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Shape and size of two-dimensional percolation clusters with and without correlations

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Abstract. The statistical analysis previously used for the temperature behaviour of clusters for the Ising model is applied to Monte Carlo samples of percolation clusters. Three cases are considered: (*a*) positive correlation ($T = 2T_c$ ferromagnetic); (*b*) random ($T = \infty$); (*c*) negative correlation ($T = 2T_c$ antiferromagnetic). It is found that the exponents which characterise the decay of the cluster-size distributions do not depend on correlation. These distributions can be fitted over their whole range by assuming that percolation critical exponents are independent of correlation, but the scaling functions which then result do depend on correlation. Statistical parameters which are related to the compactness or ramification of clusters change smoothly with correlation. However, some features of negative correlation are significantly different in behaviour.

1. Introduction

In a previous paper (Domb and Stoll 1977) we introduced a number of statistical parameters to characterise the shape and size of clusters in the two-dimensional Ising model. We then took advantage of Monte Carlo data obtained with a two-dimensional one-spin-flip Ising model (Glauber model) to estimate how these parameters varied with temperature, especially in the neighbourhood of the critical temperature T_c. A parameter λ to which we devoted particular attention was related to the cyclomatic number c of the cluster, and measured its degree of compactness or ramification.

The same model can be used to provide data on percolation clusters, the concentration being controlled by the magnetic field. Random percolation corresponds to the limit of very high temperatures, and correlated percolation to finite temperatures. We have given some typical examples of the results obtained in previous publications (Domb 1978, Stoll *et al* 1978, Stoll and Domb 1978). In the present paper we aim to furnish detailed numerical estimates for percolation to parallel those previously obtained for the Ising model.

In addition to comparing the Ising and percolation transitions, we shall focus attention on the effect of correlation on percolation behaviour. A number of authors have discussed percolation with positive correlations, i.e. in ferromagnetic Ising systems (e.g. Coniglio *et al* 1977, Odagaki *et al* 1975), and the suggestion has been made by Coniglio *et al* that universal features like critical exponents remain unchanged in the presence of correlation. Support for this suggestion is contained in a recent paper by Klein *et al* (1978). To the best of our knowledge the only previous discussion on

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percolation with negative correlations, i.e. in antiferromagnetic Ising systems, is by Kikuchi (1970).

We shall present sets of percolation data corresponding to: (*a*) $T=2T_c$ ($J>0$, ferromagnetic); (*b*) $T=\infty$ (random); (*c*) $T=2T_c$ ($J<0$, antiferromagnetic). We find that some characteristics are indeed universal and independent of correlation, but others do not fit the universality pattern. By comparing the three sets of data we will see qualitatively how correlation affects the shape and size of clusters in the critical region.

2. Critical concentration

Qualitatively one would expect positive correlation to enhance the growth of large clusters and hence to decrease p_c, whilst negative correlation should increase p_c. This is borne out by the numerical data.

As a method of estimating p_c we found it convenient to use $P(p)$, the fraction of particles in the infinite cluster, which rises very steeply for $p>p_c$. The critical exponent β has been estimated as being close to $\frac{1}{7}$ (Sykes *et al* 1976). Hence, if we plot $P(p)^7$, the result should be close to a straight line. Even if the exponent β is slightly in error, the change in the estimate of p_c is small. The very recent estimate of $\beta=0{\cdot}139\pm0{\cdot}003$ by Blease *et al* (1978) differs only marginally from the above value.

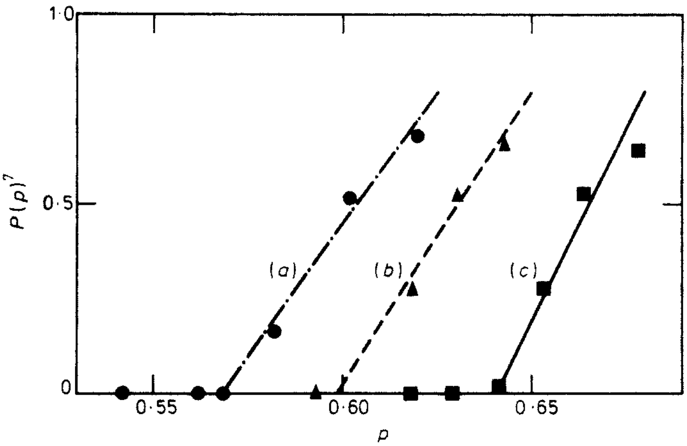

Figure 1. Determination of p_c by $P(p)^7$: (*a*) ferromagnetic; (*b*) random; (*c*) antiferromagnetic. (Same key for all other figures.)

