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Monte Carlo study of the percolating cluster for the square lattice site problem

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Abstract. Clusters which just span finite lattices of various sizes have been generated using a Monte Carlo method. These have been analysed to form estimates of the mean values of cyclomatic index, valence and perimeter. In addition the shortest spanning self-avoiding walk has been characterised. The ramified nature of these clusters is discussed in terms of these properties.

1. Introduction

Monte Carlo methods were first used in percolation theory by Hammersley and co-workers (Vyssotsky *et al* 1961, Frisch *et al* 1962) and, since then, various attempts have been made to estimate the critical density (p_c) and some critical exponents (e.g. Dean 1963, Dean and Bird 1967, Kirkpatrick 1976, Hoshen *et al* 1979) for various lattices. More recently these methods have proved useful in investigating various properties of clusters, both above and below p_c, such as the perimeter (Domb *et al* 1975, Stoll and Domb 1978) and the cyclomatic index (Stoll and Domb 1979). These results are of particular interest because properties such as the perimeter and cyclomatic index were invoked by Domb (1974) to characterise the degree of ramification of a cluster. Other workers (Stauffer 1978, Shlifer *et al* 1979) have focused attention on the radius of gyration of a cluster and on the 'backbone' of the percolating cluster (i.e. the part of the cluster contributing directly to the percolation process).

In this paper we consider percolation on a set of finite square lattices and examine properties of the clusters at various occupation densities, paying particular attention to the cluster which just spans the finite lattice (the 'percolating clusters'). We estimate various properties of the clusters and examine our results in the light of several suggestions made in the papers mentioned above. We are especially concerned with the extent to which the percolating cluster at the percolation threshold can be considered ramified and to what extent it resembles a walk-like graph.

2. Monte Carlo approach

Most Monte Carlo work has employed periodic boundary conditions in an attempt to avoid the inherent limitation of working with a finite system. We have chosen, instead, to use free boundaries but to carry out the calculations on systems with a variety of sizes

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and to attempt to extrapolate the results, especially for percolating clusters, to infinite systems. Otherwise the Monte Carlo technique used is that described by Dean (1963) and involves successively filling empty lattice sites until some maximum density of occupied sites is achieved. Each realisation of the process gives data for all densities (p) less than this designated maximum (in this case, for $p \leq 0{\cdot}75$). When each new site is filled the system is examined to determine if a cluster spans the lattice (i.e. contains a connected path from the North to South or from the East to West sides of the lattice). The cluster which first does this is referred to as the 'percolating cluster' and the value of p at which this occurs is an estimator of p_c for this particular finite system. We form averages of various properties of these percolating clusters at p_c. These calculations have been carried out for various $m \times m$ lattices where $m = 10$, 20, 40, 100 and 200. The number of realisations used was typically 600.

3. Properties of the percolating cluster at the percolation threshold

Estimates of various properties of the percolating cluster are given in table 1 for each finite lattice studied. Primarily as a test of the technique used here we have calculated the average value of p at which percolation first occurs on an $m \times m$ lattice, $p_c(m)$. This quantity increases with increasing m and we have attempted to extrapolate against m^{-1}.

Table 1. Properties of the percolating cluster.

Size of lattice		10×10	20×20	40×40	100×100	200×200
Direct estimate of p_c		0·5544	0·5667	0·5783	0·5854	0·5888
Fraction of sites with valence	1	0·18	0·15	0·14	0·13	0·13
	2	0·44	0·40	0·38	0·37	0·36
	3	0·31	0·35	0·36	0·37	0·37
	4	0·07	0·10	0·12	0·13	0·14
Average valence		2·28	2·41	2·47	2·50	2·51
$\langle c \rangle / \langle n \rangle$		0·181	0·221	0·243	0·252	0·257
$\langle b/n \rangle$		0·792	0·756	0·730	0·709	0·697
Average length, s, of shortest spanning self-avoiding walk		11·95	28·3	63·0	183·0	—
'Thickness', t, of shortest spanning walk		2·8	4·2	6·7	13·2	—
'Relative thickness', t^*, of shortest spanning walk		0·234	0·149	0·107	0·072	—

The results are shown in figure 1. The extrapolation is reasonably smooth and suggests that the value for an infinite lattice is $p_c = 0{\cdot}594 \pm 0{\cdot}003$. Dean and Bird (1967) found 0·591 using a similar Monte Carlo method, while Neal (1972) estimated 0·593. The most recent series analysis result (Sykes *et al* 1976, Gaunt *et al* 1976) is $0{\cdot}593 \pm 0{\cdot}002$.

