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# Structure of backbone perimeters of percolation clusters

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**Abstract.** We study perimeters of backbones of percolation clusters at the percolation threshold in two dimensions. These perimeters are self-avoiding for all lattices. We simulate these perimeters by three independent processes, measure the average size of them and study their variation with length. We find the exponent characterising this variation to be $0.744 \pm 0.012$. It seems likely that these perimeters are in the self-avoiding walk universality class.

## 1. Introduction

Recently there has been considerable interest in the study of different types of growing self-avoiding random walks (for a review see Peliti and Pietronero 1987). The primary motivation behind these studies is to explain polymer chain configurations at the $\theta$ point (Flory 1949). The statistics of long-chain polymer molecules in solution is governed by two competing intermolecular forces, a hard-core repulsion of the monomers of the chain at short distances, and a long-range attractive interaction. At high temperatures and in good solvents long-range attraction is weak, and the polymers have extended-coil configurations described by ordinary self-avoiding walks (SAW). On the other hand, at low temperatures and in poor solvents where attractive interaction is strong the polymer is found to be in a tightly coiled compact state described by a Hamiltonian walk (HW). At the $\theta$ temperature both contributions effectively cancel each other and chains behave essentially as ideal random walks characterised by an average size exponent $\nu_\theta$ different from both $\nu_{SAW}$ and $\nu_{HW}$, the values at the high and low temperature limits respectively. By analogy with magnetic phase transitions de Gennes showed that the $\theta$-point transition corresponds to a tricritical point (de Gennes 1975). Over the last few decades, the study of linear polymers at the $\theta$ point has attracted a lot of attention in its own right. Howeve, until recently there were few definite results owing to the difficulty of simulating $\theta$-point statistics by numerical methods.

Kremer and Lyklema (1985a) introduced and studied the indefinitely growing self-avoiding walk (IGSAW) as a possible candidate for linear polymers at the $\theta$ point. This is a two-dimensional walk in which the self-avoiding restriction is always maintained, but this walk is never trapped like ordinary SAW as it recognises and avoids cages likely to trap it—in this way it grows indefinitely. Specifically, this is done by assigning an angle, the winding angle with respect to the origin, to each site on the walk. The walker first identifies the unvisited sites among its nearest neighbours, then from these sites it selects those which will never lead to any trapping using the knowledge of winding angles. One of these accessible sites is then selected at random for the next step. Statistics of this walk have been investigated by exact enumeration and

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high-precision Monte Carlo data (Kremer and Lyklema 1985a, b) who found a value of the average size exponent $\nu_{\text{IGSAW}} = 0.567$ different from the values of other known walks. Weinrib and Trugman (1985) showed that this walk actually corresponds to the perimeter of percolation clusters at the percolation threshold. This correspondence is exact for site percolation on the triangular lattice, and its perimeter on the dual honeycomb lattice. For other lattices this correspondence is not exact, but the critical behaviour of these two objects is the same. This was shown by Ziff (1986), using a random walk algorithm to generate the perimeter of the site percolation clusters at the percolation threshold (Ziff *et al* 1984). This correspondence was generalised to dressed self-avoiding walks by Gouyet *et al* (1987). Very recently Duplantier and Saleur (1988) showed that percolation perimeters, or IGSAW, actually do represent $\theta$-point polymer statistics, an analogy proposed earlier by Coniglio *et al* (1987).

Here in this paper we study the external perimeters of the *backbones* of the percolation clusters at the percolation threshold. We generate percolation clusters at the percolation threshold and then remove all dangling ends to get the backbone. In the case of bond percolation, we isolate the number of occupied bonds of the resulting structure which are exposed to the external region. These bonds constitute the external perimeter of the backbone. For site percolation we convert the cluster to a bond cluster by joining all pairs of neighbouring occupied sites and measure the external perimeter in the same way. These perimeters are self-avoiding and cannot self-intersect on any lattice. These backbone perimeters are more straightforward than those for percolation cluster perimeters, which are much more tortuous due to the presence of dangling ends. Therefore one might expect a higher value of the average size exponent for backbone perimeters compared to that of cluster perimeters of IGSAW, and indeed we have obtained a higher value. We have studied the backbone perimeters of percolation clusters at the percolation threshold by three independent methods and measured their average sizes as a function of length. Our estimate for the associated exponent is $0.744 \pm 0.012$.