In figure 1 we show these plots in the three cases, and it will be seen that they can be reasonably fitted by straight lines. We have not been able to detect any significant difference in this critical exponent between the three cases, but the data are not very sensitive for fitting β. Our estimates of p_c in the three cases are (*a*) $0{\cdot}569\pm0{\cdot}01$; (*b*) $0{\cdot}598\pm0{\cdot}01$; (*c*) $0{\cdot}641\pm0{\cdot}01$. The value for random percolation (*b*) is larger than the value of Sykes *et al* (1976) by 0·005, the shift to a larger value being caused by a finite-size effect. We used a 110×110 square lattice spin system with periodic boundary conditions. The proper way to treat this effect is by finite-size scaling (see e.g. Reynolds *et al* 1978). The size b of the lattice is varied, and the finite-size deviation from the true p_c (corresponding to an infinite lattice) is assumed to be of the form $b^{-1/\nu}$

We hope to undertake an investigation of this kind, but as a preliminary approximation we would expect that the values of (a) and (c) need to be decreased by a comparable amount.

For the ferromagnetic case it is known that p_c becomes 0·5 at $T = T_c$, and remains at 0·5 in the phase equilibrium region for $T < T_c$ (Coniglio *et al* 1977). For the antiferromagnetic case the behaviour at lower temperatures is much less clear, since one enters the region of critical field behaviour of an antiferromagnet. It is reasonable to expect that p_c will increase further as the temperature is lowered, but the limiting value as $T \to 0$ depends on the competition between the ferromagnetic and antiferromagnetic phases near the critical field H_c. It must be related to the critical concentration (~0·77) at which an ordered antiferromagnetic phase first appears (Brooks and Domb 1951). We shall return to a discussion of the behaviour of p_c as a function of temperature at the end of § 3.

3. Cluster-size distribution

For random percolation the asymptotic form of distribution of n-clusters has been established rigorously (Kunz and Souillard 1978a, Schwartz 1978) as follows:

$$z(n, p) \sim A(n) \exp(-b(p)n^{1/2}), \qquad p > p_1 > p_c, \tag{1}$$

$$z(n, p) \sim C(n) \exp(-d(p)n), \qquad p < p_2 < p_c, \tag{2}$$

where $z(n, p)$ is the number of n-clusters at concentration p. The arguments of Hankey (1978) indicate that (1) should be valid for any $p > p_c$. Monte Carlo data were found to fit well to formula (1) for all $p > p_c$ (Stoll and Domb 1978); for $p < p_c$ the asymptotic form (2) does not set in until n is much larger, but sufficiently extensive data were available to give evidence of the exponential decay (Müller–Krumbhaar and Stoll 1976).

Some of the rigorous arguments can be extended to correlated percolation (Kunz and Souillard 1978b). We have found numerical evidence for an equally good fit to formula (1). Here we have plotted the function

$$\ln\text{–}\ln(z(n, p)/z(n, p_c)) \tag{3}$$

against $\ln n$, and the results are shown in figure 2(a) ($p/p_c = 1·17, 1·11, 1·07, 1·04$) and figure 2($c$) ($p/p_c = 1·06, 1·04, 1·02$). The results for random percolation are reproduced for comparison in figure 2(b) ($p/p_c = 1·09, 1·07, 1·05$).

The scaling hypothesis (see e.g. Stauffer 1978a) would require $b(p)$ to be proportional to $(p - p_c)^{1/2\sigma}$, or taking the same value for σ in all three cases ($\sigma = \frac{7}{18}$) to $(p - p_c)^{9/7}$. The data can be well fitted by such a formula provided that we choose a value of p_c lower than that of the previous section, i.e. (a) 0·558, (b) 0·589, (c) 0·637. The finite-size effect does not enter in the same way as in the previous section, and, if we take random percolation as a standard, the true value for an infinite system is close to the average of the two sets of values given previously, i.e. (a) 0·563, (b) 0·593, (c) 0·639.

In relation to data for $p < p_c$, we have found it more convenient to try to fit the conjectured form of complete distribution

$$z(n, p)/z(n, p_c) \sim \exp(a(p)n^{\sigma} - d(p)n) \tag{4}$$

rather than just the exponential decay. Taking the same value of σ, the resultant fit to