The average valence of a site in the percolating cluster increases with m and appears to be tending to a limit in the region of 2·52 for an infinite lattice. A large fraction of sites have valence greater than two (at least 50%) so that, at this detailed level, the cluster does not resemble a self-avoiding walk. The cyclomatic index, c, of a cluster can be obtained from the average valence, $\bar{v}$, of a site in the cluster, and the number of sites,

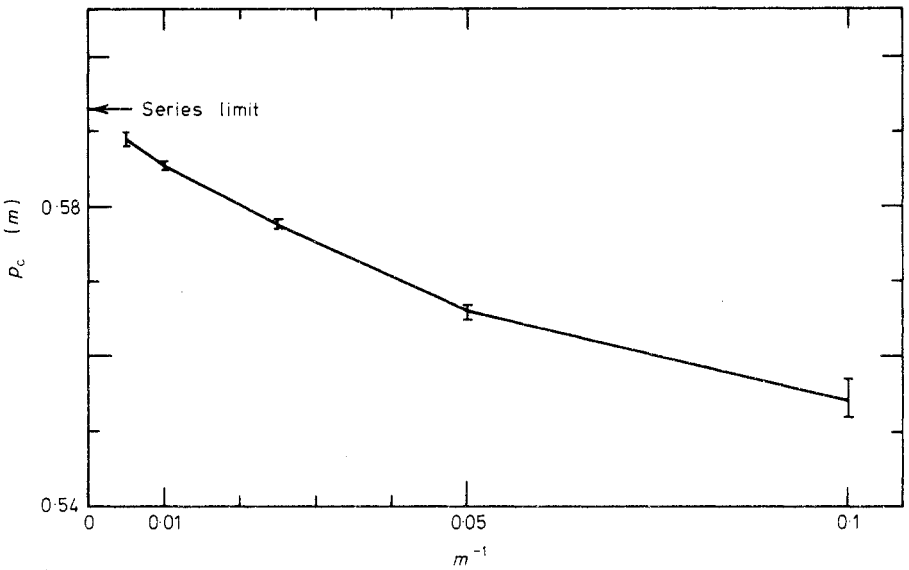

Figure 1. Lattice size dependence of estimates of the critical density.

n, in the cluster using Euler's relation, giving

$$c/n = \tfrac{1}{2}(\bar{\nu} - 2) + n^{-1} \tag{1}$$

and hence, for an infinite lattice,

$$\lim_{n\to\infty} \{c/n\} = \tfrac{1}{2}(\bar{\nu} - 2). \tag{2}$$

Averaging over all realisations gives

$$\left\langle \lim_{n\to\infty} \{c/n\} \right\rangle = \tfrac{1}{2}(\langle\bar{\nu}\rangle - 2) = \tfrac{1}{2}(2{\cdot}52 - 2) = 0{\cdot}26. \tag{3}$$

In table 1 we also give the ratio of averages over all percolating clusters $\langle c\rangle/\langle n\rangle$ for finite lattices which differs from this in using ratios of averages instead of averages of ratios. The m dependence of this quantity is shown in figure 2. Again the extrapolation is smooth and the limiting value is also in the region of 0·26. This is in close agreement with the value obtained by Stoll and Domb (1979) and Cherry and Domb (1980). Since the maximum cyclomatic index per site in the cluster is unity for an infinite cluster, this means that about 26% of the maximum possible number of cycles are actually present. While this number is much less than the value of 100% for a completely compact cluster† it is also much greater than the value zero expected for a tree or, in particular, for a self-avoiding walk. Again, at least on this scale, the percolating cluster does not resemble a walk.