In § 2 we describe the study of backbones of actual percolation clusters for bond percolation on a square lattice at the percolation threshold. In § 3 we describe the study of backbone perimeters by generating perimeters for site percolation on a square lattice using a random walk algorithm. In § 4, we describe the same study this time generating backbone perimeters by IGSAW on a triangular lattice, while § 5 contains our conclusion.

## 2. Simulation of the actual percolation clusters

We have studied bond percolation on a square lattice at the percolation threshold $p_c$ ($=\frac{1}{2}$). For a square lattice of size $L$ every bond is occupied with probability $p_c$ and vacant with probability $(1-p_c)$. We considered those configurations for each of which an 'infinite' cluster exists, spanning the whole lattice from top to bottom. We separated the infinite cluster following the algorithm by Hoshen and Kopelman (1976) and removed all its dangling ends, obtaining the percolation backbone using the recently introduced algorithm of Roux and Hansen (1987).

To get the backbone perimeter, we consider the clusters of the smallest squares on this lattice. Two squares separated by a vacant bond belong to the same cluster. A distinct cluster of such squares is surrounded by occupied bonds. We number these clusters of squares following the algorithm of Hoshen and Kopelman (1976). After

numbering we note the number of squares on the leftmost column of the lattice. Then, among all occupied bonds of the lattice, we choose those bonds which have exactly one square on one side having the same number as the left-side squares (see figure 1). These bonds constitute the left perimeter, and its length is measured. In the same way we count the number of bonds on the right perimeter. We assign the mean of these left- and right-perimeter lengths as the perimeter of the backbone of this configuration.

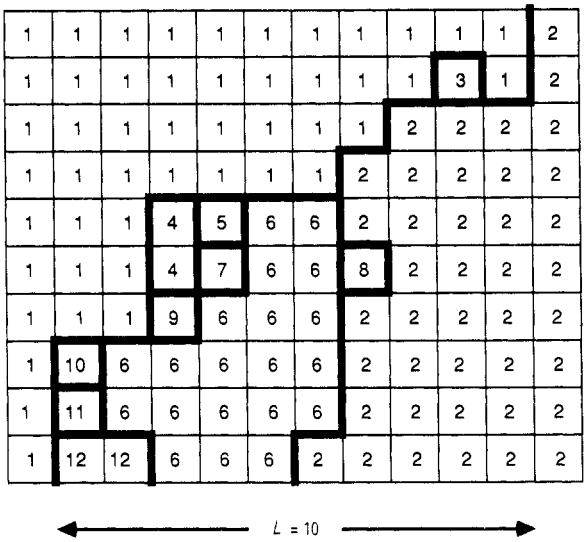


**Figure 1.** Backbone of an infinite bond percolation cluster on the square lattice of size $L = 10$. Clusters of smallest squares are numbered. Occupied bonds with squares on one of its two sides of number 1 constitute the left perimeter, and its length is 22. Similarly the right perimeter is of length 17.

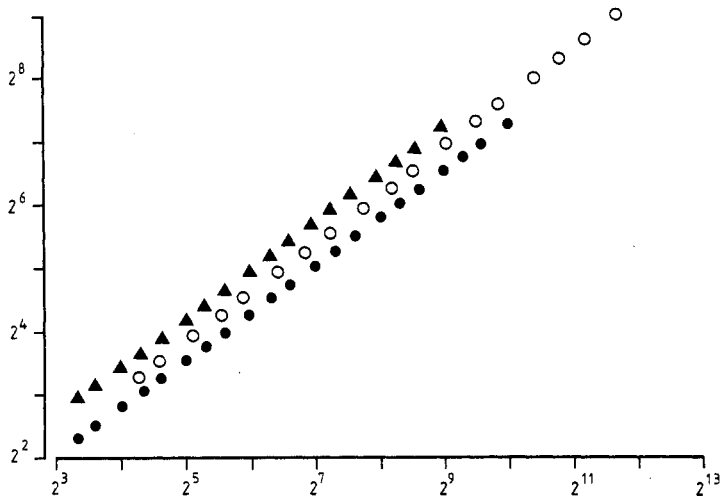


**Figure 2.** Points denoted by (○) represent log $L$ against log$\langle P_L \rangle$ of § 2. Points denoted by (●) represent by log $\langle R_N \rangle$ against log $N$ of § 3. Points denoted by (▲) represent log$\langle R_N \rangle$ against log $N$ of § 4. Least-square fits of different symbols give estimates of slopes 0.753, 0.737 and 0.745 respectively.