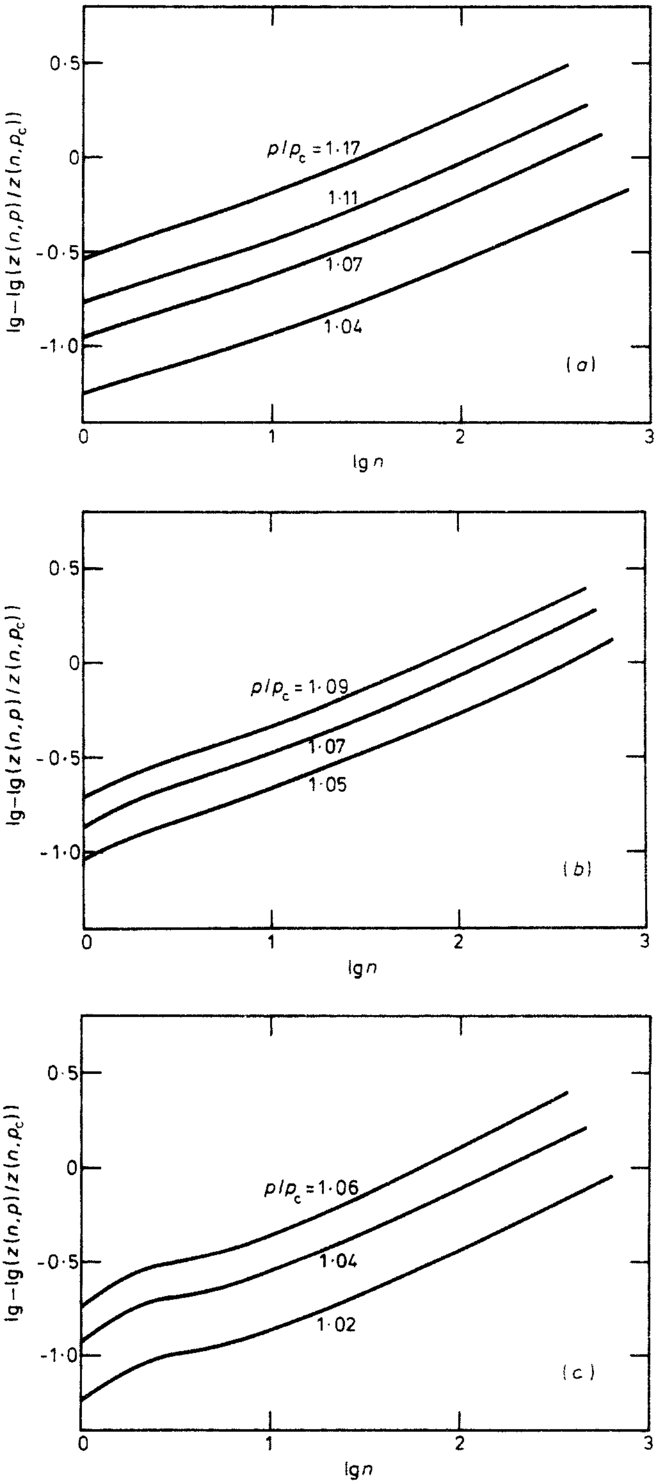

Figure 2. Asymptotic decay of clusters for $p > p_c$, with $z(n, p)$ representing the number of n-clusters at concentration p.

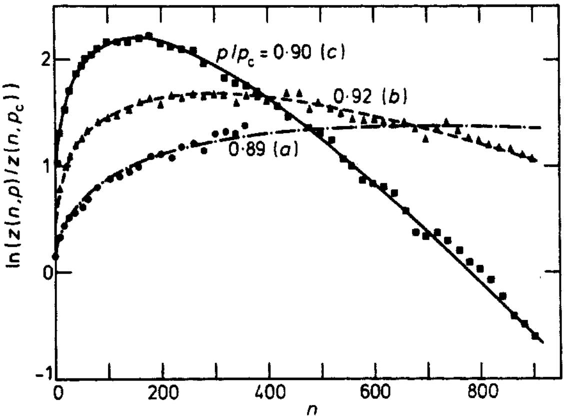

Figure 3. Distribution of n-clusters for $p < p_c$, with $z(n, p)/z(n, p_c) = \exp(a(p)n^{\sigma} - d(p)n)$, $\sigma = \frac{7}{18}$.

the data is shown in figure 3 (the division by $z(n, p_c)$ helps to remove the odd–even oscillations for small n). For random percolation a similar fit to the data has recently been given in the comprehensive study by Leath and Reich (1978).

Scaling theory now suggests that $a(p)$ should be proportional to $p - p_c$ and $d(p)$ to $(p - p_c)^{1/\sigma}$. If we fit p_c from this formula, we obtain different and somewhat larger values than those in the previous section, but they are less well defined since the data are more sparse; we do not think that too much significance should be attached to these deviations. To avoid suggesting excessive accuracy we have taken the following values of p_c for the calculations involved in the rest of this paper: (*a*) 0·56, (*b*) 0·59, (*c*) 0·64. We think that these should be within 1% of the true critical concentrations.

Our value (*a*) differs significantly from that of 0·544 obtained by Odagaki *et al* (1975). These authors give no estimate of their expected error and do not take account of the finite-size effect. We think that the method they use to estimate critical concentration is insensitive, and that the values they quote for large T represent too rapid a change near $1/T = 0$. The pattern of behaviour indicated by Kikuchi (1970) in his approximate treatment of the problem,

$$p_c = (q-1)/(q-1)^2 - 4(q-1)^2[1 - \exp(4J/kT)] \tag{5}$$

for a lattice of coordination number q seems to provide a reasonable qualitative picture of the dependence of p_c on T, but the method he used is too crude to give numerical results of sufficient accuracy to compare with our own.

Attention should be drawn to a number of features of the cluster-size distribution curves in figure 3. They all have the same characteristic shape (described by Stauffer 1978a), rising to a maximum and then decaying exponentially. However, the actual value of the maximum differs in the three cases—(*a*) 4·0, (*b*) 5·4, (*c*) 9·1— and these differences seem well beyond any expected margin of error. This means that the curves cannot be scaled, and that it is not possible to find a universal scaling function which will fit all three sets of data.

Our estimate of 5·4 for the maximum in the case of random percolation differs somewhat from the value of 4·8 given recently by Stauffer (1978c). We have found it better to use data removed from p_c to estimate this maximum, since near p_c the maximum occurs in the large-cluster region where statistical data are not too good.

