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Valences of sites in percolating and non-percolating clusters

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Abstract. We present some exact enumeration data and appropriate Padé mimic functions for the p dependence of the fraction of sites in finite clusters for the square lattice site problem having given valence. In addition, we report Monte-Carlo results on the corresponding quantities for sites in infinite clusters and use these data to investigate the degree of ramification of infinite clusters at and above the percolation threshold.

1. Introduction

There have been a number of recent attempts to characterise the degree of ramification of clusters in random percolation processes by using 'local' properties such as the cyclomatic index of the cluster (Domb and Stoll 1977, Cherry and Domb 1980, Middlemiss *et al* 1980) and closely related quantities such as the mean valence of a site in the cluster (Middlemiss *et al* 1980, Gaunt *et al* 1980). In this paper we are concerned with more detailed information of the same type, namely the probability that a randomly chosen site has given valence. In § 2 we discuss the density dependence of these quantities for sites in finite clusters on the square lattice. For densities $p < p_c$, the critical density, this can be calculated exactly and for $p > p_c$ we use series analysis techniques to construct Padé mimic functions. In § 3 we present Monte-Carlo data for the distribution of the valences of sites in infinite clusters and show how these data can be used to characterise the extent to which the clusters resemble trees.

2. Finite clusters

Consider a site percolation process on a lattice with coordination number Q, at density p; that is, sites on the lattice are occupied, uniformly and independently, with probability p. The valence of an occupied site is the number of occupied sites which are near neighbours of this site and we define f_i^F as the fraction of sites in *finite* clusters having valence i. For densities below the critical density, all clusters are finite clusters and

$$f_i^F(p) = \binom{Q}{i} p^i (1-p)^{Q-i} \qquad p \leq p_c. \tag{2.1}$$

To describe the high-density behaviour of f_i^F we define $C(n, t, i)$ to be the number (per lattice site) of sites having valence i, in clusters of n sites having perimeter t. Then f_i^F is given by

$$f_i^F = \sum_{n,t} C(n, t, i)p^n q^t \Big/ \sum_{n,t,i} C(n, t, i)p^n q^t \tag{2.2}$$

where $q = 1-p$. We have calculated $C(n, t, i)$ for $n \leq 16$ for the square lattice. The expansion in powers of p must agree with equation (2.1) and this gives a useful check on the coefficients $C(n, t, i)$. For the high-density branch we expand in powers of q giving

$$f_0^F(q) = 1 - 4q^2 - 8q^3 - 7q^4 + 36q^5 - 2q^6 + 256q^7 - 452q^8 + 1068q^9 - 7372q^{10} + 216\,24q^{11} - 691\,90q^{12} + \ldots \tag{2.3}$$

$$f_1^F(q) = 4q^2 + 4q^3 - 4q^4 - 60q^5 - 8q^6 - 108q^7 + 448q^8 - 68q^9 + \ldots \tag{2.4}$$

$$f_2^F(q) = 4q^3 + 6q^4 + 20q^5 - 42q^6 - 96q^7 - 164q^8 + 56q^9 + \ldots \tag{2.5}$$

$$f_3^F(q) = 4q^4 + 4q^5 + 36q^6 - 36q^7 + 64q^8 - 596q^9 + \ldots \tag{2.6}$$

$$f_4^F(q) = q^4 + 16q^6 - 16q^7 + 104q^8 - 460q^9 + \ldots. \tag{2.7}$$

As expected, $f_0^F \to 1$ and $f_i^F \to 0$, $i > 0$, as $q \to 0$ since at sufficiently high densities finite clusters will consist of isolated sites. As additional checks, we note that $\Sigma_i f_i^F = 1$ and the mean valence of sites in finite clusters $\langle v \rangle_F = \Sigma_i i f_i^F$. The q expansion of $\langle v \rangle_F$ follows from (2.3) to (2.7), and the series so derived agrees with that given by Gaunt *et al* (1980).