We considered lattices of 18 different sizes, with $L = 10, 12, 16, 20, 24, 32, \ldots, 360, 384, 512$. For $L = 10, 12, 16$ we averaged over 32 000 percolating configurations. The number of configurations studied for a particular lattice size $L$ was reduced by a factor of two when the lattice size was doubled. Finally, for $L = 360, 384$ and 512 we simulated 1000 percolating configurations each. We averaged the perimeter lengths for each lattice size $L$, and tried to fit this average length $\langle P_L \rangle$ for various lattice sizes $L$ to the form $L \sim \langle P_L \rangle^{\nu}$. To get the value of $\nu$ we plotted $L$ against $\langle P_L \rangle$ on a log-log scale (see figure 2). The points fit very well to a straight line. A least-squares fit to these data gives the value of the size exponent $\nu = 0.753$. Similar measurements for site percolation on the square lattice at the percolation threshold (using $p_c = 0.592\,745$, Ziff and Sapoval (1986)) gives for the size exponent $\nu = 0.741$.

## 3. Simulation of percolation cluster perimeters

Here we generate the site percolation cluster perimeters on the square lattice at the percolation threshold by a random walk algorithm introduced by Ziff *et al* (1984). This method generates only the cluster perimeters without generating the actual percolation clusters. Let us briefly describe the method.

The sites of the lattice are divided into three categories, namely blank, vacant and occupied. The process starts with a lattice full of blank sites except for a vacant-site-occupied-site pair at the centre. The clusters are grown by the following algorithm.

(i) A direction is defined by drawing an arrow from the vacant site to the occupied site and the random walker goes to the occupied site.

(ii) With the walker oriented by the arrow, the site to the left of the present site is tested for type, as follows.

(a) If the site is already occupied then an arrow is drawn from the present position to the new occupied site, the random walker goes to this occupied site and process (ii) is repeated.

(b) If the site is vacant then testing is repeated, but with the site colinear with the arrow chosen; if this is also vacant, the site to the right is tested; if this is also vacant the backward site is tested.

(c) If the site is blank, then this site is occupied with probability $p$ and vacant with probability $(1-p)$. This process stops when the initial site is traversed again in the initial direction.

We generate long percolation cluster perimeters of occupied sites on the square lattice at its percolation threshold $p_c$ by this method. Then we determine the backbone of this cluster between initial occupied sites and the final occupied sites. This is done by numbering the occupied sites during the process of generation of the perimeter. In this process the random walker assigns a number to each occupied site. Whenever a new occupied site is faced, the walker assigns a new number to this site, one greater than the number of the presently occupied site. When an occupied site is revisited the number of that site is unchanged. However, corresponding to every site number we keep in memory the position of the latest occupied site visited having this number. Finally, when the process is terminated the sites in memory represent the backbone of the perimeter. In our case this backbone is also its perimeter (see figure 3).

We restrict the length of the backbone perimeter to $N$, and calculate the end-to-end distance. We simulated backbone perimeters of 21 different lengths, namely $N = 10, 12, 16, 20, 24, 32, \ldots, 640, 768, 1024$. For $N = 10, 12$ and 16 we averaged over 3.2

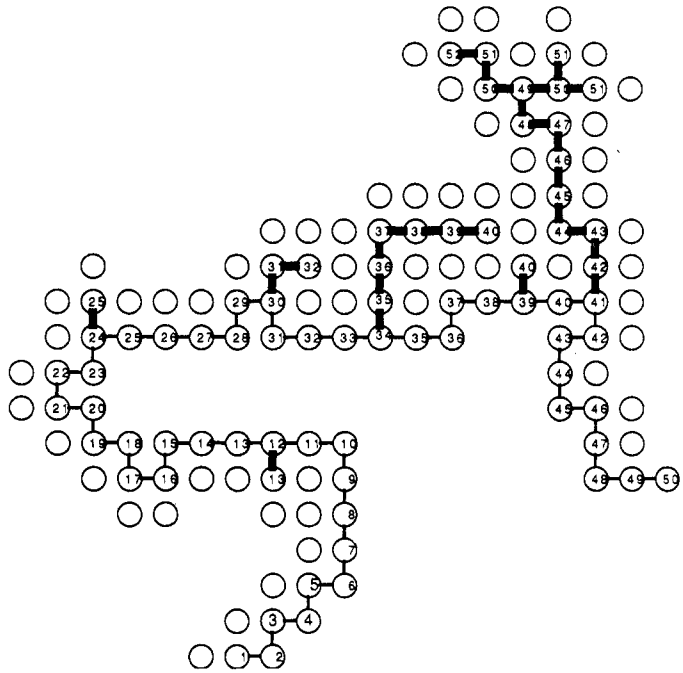

**Figure 3.** Generation of the percolation backbone perimeter of length 49 bond units. Numbered circles represent occupied sites, empty circles represent vacant sites and blank sites are not shown. All connected circles constitute the perimeter of the percolation cluster. Thin and thick line connections correspond to the backbone and to dangling ends respectively.