4. Cyclomatic number and compactness of clusters

The cyclomatic number c of clusters is defined by

$$c(n, l) = l - n + 1,$$

where n is the number of points and l the number of lines in the cluster. $c(n, l)$ represents the number of independent cycles and provides a measure of its compactness. For trees $c = 0$, and small values of c correspond to ramified clusters.

In figure 4 we have plotted $\bar{c}(n)$, the statistical average over different l for a given n, as a function of n for various values of p/p_c. For the ferromagnetic and random cases (figures 4(a) and (b)) the behaviour is similar to that of the ferromagnetic Ising model as a function of temperature. The curves do not manifest much curvature and rapidly approach their asymptotic linear value. The limiting slope for large n is a measure of the coefficient of compactness

$$\lambda = \lim_{n\to\infty} (\mathrm{d}\bar{c}/\mathrm{d}n). \tag{6}$$

However, there is a marked difference of behaviour in the antiferromagnetic case (figure 4(c)). The curves start with a relatively small slope, and a quite rapid change in slope occurs when a particular size n_0 is reached. The value of n_0 depends on the value of p. For small p it is quite small, but as p approaches p_c it becomes larger and larger until it disappears. This 'size effect' seems to be related to the ease with which the cyclomatic number can be increased by overturning spins in groups which have antiferromagnetic ordering.

The coefficient of compactness, λ, is plotted in figure 5. Again the pattern of behaviour is similar in the ferromagnetic and random cases (figures 5(a) and (b)), although the numerical values are significantly larger in the former case. As one might reasonably expect, the effect of the correlation is to produce more compact clusters.

But the behaviour in the antiferromagnetic case is again significantly different (figure 5(c)). The coefficient of compactness *decreases* up to the neighbourhood of p_c, and starts to increase only when an infinite cluster has formed. The ramification of the infinite cluster itself for a given p/p_c increases significantly as one goes from (a) to (c).

5. Average number of spins per cluster

In order to estimate how the average number of spins per cluster changes with increasing p, it is convenient first to calculate $\langle C\rangle_{\text{site}}$, the average number of clusters per site, defined by

$$\langle C\rangle_{\text{site}} = \sum z(n). \tag{7}$$

The behaviour shown in figure 6 follows a similar pattern of steady decrease in all three cases. As one would expect, there is a larger number of small clusters in the antiferromagnetic case, whereas the ferromagnetic interaction induces the smaller clusters to coagulate.

If the number of spins per cluster is defined by

$$\langle n\rangle_{\text{cluster}} = \frac{\text{average number of spins}}{\text{average number of clusters}} = \frac{\Sigma nz\,(n)}{\Sigma z\,(n)}, \tag{8}$$