To investigate the valence of sites in an infinite cluster, we define $P_i(p)$ to be the probability that a randomly chosen occupied site *with valence i* is in an infinite cluster and $P(p)$ to be the probability that a randomly chosen occupied site is in an infinite cluster. If $f_i(p)$ is the probability that a randomly chosen occupied site has valence i, irrespective of whether it lies in a finite or infinite cluster, then

$$P(p) = \sum_{i=1}^{Q} f_i(p) P_i(p). \tag{2.8}$$

$f_i(p)$ is an analytic function of p (in fact given by the right-hand side of (2.1) for all p) and $P(p)$ has a singular point at p_c so that at least one of the functions $P_i(p)$ must be singular at p_c. For $p < p_c$, $P_i(p) = 0$, $\forall i$ and, since typical infinite clusters contain sites of all valences greater than zero, we expect that for some values of p, $P_i(p) > 0$ for all $i > 0$, so that $P_i(p)$ will be a non-analytic function of p, for all $i > 0$. Since $P(p)$ is expected to have only one singular point we expect each of the $P_i(p)$, $i > 0$, to be singular at p_c.

If $f_i^I(p)$ is the probability that a randomly chosen site in an infinite cluster has valence i then

$$f_i(p) = P(p) f_i^I(p) + (1 - P(p)) f_i^F(p). \tag{2.9}$$

Following the arguments of Gaunt *et al* (1980) it is easy to show that, if $P(p)$ is continuous at p_c, then $f_i^F(p)$ is continuous at p_c and either

$$f_i^F(p_c) = f_i^I(p_c) \tag{2.10}$$

or

$$f_i(p) - f_i^F(p) \sim P(p) \qquad \text{as } p \to p_c+. \tag{2.11}$$

One can calculate $f_i^F(p_c)$ from (2.1) and these values are quite different from Monte-Carlo estimates of $f_i^I(p_c)$ (Middlemiss *et al* 1980) so that we expect that, close to p_c, $f_i^F(p)$ will behave as in (2.11).

We have evaluated a sequence of Padé approximants (Gaunt and Guttmann 1974) to (2.4) to (2.7) and the results are given in figures 1 and 2, together with the values of $f_i^F(p)$ calculated from (2.1) for $p < p_c$. In figure 1, the high-density branch for $f_1^F(p)$ is taken from the [5/3] approximant and the error bar shown is an estimate of the uncertainty at that point derived from the behaviour of the other approximants. The value at that point is above $f_1^F(p_c)$ calculated from (2.1) so that either f_1^F has a discontinuity (which would imply that $P(p)$ goes to zero discontinuously as $p \to p_c+$) or, more likely, it goes through a maximum between p_c and $p = 0{\cdot}75$. For $f_2^F(p)$ we show the [5/3] and [6/3] approximants which probably represent upper and lower limits on the

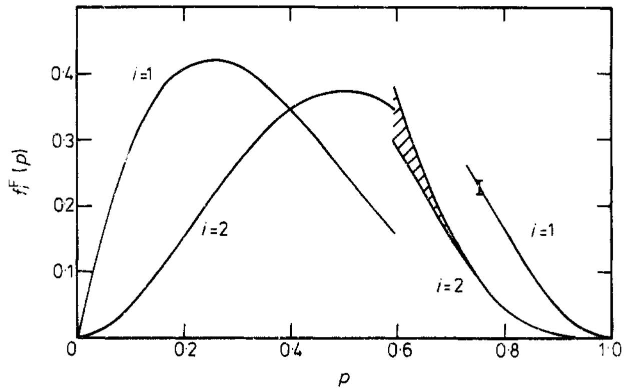

Figure 1. The p dependence of the fractions f_1^F and f_2^F of sites in finite clusters with valences 1 and 2.