million configurations. The number of configurations studied for a particular perimeter length $N$ is reduced by a factor of two when the perimeter length is doubled. Finally, for $N = 640$, 768 and 1024 we simulated 50 000 configurations each. We averaged these end-to-end distances for each perimeter length $N$ and tried to fit this average length $\langle R_N \rangle$ for various perimeter lengths $N$ to the form $\langle R_N \rangle \sim N^{\nu}$. In figure 2 $\langle R_N \rangle$ is plotted against $N$ on a log-log scale. A least-squares fit of these data gives the value of the size exponent $\nu = 0.737$.

## 4. Simulation of the indefinitely growing self-avoiding walks

We generated perimeters of backbones of percolation clusters by indefinitely growing self-avoiding walks. To explain this, let us consider the correspondence between IGSAW and percolation cluster perimeters in some detail, following Weinrib and Trugman (1985).

Consider site percolation clusters on a triangular lattice at the percolation threshold $p_c = \frac{1}{2}$. The perimeter of such a cluster is defined by those bonds on the dual honeycomb lattice which separate occupied sites from unoccupied sites on the triangular lattice. The probability that a bond on the dual honeycomb lattice will be occupied by the perimeter will depend on the probability that a site on any of its two sides is occupied. It has been shown (Weinrib and Trugman 1985) that the probability distribution for

the bonds on the perimeter will follow exactly the same probability distribution IGSAW steps on the honeycomb lattice. Now two sites (separated by more than three bonds) on such a perimeter will be at nearest (NN), next nearest (NNN) or next-to-next nearest (NNNN) neighbour distance only when the portion of the perimeter between this pair of sites surrounds some dangling ends of the percolation cluster. Therefore to get the perimeter of the backbone of the percolation cluster we have to remove that portion of the percolation cluster perimeter between two sites placed at NN, NNN and NNNN positions. In figure 4 these site pairs are marked by 11, 22 and 33. The sites 44 are also nearest neighbours but the portion of the perimeter between these two sites surrounds a dangling end of thee unoccupied site cluster, and we do not try to remove it. The resulting structure therefore gives the perimeter of the backbone.

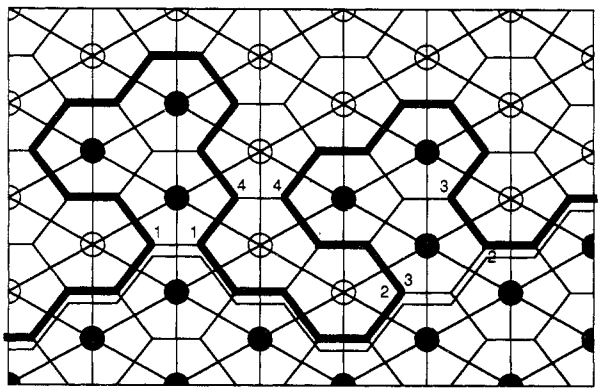


**Figure 4.** Percolation cluster (full circles) on the triangular lattice and its perimeter (thick curve) on the honeycomb lattice. Portions of this perimeter between pairs of points 11, 22 and 33 surround dangling ends of the cluster whereas 44 corresponds to a dangling end of an unoccupied site cluster. The backbone perimeter obtained from the cluster perimeter is shown by the thin line.

From the point of view of IGSAW, when the walker comes to NN, NNN and NNNN sites of its previous path it faces a possibility of future trapping. The dangling ends of the percolation clusters correspond to trapping situations on the IGSAW. Therefore, as an equivalent procedure, instead of generating the perimeter of percolation clusters we can use IGSAW on a honeycomb lattice to get the percolation backbone perimeter on the triangular lattice. To do this, a long IGSAW is generated and all NN, NNN and NNNN site pairs are determined. Then those pairs of sites which differ in winding angle by the same sign (to avoid the situation marked 44 in figure 4) are short circuited. For two different signs, + and −, we get two perimeters, left and right. Though the correspondence between IGSAW and percolation perimeters is not exact on lattices other than the honeycomb lattice, we believe from universality considerations that such a construction of backbone perimeters from IGSAW on other lattices would yield similar results. With this belief, we have simulated IGSAW on the triangular lattice to use the knowledge that, on this lattice, to check for possible caging it is enough to look at nearest neighbours only (Kremer and Lyklema 1985b) (see figure 5).

