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Mean valence of sites in non-percolating clusters

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Abstract. We present Monte Carlo and series results for the mean valence $\langle v\rangle_F$ of non-percolating clusters on the square lattice and corresponding series results for the simple cubic lattice. Mimic functions have been constructed from the series which, for the square lattice, agree well with the Monte Carlo data, for a wide range of densities. We have shown that if the percolation probability is continuous at p_c then $\langle v\rangle_F$ is continuous at p_c, and have presented a heuristic argument which indicates that $\langle v\rangle_I$, the mean valence of a site in a percolating cluster, is greater than $\langle v\rangle_F$, at p_c. This allows us to infer the asymptotic behaviour of $\langle v\rangle_F$ in the region of p_c.

Recently, Stauffer (1979) and Essam (1980) have reviewed the theory of percolation processes from the viewpoint of the statistics of the percolating and non-percolating clusters. Domb has drawn attention to the importance of ramified clusters close to p_c and, in particular, Domb and coworkers (Domb and Stoll 1977, Stoll and Domb 1979, Cherry and Domb 1980) have characterised the degree of compactness or ramification of clusters in a percolation process, by a parameter (λ) defined as the fraction of the maximum number of possible cycles which are present in the cluster. Stoll and Domb (1979) have used Monte Carlo methods to estimate λ for the square lattice at densities $0{\cdot}85 \leqslant p/p_c \leqslant 1{\cdot}1$, where p_c is the critical percolation density. Cherry and Domb (1980) have used series methods to estimate the p-dependence of λ, for all $p \geqslant p_c$, for the *infinite* cluster on the square, triangular and simple cubic lattices.

Closely related to the cyclomatic index (and hence λ) is the mean valence of a site in a cluster, and we examine here the p-dependence of this quantity, for all p, for *finite* clusters on the square and simple cubic lattices. The dependence of the mean valence of sites in a finite cluster on p for $p > p_c$ is of interest, since it characterises the behaviour of non-percolating clusters in the presence of the percolating cluster.

We can denote the mean valence of sites in *finite* clusters as $\langle v\rangle_F$ and the mean valence of sites in *all* clusters as $\langle v\rangle_E$. It is easy to derive the p-dependence of $\langle v\rangle_E$. Since the sites are occupied uniformly and at random, the expectation of the valence of an occupied site belonging to *any* cluster on the square lattice is given by

$$\langle v\rangle_E = 4pq^3 + 12p^2q^2 + 12p^3q + 4p^4 \tag{1}$$

where $q = 1-p$. This immediately gives $\langle v\rangle_E = 4p$ and, more generally, for a lattice of coordination number Q,

$$\langle v\rangle_E = Qp. \tag{2}$$

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Denoting the mean valence of sites in an *infinite* cluster by $\langle v\rangle_I$, we can relate this to $\langle v\rangle_F$ and $\langle v\rangle_E$ through the equation

$$P(p)\langle v\rangle_I+(1-P(p))\langle v\rangle_F=\langle v\rangle_E=Qp \tag{3}$$

where $P(p)$ is the probability that a randomly chosen occupied site is a member of the infinite cluster, i.e. the percolation probability. We note that for $p<p_c$, $\langle v\rangle_F=Qp$, since $P(p)$ is then zero. As $p\to p_c-$, $\langle v\rangle_F\to Qp_c$. For $p>p_c$ we can write

$$\langle v\rangle_F=(Qp-P(p)\langle v\rangle_I)/(1-P(p)) \tag{4}$$

and, provided that $P(p)$ is continuous, as $p\to p_c+$, $\langle v\rangle_F\to Qp_c$ (since $\langle v\rangle_I$ is bounded). Hence $\langle v\rangle_F$ is continuous at p_c.

For any p, $\langle v\rangle_F$ can be written as

$$\langle v\rangle_F=\sum_{n,t,v}C(n,t,v)p^nq^tv\Big/\sum_{n,t,v}C(n,t,v)p^nq^t$$

$$=\sum_{n,t,v}C(n,t,v)p^nq^tv/p(1-P(p)) \tag{5}$$

where $C(n, t, v)$ is the number of sites of valence v in an n-cluster with perimeter t. We have derived $C(n, t, v)$ for $n\leqslant 16$ for the square lattice and for $n\leqslant 11$ for the simple cubic lattice.