We have also calculated the expectation of the ratio of the number of perimeter sites of the percolating cluster to the number of sites in the cluster, which we write as $\langle b/n\rangle$. This quantity decreases with m, tending to a limiting value of about 0·69. Hankey (1978) and Reich and Leith (1978) have shown that this ratio should equal $(1-p_c)/p_c$

† See also Temperley's (1976) results on the cyclomatic index of the average bond cluster at the percolation threshold.

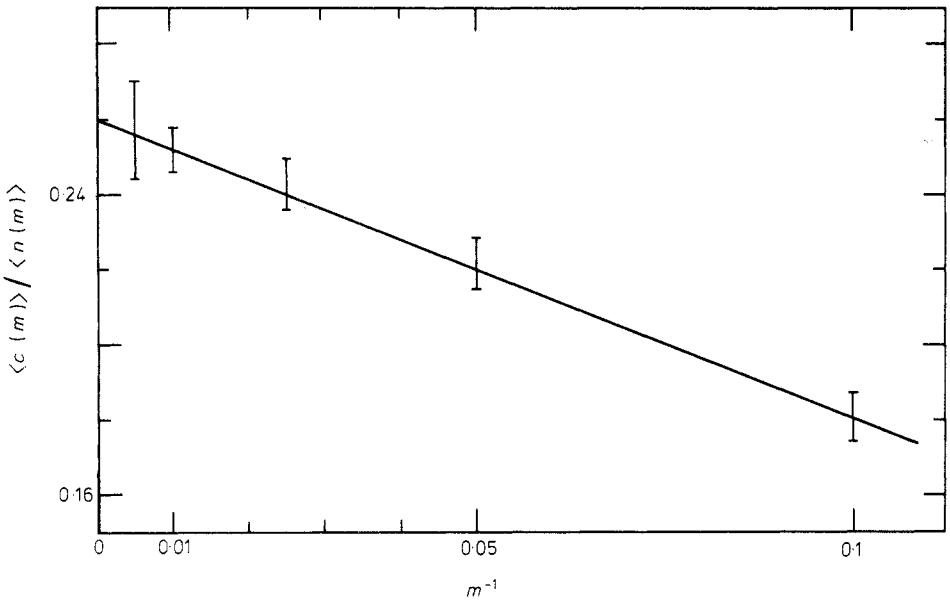

Figure 2. Lattice size dependence of estimates of the cyclomatic index of the percolating cluster.

and, using the series estimate of $p_c = 0{\cdot}593$, we obtain $\langle b/n \rangle = 0{\cdot}686$. Even for a finite lattice, the relationship seems to hold, at least approximately, as we see by inserting the finite lattice estimates $p_c(m)$ into this expression.

These properties are all non-metric. An alternative way to characterise a cluster is by a metric property and as an example we consider the *span* in the non-percolating direction. For a finite $m \times m$ lattice we call the average span in the percolating direction (N → S or W → E) the 'length' $l(m) = m - 1$, since a percolating cluster must just span the lattice. The 'width' $w(m)$ is the average span in the non-percolating direction and we can enquire how $w(m)$ depends on m. The area of the smallest rectangle which can contain the percolating cluster is $w(m)l(m)$ and we expect this to be a non-zero fraction of the total number of lattice sites, m^2. Since $l(m) = m - 1$, this implies that $w(m) = 0(m)$, and the numerical data suggest that $w(m) \sim 0{\cdot}79m$. To obtain a visual impression of the density of sites in a percolating cluster consider a cluster which percolates in the y direction (N → S) and which has vertices at the lattice positions $\{(x_i, y_i), i = 1, 2, \ldots, n\}$. We define the x-centre of the cluster as

$$x_c = \tfrac{1}{2}(\min x_i + \max x_i) \tag{4}$$

and examine the number of sites in the cluster with x coordinate equal to x_c, $x_c \pm 1$, $x_c \pm 2, \ldots$, and then average these numbers over all percolating clusters. This is the average density of occupied sites around the x-centre, $\rho(x)$. The dependence of $\rho(x)$ on x for $m = 200$ is shown in figure 3. The clusters appear to be quite diffuse in the x direction, occasionally reaching one edge of the lattice. (The symmetry comes from averaging over *all* percolating clusters.)