We have generated 1000 configurations of such IGSAW. Each of these configurations has a left or right perimeter greater than 2048 steps. Then average distances $\langle R_N \rangle$ on these perimeters are calculated for points separated by $N = 16, 32, \ldots, 512$ steps and

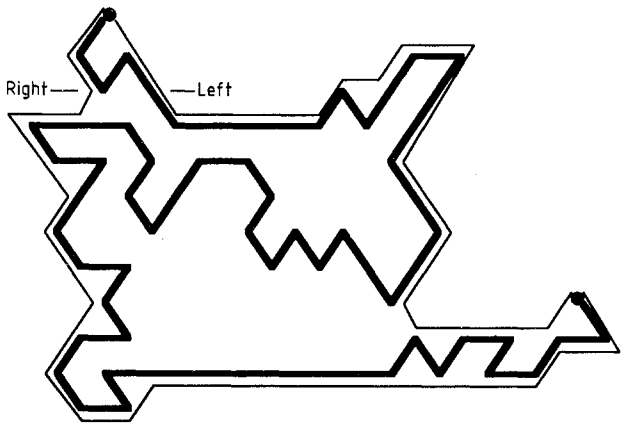


**Figure 5.** Indefinitely growing self-avoiding walk of length 64 steps on the triangular lattice (shown by thick line). The left and right backbone perimeters constructed from this walk are of length 22 and 25 respectively.

they are further averaged over 1000 configurations, and over both sides. Similar calculations are done for 12, 24, ..., 384 steps and 10, 20, ..., 320 steps. We plot $\langle R_N \rangle$ and $N$ on a log-log scale (see figure 2). A least-squares fit of these data gives the value of the size exponent $\nu = 0.745$.

## 5. Conclusion

In this paper we have studied perimeters of the backbones of the percolation clusters at the percolation threshold in two dimensions by three independent methods. First, we generated actual bond and site percolation clusters at the percolation threshold on the square lattice and measured the average length of the perimeters of the backbones as a function of lattice size (§ 2). Second, percolation cluster perimeters were generated by a random walk algorithm for site percolation on the square lattice at the percolation threshold and the average end-to-end distance of the perimeter of the backbone was measured as a function of perimeter length (§ 3). Third, indefinitely growing self-avoiding walks were generated on the triangular lattice. As these walks represent perimeters of percolation clusters at the percolation threshold we used them to generate equivalent percolation backbone perimeters by chopping off portions of the walk corresponding to dangling ends. We measured the average end-to-end distance as a function of this perimeter length. In each case we calculated the exponent related to the average size and length of these perimeters. All these three independent methods give very close estimates of the exponent, and we finally estimate a value of $\nu = 0.744 \pm 0.012$. This value is very close to the average size exponent for ordinary self-avoiding walks in two dimensions, which is exactly equal to $\frac{3}{4}$ (Nienhuis 1982). Therefore it seems likely that perimeters of percolation backbones may belong to the same universality class as that of ordinary SAW. This result is not very surprising since considering the backbone instead of the whole cluster amounts to adding repulsive interactions to a $\theta$ point, which results in self-avoiding walk behaviour.

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*Note added.* After submission of the paper we came to know about the works of Grossman and Aharony (1986, 1987). Here the external perimeter of a percolation cluster is measured by throwing particles to the percolation cluster and estimating the length accessible to them. The fractal dimension of this perimeter was estimated to be nearly $\frac{4}{3}$. We find this work and our work are complementary in the following sense and expect the results should be the same. Consider two pictures: the first is an infinite cluster of occupied sites in a sea of vacant sites and the second is just the 'negative' of the first. By negative we mean all the occupied sites have become vacant and the vacant sites are made occupied. Then the external accessible perimeter and the perimeter of the backbone of the first picture will be the internal perimeter of the backbone and the internal accessible perimeter of the occupied cluster on the second picture respectively. At the percolation threshold they should be the same.

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