Below p_c, $P(p)=0$ and, expanding the numerator in (5) in powers of p, we obtain $\langle v\rangle_F=Qp$, as expected. This forms a useful check on the coefficients $C(n, t, v)$. At high densities ($p>p_c$) one can expand $\langle v\rangle_F$ in powers of q, giving

$$\langle v\rangle_F=4q^2+12q^3+24q^4-8q^5+80q^6-472q^7+728q^8-3584q^9+\ldots \tag{6}$$

for the square lattice, and

$$\langle v\rangle_F=6q^4-6q^5+48q^7-120q^8+144q^9+144q^{10}-1056q^{11}+2604q^{12}-3480q^{13}$$
$$+48q^{14}+13\,332q^{15}-37\,008q^{16}+47\,064q^{17}+22\,482q^{18}$$
$$-256\,026q^{19}+612\,054q^{20}+\ldots \tag{7}$$

for the simple cubic lattice. For the square lattice it is known (Sykes and Glen 1976) that the coefficient of q^{14} in the high-density expansion of the mean number of clusters, $K(q)$, contains contributions from clusters with more than sixteen sites. Hence the coefficients of the expansion of the numerator in (5) are known only through q^{13}, which implies that (6) is known only through q^9. Less detailed configurational data are available for the simple cubic lattice, the perimeter polynomials are only known up to $D_{11}(q)$ (Sykes *et al* 1976a) and, as a result, the last two terms in (7) are subject to some doubt. However, any errors in these coefficients will be small and should have no appreciable effect on the extrapolations.

The expansion in powers of q could also be obtained (Essam, private communication) by noticing that for $p>p_c$ $\langle v(p)\rangle_I=Qp\bar{P}(p)/P(p)$ where $\bar{P}(p)$ is the probability that a randomly chosen occupied *bond* is a member of an infinite *site* cluster.

We note that by expanding

$$\sum_{n,t}C(n,t,v)p^nq^t\equiv\sum_r a_r(v)q^r \tag{8}$$

we can compare our data for $a_r(v)$ with that of Cherry and Domb (1980), who gave $a_r(v)$

up to $r = 12$ for the square lattice, and up to $r = 24$ for the simple cubic lattice. Our data agree with theirs and, in addition, we find

$$a_{13}(1) = -2204, \quad a_{13}(2) = 630, \quad a_{13}(3) = -580, \quad a_{13}(4) = -559 \tag{9}$$

for the square lattice and, with the proviso discussed above,

$$a_{25}(1) = 19\,032, \quad a_{25}(2) = 19\,104, \quad a_{25}(3) = 2856, \quad a_{25}(4) = -8070,$$
$$a_{25}(5) = 7182, \quad a_{25}(6) = 1705, \quad a_{26}(1) = -48\,618, \quad a_{26}(2) = -36\,855,$$
$$a_{26}(3) = -12\,480, \quad a_{26}(4) = 9798, \quad a_{26}(5) = -13\,014, \quad a_{26}(6) = -3161 \tag{10}$$

for the simple cubic lattice.

In order to characterise $\langle v \rangle_F$ for $0 \leqslant q < q_c$ we have formed Padé approximants (Gaunt and Guttmann 1974) to the series (6) and (7). For the square lattice the last few approximants are in good agreement with one another for $q \leqslant 0{\cdot}3$ (for which the spread in the last five approximants is at most 10%). Since $\langle v \rangle_F$ is continuous at p_c, the high- and low-density branches must match and equal $4p_c \simeq 2{\cdot}372$. The value of the [3/4] approximant at p_c is 2·411, a discrepancy of only $1\frac{1}{2}$%. The p-dependence of $\langle v \rangle_F$ is shown in figure 1 for this lattice. We have carried out a similar analysis for the simple cubic lattice, for which the [9/10] approximant matches the low-density branch to within less than 2%. The mimic function is exhibited in figure 2.