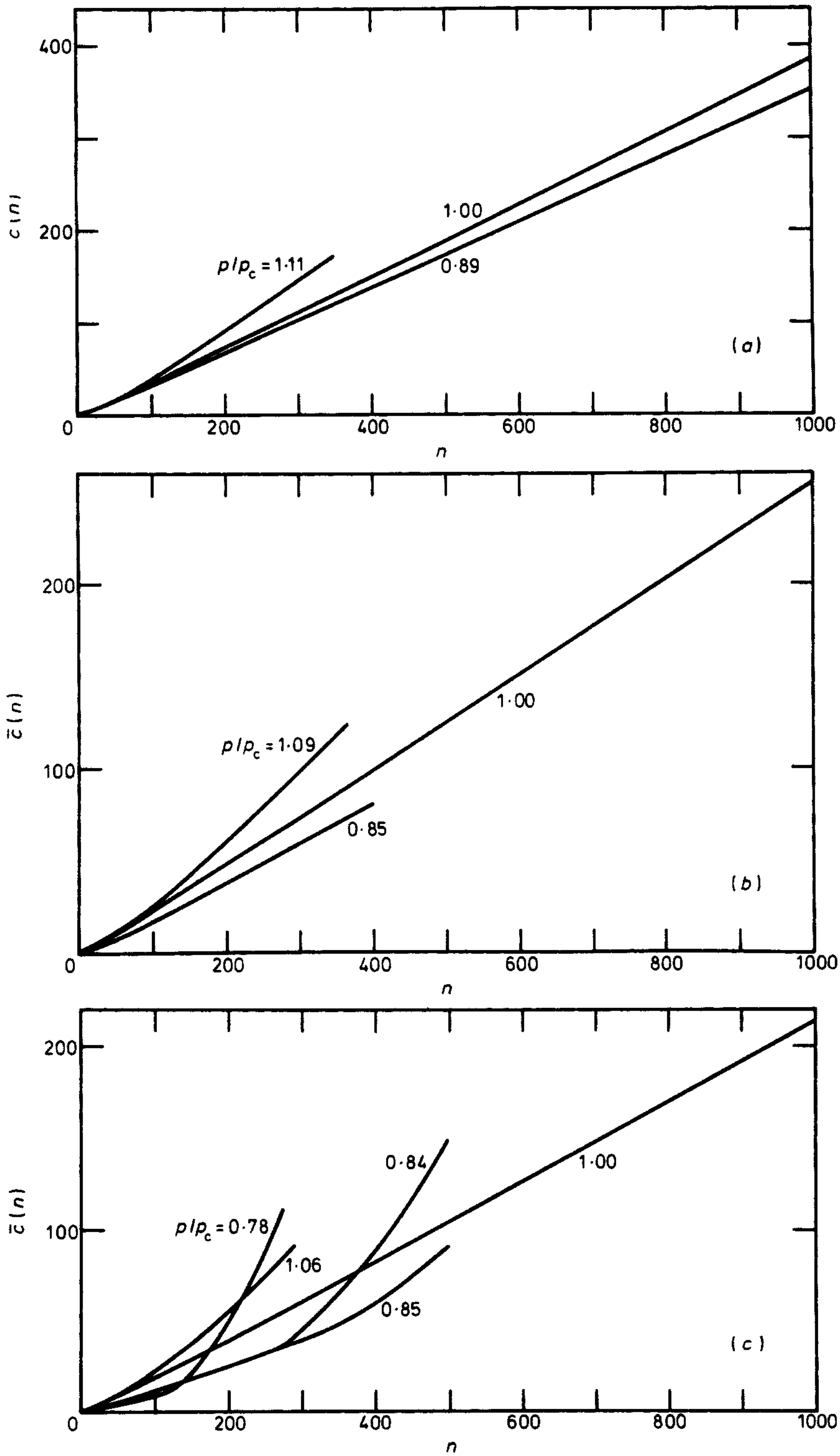

Figure 4. Average cyclomatic number against n for various p/p_c, with $c(n, l)$ representing the cyclomatic number of an n-cluster with l links, and $\bar{c}(n)$ the average over different l.

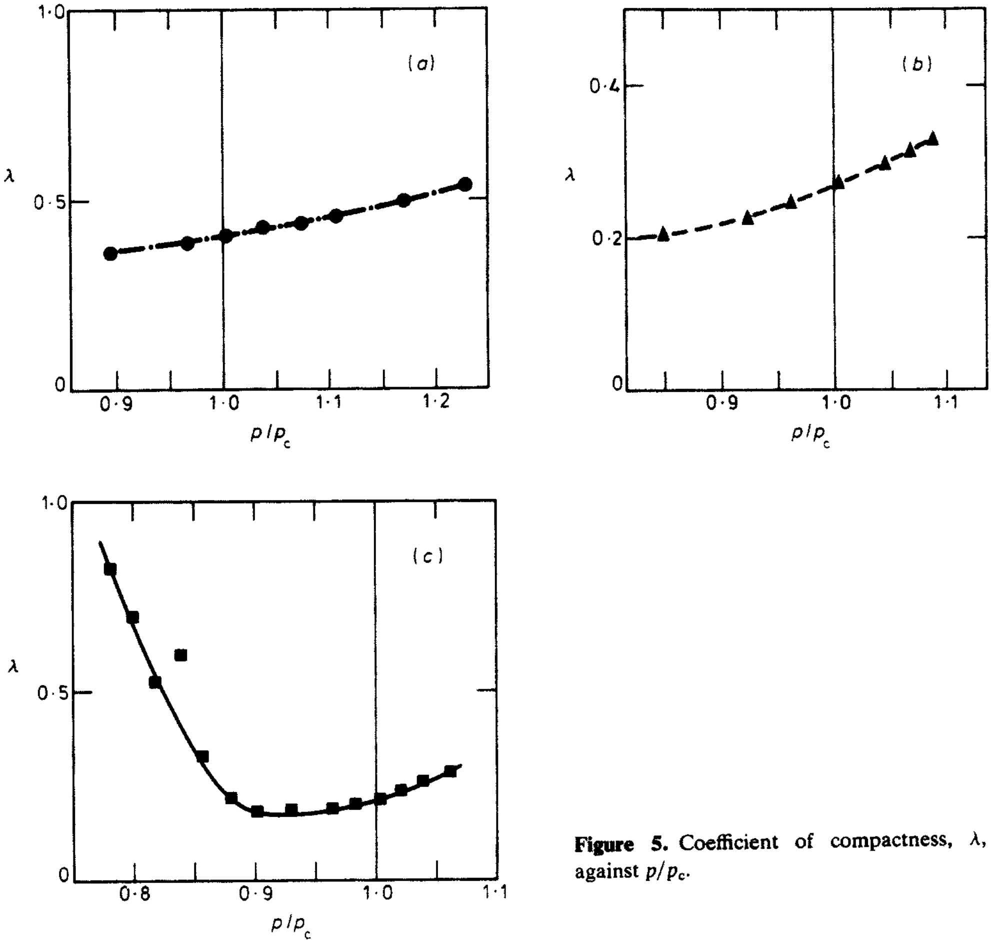

Figure 5. Coefficient of compactness, λ, against p/p_c.