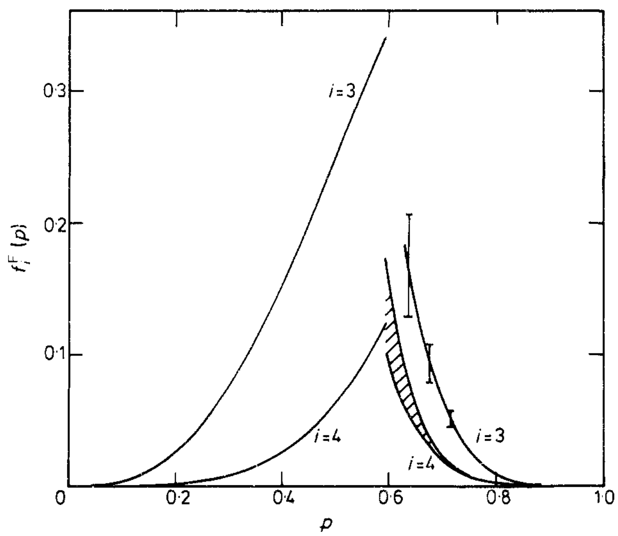

Figure 2. The p dependence of the fractions f_3^F and f_4^F of sites in finite clusters with valences 3 and 4.

true behaviour of the high-density branch. This is consistent with continuity at p_c and monotonicity above p_c. The same behaviour is indicated for $f_3^F(p)$ and $f_4^F(p)$ in figure 2 where we give estimates (with typical error bars) of the high-density branches. For $f_3^F(p)$ the central estimates are based on the [6/2] approximant, while for $f_4^F(p)$ the upper and lower limits shown are the [6/2] and [7/2] approximants.

3. Infinite clusters

Domb and Cherry (1980) have used series expansion data on finite clusters to deduce information about infinite clusters through an equation analogous to (2.9). Instead we use a Monte-Carlo technique to obtain information on the value of $f_i^I(p)$ for a series of *finite* lattices and attempt to extrapolate to the infinite lattice case. Middlemiss *et al* (1980) have carried out similar calculations, but concentrated on the behaviour of the percolating cluster at p_c. Here we present data for a range of p values above the percolation threshold.

In figure 3 we give the extrapolated values of $f_i^I(p)$ for $p > p_c$. The Monte-Carlo approach becomes inefficient above $p \simeq 0{\cdot}9$ but we have derived the first few terms in the q expansions of f_i^I. These can conveniently be obtained by considering holes in an otherwise completely filled lattice of N sites and taking the limit $N \to \infty$. For instance,

$$\begin{aligned} f_4^I(q) = \lim_{N\to\infty} \; & \{N(1-q)^N + N(N-5)q(1-q)^{N-1} + [4N(N-8) + 2N(N-9) \\ & + \tfrac{1}{2}N(N-10)(N-13)]q^2(1-q)^{N-2} + \ldots\} \\ & \times \{N(1-q)^N[1 + (N-1)q + \tfrac{1}{2}N(N-1)q^2 + \ldots]\}^{-1} \\ = {} & 1 - 4q + 6q^2 + O(q^3). \end{aligned} \tag{3.1}$$

Similarly,

$$f_3^I(q) = 4q - 12q^2 + O(q^3) \tag{3.2}$$

$$f_2^I(q) = 6q^2 + O(q^3) \tag{3.3}$$

and

$$f_1^I(q) = 4q^3 + O(q^4). \tag{3.4}$$

As $q \to 0$ f_1^I and f_2^I approach zero with zero slope, f_3^I approaches zero linearly and f_4^I approaches unity linearly. Indeed f_3^I and f_4^I have limiting gradients of the same magnitude but opposite sign. The other interesting feature of figure 3 is the maximum exhibited by f_3^I. This can be understood qualitatively by considering the holes created in an initially filled lattice as q increases. At first most holes will be separated and their neighbouring sites will have valence three. At higher q, the probability of clusters of holes increases and an increasing fraction of the neighbouring sites will have lower valence so that f_3^I will start to decrease.