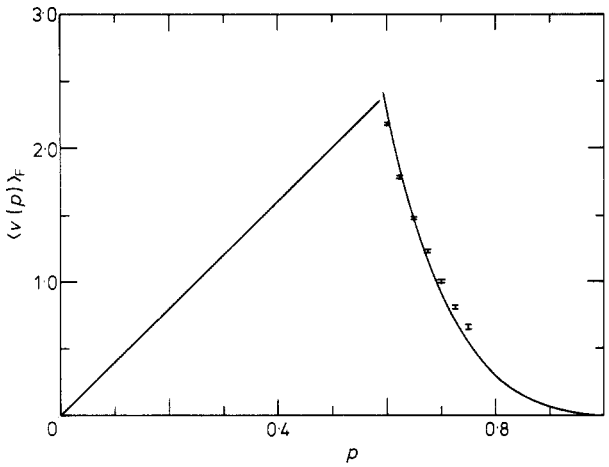

Figure 1. Average valence $\langle v(p) \rangle_F$ of sites in finite clusters on the square lattice. The full line is the Padé mimic function. Points with error bars are Monte Carlo estimates.

For the square lattice we have also calculated $\langle v \rangle_F$ using a Monte Carlo procedure based on that described by Dean (1963). We have used a variety of finite $m \times m$ lattices with fixed boundary conditions, ranging from $m = 10$ to $m = 200$. The results for the $m = 200$ and $m = 20$ cases are shown in figure 3. The linearity is readily apparent in this data for $p \leqslant 0{\cdot}5$, but there is a rounding effect close to p_c due to the distribution of p-values at which percolation first occurs in the sample. The deviation from a gradient of 4 for $m = 20$ is also a finite lattice effect. Some of the Monte Carlo points for $m = 200$ are also plotted in figure 1 for comparison with the series results. The agreement is very

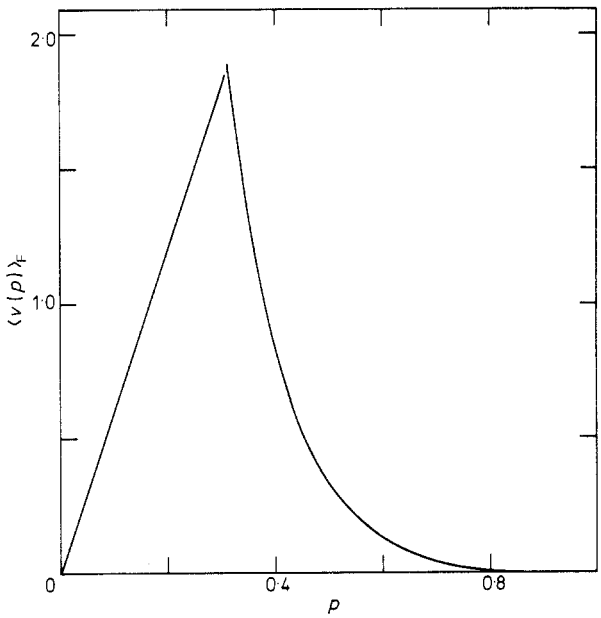

Figure 2. Mimic function for $\langle v(p)\rangle_F$ on the simple cubic lattice.

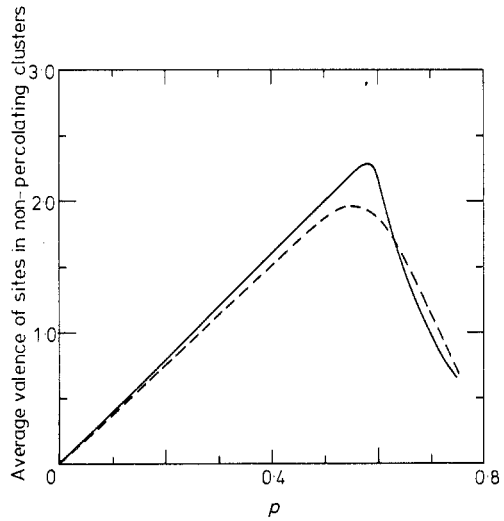

Figure 3. Monte Carlo data for the average valence of sites in finite clusters on *finite* square lattices. —— 200×200, - - - 20×20.

satisfactory, especially for p near to p_c where the series results are less reliable. At higher p, where the discrepancies are more marked, the Monte Carlo data are not of such good quality and the series results are probably to be preferred.