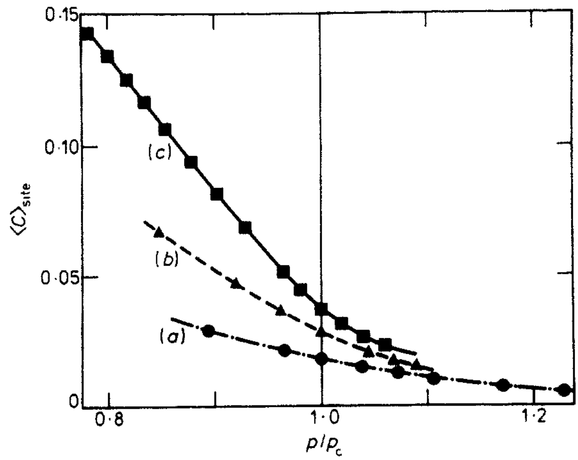

Figure 6. Average number of clusters per site, $\langle C\rangle_{\text{site}}$, against p/p_c.

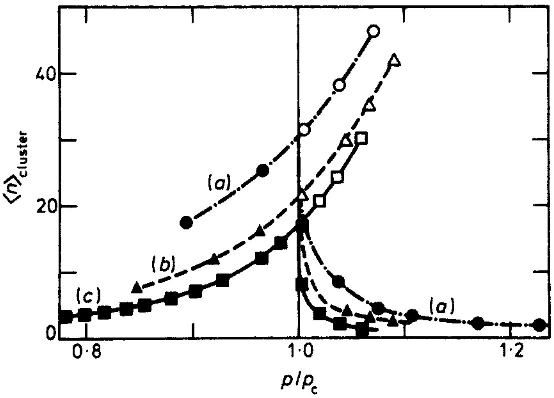

Figure 7. Average number of spins per cluster, $\langle n \rangle_{cluster}$, against p/p_c. The open circles, squares and triangles correspond to *all* clusters, including the spanning cluster.

the behaviour of $\langle n \rangle_{cluster}$ as a function of p/p_c is shown in figure 7. The general pattern is the same in all three cases and is similar to that of ferromagnetic Ising clusters as a function of T/T_c, but there is a steady decrease in numbers from (a) to (c) for a given p/p_c. At critical concentration the average numbers of spins per cluster are 33, 21 and 15 respectively.

Finally, we estimate the value of the average number of cycles per site, $\langle \bar{c} \rangle_{site}$, using the definition

$$\langle \bar{c} \rangle_{site} = \sum \bar{c}(n) z(n). \tag{9}$$

This quantity can be calculated exactly for the ferromagnetic Ising model at T_c (Temperley and Lieb 1971), and the Monte Carlo data fitted in well with the exact calculation. Unfortunately the corresponding calculation for random percolation applies to the *bond* rather than the *site* problem, and no direct comparison is therefore possible. The general pattern of behaviour is again similar to that of the ferromagnetic Ising model and is shown in figure 8.

6. Properties of the infinite cluster

For the infinite cluster $(p > p_c)$ Hankey (1978) has recently established a number of important results. It is possible to define a 'bulk entropy' per particle which is independent of lattice structure and is given by

$$S(p) = [-p \ln p - (1-p) \ln(1-p)]/p. \tag{10}$$

This is just the entropy per particle of a random mixture of particles and holes. Defining the total number of holes adjacent to particles of the cluster as s, and writing