The detailed valence data can be used to characterise the extent to which the infinite cluster is tree-like in a way analogous to Domb's use of the cyclomatic index. Consider a cluster of n sites, n_i of which have valence i. For the case of direct interest here, where the maximum valence is four, it is easy to show that

$$n_1 \leqslant 2n_4 + n_3 + 2 \tag{3.5}$$

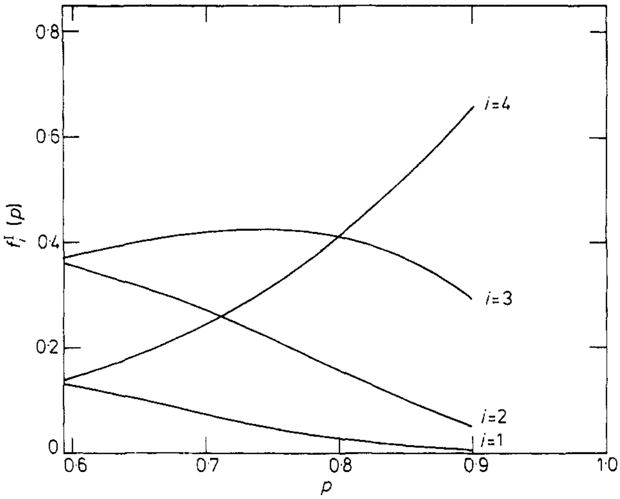

Figure 3. The p dependence of the fraction f_i^{I} ($i = 1, 2, 3, 4$) of sites with valence i in the infinite cluster.

where the equality holds if and only if the cluster is a tree. For an infinite cluster it is convenient to define

$$\mu(p) = (2f_4^{\mathrm{I}} + f_3^{\mathrm{I}} - f_1^{\mathrm{I}})/(2f_4^{\mathrm{I}} + f_3^{\mathrm{I}}) \tag{3.6}$$

which is zero for a tree and has a maximum value of unity. μ can be regarded as a 'compactness' parameter, analogous to Domb's parameter λ. From (3.1) to (3.4) we obtain

$$\mu(q) = 1 - 2q^3 + \mathrm{O}(q^4) \tag{3.7}$$

as the small-q behaviour. Our estimate of the p dependence of μ is shown in figure 4. As p decreases μ decreases, as expected, but $\mu(p_c)$ is about 0·8; that is, the infinite cluster

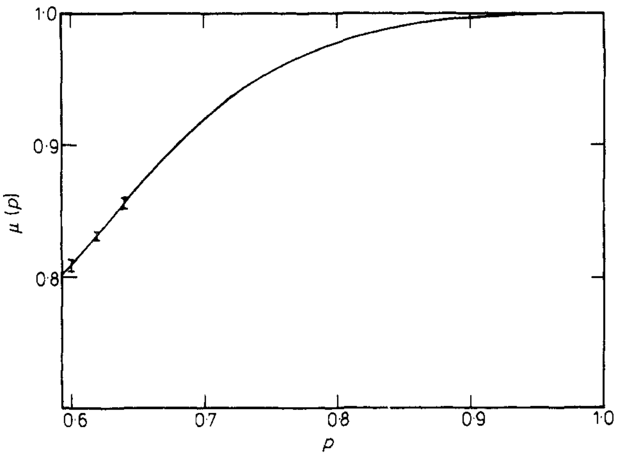

Figure 4. The p dependence of the compactness parameter $\mu(p)$.

becomes more tree-like as p decreases but is still far from being a tree even at p_c. This is in qualitative agreement with the conclusion of Cherry and Domb (1980) that about 26% of the possible cycles are present at p_c for this system.

4. Conclusions

Perhaps the most interesting aspect of this work concerns the degree of compactness of the infinite cluster. If the infinite cluster were ramified close to p_c we would expect f_2^I to be large and f_1^I to be close to $2f_4^I + f_3^I$. In fact, f_2^I and f_3^I are very similar at p_c and f_1^I is close to f_4^I but much smaller than f_3^I. It thus appears that on this local scale the compactness decreases as p decreases, but the infinite cluster is not especially ramified at p_c. Other ways of characterising the infinite cluster (e.g. the dependence of the perimeter on the cluster size (Hankey 1978), the radius of gyration (Stauffer 1978) and the relative 'thickness' of the shortest walk spanning the cluster (Middlemiss *et al* 1980) suggest that it is ramified at p_c but these properties are in a sense more global. Domb's coefficient of compactness, λ, can be related through the average valence of a site in the infinite cluster to a combination of the f_i^I and seems therefore to be a characterisation of the compactness, intermediate between the local one adopted in this paper and the global ones referred to above. The degree of ramification depends on the definition of 'ramified'!

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