If we assume that $P(p)$ is continuous at p_c, then we can investigate more closely the behaviour of $\langle v\rangle_F$ as $p\to p_c+$ by writing $\langle v\rangle_I$ as

$$\langle v\rangle_I = P(p)^{-1}(Qp-\langle v\rangle_F)+\langle v\rangle_F. \tag{11}$$

Since $P(p) \to 0$ as $p \to p_c+$, and $\langle v \rangle_I$ is bounded, $Qp - \langle v \rangle_F$ must go to zero at least as rapidly as $P(p)$. We then have two possibilities: (i) $Qp - \langle v \rangle_F \to 0$ more rapidly than $P(p) \to 0$, in which case $\langle v \rangle_I = \langle v \rangle_F$ at p_c, or (ii) $Qp - \langle v \rangle_F \to 0$ at the same rate as $P(p) \to 0$. In this case, writing $P(p) \sim B(p - p_c)^{\beta}$ we have $Qp_c - \langle v \rangle_F \sim B'(p - p_c)^{\beta'}$ for $p = p_c{}^+$, with $\beta' = \beta$. That is, the exponent characterising the behaviour close to the critical density is the *same* for the two functions, and $\langle v \rangle_I = \langle v \rangle_F + B'/B$ at p_c. For the square lattice $\langle v(p_c) \rangle_F = 4p_c = 2{\cdot}372 \pm 0{\cdot}008$ (Sykes *et al* 1976b) and recent Monte Carlo data (Middlemiss *et al* 1980) suggest $\langle v(p_c) \rangle_I = 2{\cdot}52 \pm 0{\cdot}01$. This result comes from an extrapolation from finite lattice data, but the extrapolation appears to be quite smooth and a value as low as 2·372 seems to be completely inconsistent with the Monte Carlo results. This leads to the view that, for the square lattice, $\langle v \rangle_F \sim Qp_c - B'(p - p_c)^{\beta}$, as $p \to p_c+$, with $\beta \simeq \frac{1}{7}$ (Sykes *et al* 1976c) and $B' = 0{\cdot}23 \pm 0{\cdot}03$, where we have used the value $B = 1{\cdot}530 \pm 0{\cdot}015$ (Sykes *et al* 1976c). An alternative proof that $\beta' = \beta$ can be constructed by using the relationship between $\langle v \rangle_I$ and $\bar{P}(p)$ (see above) and extending to the site problem the inequalities between $P(p)$ and $\bar{P}(p)$ derived by Blease *et al* (1978). We note that if $P(p)$ has a discontinuity at p_c then (11) gives no information about β', but the inequality $\langle v(p_c+) \rangle_I \neq \langle v(p_c+) \rangle_F$ would then imply that $\langle v \rangle_F$ is discontinuous.

The way in which the average valence of a site depends on the size of the cluster containing it is also of interest, and we define $\langle v(n, p) \rangle$ as the average valence of a site in a cluster of n sites at density p. We have calculated this quantity at $p = p_c$, for small n, from Monte Carlo data. The n-dependence is shown in figure 4 for a finite (100×100) lattice. Not surprisingly, $\langle v(n, p_c) \rangle$ appears to be a monotone non-decreasing function of n, approaching the limit for the percolating cluster found by Middlemiss *et al* (1980). This limiting value is shown as a dashed line in the figure. In order to obtain $\langle v(p_c) \rangle_F$ from these results, one needs the distribution of cluster sizes $\rho(n, p_c)$. This quantity is known (e.g. Hoshen *et al* 1979) to be a rapidly decreasing function of n, and our data, for the 100×100 finite lattice, are also shown in figure 4. The mean valence over *all* clusters is given by

$$\langle v(p_c) \rangle_F = \int_1^{\infty} \langle v(n, p_c) \rangle \rho(n, p_c)\, \mathrm{d}n. \tag{12}$$

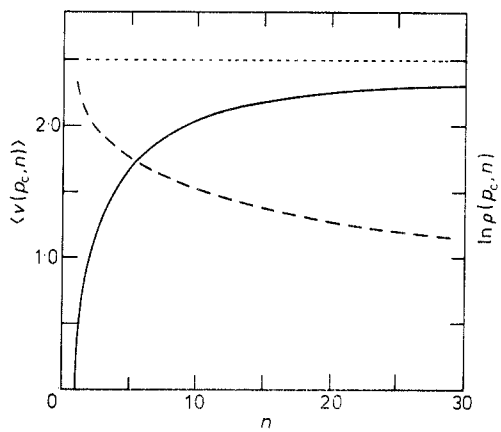

Figure 4. Average valence of sites in clusters of n sites (full line) and cluster size distribution function (broken line) in arbitrary units.