$$s/n = a, \tag{11}$$

we have for the infinite cluster

$$a = (1-p)/p. \tag{12}$$

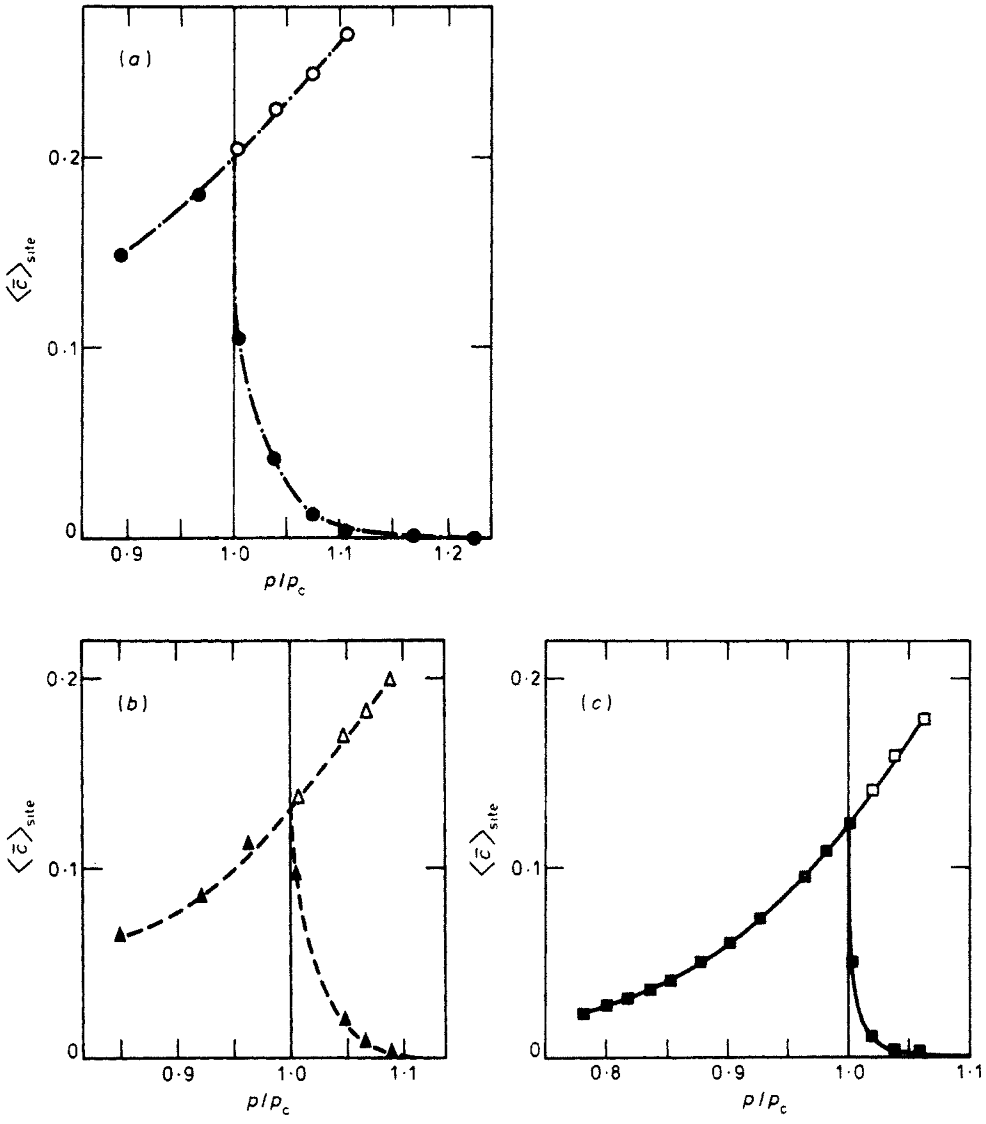

Figure 8. Average number of cycles per site, $\langle \bar{c} \rangle_{site}$, against p/p_c. The open circles correspond to *all* clusters, including the spanning cluster.

In terms of a the entropy in (10) can be written as

$$(1+a)\ln(1+a)-a\ln a. \tag{13}$$

Relation (12) was conjectured empirically from Monte Carlo data independently of Hankey's derivation (Stoll and Domb 1978). It is of interest to see what happens to s/n when correlations are taken into account, and values of s/n for the three cases considered are plotted in figure 9. The case of positive correlation is shown in figure 9(a), and it will be seen that the points all fall below the curve given by equation (12). Dr A Coniglio has informed us that he has established this result rigorously for all positive correlations.

