K sites, for K ranging up to 15; and then divide by the number of clusters of K sites, getting the average value of $\lambda_{\min}/\lambda_{\max}$ for the restricted ensemble of K -site clusters. This average is then plotted against $K^{-\theta}$ (for a suitable value of θ). Our result for $\langle \lambda_{\min}/\lambda_{\max} \rangle$ is not too different from theirs.

These anisotropy quantifiers are independent of the orientation of the principal axes of the cluster, which might be arbitrarily oriented; thus anisotropy of these sorts does not imply anisotropy of the site-site correlation function, but rather reflects the spontaneous fluctuations in shape about the expected isotropic shape. Lam [4] has studied the site-site correlation function in two dimensions, and found that for small clusters the distribution has square but not circular symmetry (so that directions parallel to the lattice axes are distinct from diagonal directions) and that for large clusters the site-site correlation becomes circularly symmetric. This may be regarded as a consequence of the breaking of rotational symmetry by the lattice; in the limit of large clusters the asymmetry is too weak to have any effect.

In order to determine the effect on our results of the small cluster anisotropy discovered by Lam we constructed larger clusters. We used the Alexandrowicz [8] method, which builds a distribution of clusters characteristic of the percolation problem at any site density p . For $p = 0.5$ it was possible to collect data on all clusters that this algorithm constructed; for $p = p_c$ it was necessary to terminate the cluster construction process if the cluster grew too large. We chose $K = 500$ as the cutoff point and constructed 5×10^4 clusters with $20 \leq K \leq 500$.

Since we cannot construct all clusters in the ensemble close to the percolation threshold, we cannot calculate $\{F\}_p$ as defined in (2). Instead we define for any function F and any K

$$[F]_K = \sum F \quad (8)$$

where the sum is restricted to the clusters having K sites, and then calculate

$$\tilde{\Delta}_D(K) = \frac{D}{D-1} \frac{[\text{Tr } Q^2]_K}{[(\text{Tr } M)^2]_K}. \quad (9)$$

For $p = 0.5$ we found $\tilde{\Delta}_2$ and Δ_2 to be of comparable size; however, for $p = p_c$, $\tilde{\Delta}_2(K)$ is a decreasing function of K which for larger K is distinctly less than our estimate for Δ_2 . Extrapolating against $K^{-0.47}$ (as recommended by Family *et al* [1]) indicates $\Delta_2(\infty) \approx 0.31$ (Quandt and Young [9] find similar results in an independent study).

Our results are given in table 1. We note reasonable agreement between our results and previous work. Considering that the ε expansions are expansions in $(6-D)$ or $(8-D)$, the low-dimensionality series are in remarkably good agreement with them.

We conclude that percolation clusters and lattice animals are prolate and significantly anisotropic; 'egg-shaped' would be a reasonable summary of our results.

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