A more interesting way to define the length of the cluster is as the length of the shortest (and therefore self-avoiding) walk which is a subgraph of the cluster and which spans the finite lattice. If the average length of this walk is $s(m)$ for an $m \times m$ lattice we

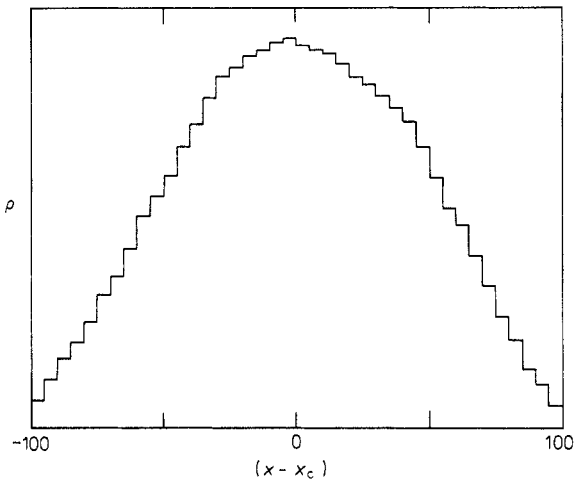

Figure 3. Density of sites (in arbitrary units) in the non-percolating direction for percolating clusters on a 200×200 lattice.

note that $s(m)$ would equal $m-1$ for a completely compact cluster, i.e. $s(m)$ would then equal $l(m)$. Our numerical data (see table 1) suggests that $s(m)/m$ is monotone increasing while $s(m)/m^2$ is monotone decreasing, i.e. $s(m) \sim m^\theta$ with $1 < \theta < 2$. (For a compact cluster, $\theta = 1$.) We can define an alternative measure of the width (which we call the thickness, $t(m)$) as

$$t(m) = n(m)/s(m) \tag{5}$$

where $n(m)$ is the number of sites in the percolating cluster. For $p > p_c$, $n(m)$ is a non-zero fraction of the total number of lattice sites so that $t(m)s(m) \sim m^2$. As $p \to p_c+$ we expect this to remain true, so that

$$t(m) \sim m^{2-\theta}. \tag{6}$$

Since $\theta < 2$ the 'walk' gets 'thicker' as m increases. However, we can define a relative thickness, or 'thickness per unit length',

$$\begin{aligned} t^*(m) &= t(m)/s(m) \\ &\sim m^{-2(\theta-1)} \end{aligned} \tag{7}$$

and since we believe that $\theta > 1$, $t^*(m) \to 0$ as $m \to \infty$.

4. Discussion

Our calculations on the infinite cluster were addressed to the question: to what degree are percolating clusters (at p_c) ramified? Not surprisingly the answer depends on what one means by ramified. Our results certainly support the idea that the perimeter, b, is proportional to the number, n, of sites in the cluster. (For a compact cluster $b = O(\sqrt{n})$.) The cyclomatic index corresponds to only about 26% of the maximum possible number of cycles being present. Related to this is the fact that the average valence of a site in the cluster is about 2·52. These values support the idea that percolating clusters are not

compact. However, they do not seem to resemble self-avoiding walks with relatively few branches or cycles. There is, of course, a shortest self-avoiding walk through the cluster from one side of the lattice to the other but this walk accounts for only a small proportion of the vertices in the cluster, namely $(s(m)+1)/n(m) \sim t(m)^{-1}$ as $m \to \infty$. Indeed the thickness, $t(m)$, of this walk seems to diverge for an infinite lattice. However, the thickness diverges less rapidly than the length of this walk and it seems to be only in this sense that the percolating cluster can be considered walk-like.

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