Writing $\langle v(n, p_c)\rangle = [\lim_{n\to\infty} \langle v(n, p_c)\rangle] - g(n) \equiv t - g(n)$, we have

$$\langle v(p_c)\rangle_F = t - \int_1^\infty g(n)\rho(n, p_c)\,dn \tag{13}$$

since $\int_1^\infty \rho(n, p_c)\,dn = 1$, and this will be strictly less than t provided only that the integral is positive. This is the case since g and ρ are both non-negative everywhere and positive, at least for sufficiently small n. This argument supports the result that $\langle v(p_c)\rangle_F < \langle v(p_c)\rangle_I$ and hence that $Qp - \langle v\rangle_F \sim P(p)$ for $p = p_c+$.

Finally, we return to explore the relationship of our results to those of Cherry and Domb (1980). For the infinite cluster on the square lattice, at any $p > p_c$, the coefficient of compactness (λ) is related to the mean valence through the equation

$$\lambda(p) = \tfrac{1}{2}\langle v(p)\rangle_I - 1 \tag{14}$$

(see e.g. Middlemiss *et al* 1980, equation (3)). From (3) and (14) we obtain

$$\lambda(p) = \tfrac{1}{2}\langle v(p)\rangle_F + [4p - \langle v(p)\rangle_F]/2P(p) - 1. \tag{15}$$

Using the Padé mimic function for $\langle v(p)\rangle_F$ and an appropriately derived mimic function for $P(p)$, we have calculated $\lambda(p)$ for $p > p_c$, using equation (15). The results are in good agreement with those of Cherry and Domb (1980) except in a small region close to p_c. The mimic functions which we have used for $\langle v(p)\rangle_F$ do not quite go to Qp_c as $p \to p_c+$, and this small error is magnified close to p_c since $P(p) \to 0$. Consequently our estimate of $\lambda(p)$, from the mimic functions, will be unsatisfactory close to p_c. One might hope to use the asymptotic form $\langle v(p)\rangle_F \sim Qp_c - B'(p - p_c)^\beta$ in conjunction with equation (15) to predict the behaviour of $\lambda(p)$ in the asymptotic region. This requires a knowledge of the way in which $(Qp - \langle v\rangle_F)/P(p)$ approaches B'/B as $p \to p_c+$, which is determined by the form of the subdominant (but confluent) singularities in the numerator and denominator. Consequently, no detailed predictions can be made about the behaviour of $\lambda(p)$ in the asymptotic region. However, equation (15) suggests that $\lambda(p)$ will exhibit power law behaviour,

$$\lambda(p) - \lambda(p_c) \sim T(p - p_c)^\theta \tag{16}$$

and θ will be determined by the most singular term in the right-hand side of equation (15). Hence $\theta \leqslant \beta$. Since β is known to be about $\frac{1}{7}$ for the square lattice, this implies that $\lambda(p)$ approaches $\lambda(p_c)$ with infinite slope. This is not apparent from the data of Cherry and Domb (1980), but this may only imply that the asymptotic region is very narrow.

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References

Blease J, Essam J W and Place C M 1978 *J. Phys. C: Solid St. Phys.* **11** 4009
Cherry R and Domb C 1980 *J. Phys. A: Math. Gen.* **13** 1325
Dean P 1963 *Proc. Camb. Phil. Soc.* **59** 397

Domb C and Stoll E 1977 *J. Phys. A: Math. Gen.* **10** 1141
Essam J W 1980 *Rep. Prog. Phys.* **43** 833
Gaunt D S and Guttmann A J 1974 *Phase Transitions and Critical Phenomena* ed C Domb and M S Green (London, New York: Academic)
Hoshen J, Stauffer D, Bishop G H, Harrison R G and Quinn G D 1979 *J. Phys. A: Math. Gen.* **12** 1285
Middlemiss K M, Whittington S G and Gaunt D S 1980 *J. Phys. A: Math. Gen.* **13** 1835
Stauffer D 1979 *Phys. Rep.* **54** 1
Stoll E and Domb C 1979 *J. Phys. A: Math. Gen.* **12** 1843
Sykes M F, Gaunt D S and Glen M 1976a *J. Phys. A: Math. Gen.* **9** 1705
—— 1976b *J. Phys. A: Math. Gen.* **9** 97
—— 1976c *J. Phys. A: Math. Gen.* **9** 725
Sykes M F and Glen M 1976 *J. Phys. A: Math. Gen.* **9** 87