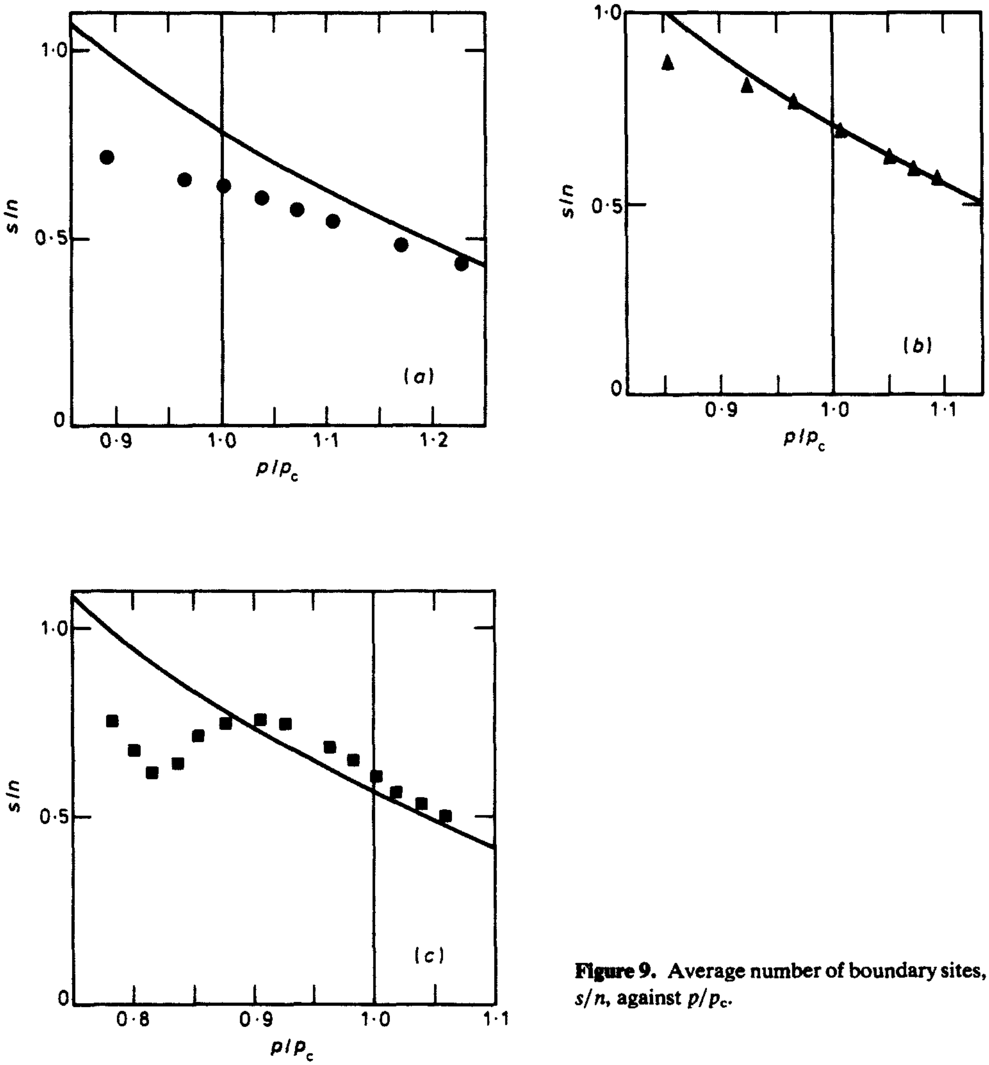

Figure 9. Average number of boundary sites, s/n, against p/p_c.

The case of random percolation is shown in figure 9(*b*). For $p<p_c$ there are only finite clusters and the points fall below the curve, as was shown by Hankey (and A Coniglio, private communication).

When the correlations are negative (figure 9(*c*)), however, the curve of s/n crosses the curve (12) at some value $p_0<p_c$, and for the infinite cluster s/n remains above the curve.

It is challenging to enquire whether any generalisations of formulae (10)–(13) are possible for the infinite cluster in correlated percolation. Clearly the entropy in (10) can be replaced by the corresponding entropy of the Ising model, ferromagnetic or antiferromagnetic. Formula (13), which relates to the number of lattice animals of given *a*, is a geometrical formula independent of correlation. Since (12) can be derived from (10) and (13) for random percolation, we think that it may be possible to calculate the appropriate generalisation for correlated percolation. We are currently undertaking detailed calculations.

7. Nature of percolation clusters

In a recent letter by Stauffer (1978b) evidence is provided for the existence of a density profile for a percolation cluster with $p > p_c$, whereas there is no such profile for $p < p_c$. These results are in accord with the discussion by Hankey (1978) to which we have referred.

Stauffer goes on to characterise clusters as droplet-like for $p > p_c$ and hydra-like when $p < p_c$. It is important to differentiate between our results, which are concerned with the local structure of percolation clusters, and Stauffer's, which deal with the long-range structure. We wish to draw attention to the fact that there is no dramatic change in compactness of clusters as p passes through p_c (as evidenced by the behaviour of λ in figure 5). To illustrate this further we have reproduced in figure 10 typical clusters arising from random percolation for $p/p_c = 0{\cdot}93$ and $p/p_c = 1{\cdot}13$, and there is little apparent difference in their structure.

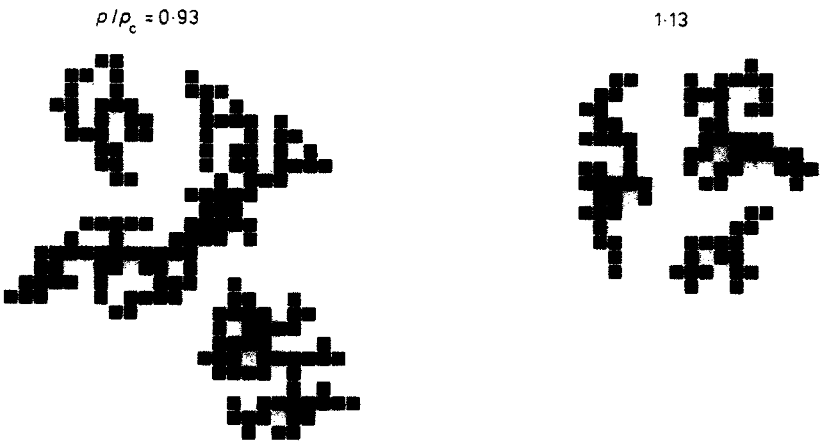

Figure 10. Typical clusters for random percolation.

Our results also show that it is possible for a percolation cluster with a particular local structure to belong to the $p < p_c$ region for random percolation and the $p > p_c$ region for percolation with negative correlations. Hence the local structure has little relevance in relation to the formation of an infinite cluster.

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References

Blease J, Essam J W and Peace C M 1978 *J. Phys. C: Solid St. Phys.* **11** 4009–16
Brooks J E and Domb C 1951 *Proc. R. Soc.* **207** 343–58
Coniglio A, Nappi C R, Peruggi F and Russo L 1977 *J. Phys. A: Math. Gen.* **10** 205–18
Domb C and Stoll E 1977 *J. Phys. A: Math. Gen.* **10** 1141–9

Domb C 1978 *Proc. 13th IUPAP Conf. on Statistical Physics, Ann. Isr. Phys. Soc.* vol 2 (Bristol: Adam Hilger) pp 61–74
Hankey A 1978 *J. Phys. A: Math. Gen.* **11** L49–55
Kikuchi R 1970 *J. Chem. Phys.* **53** 2713–8
Klein W, Stanley H E, Reynolds P J and Coniglio A 1978 *Phys. Rev. Lett.* **41** 1145–8
Kunz H and Souillard B 1978a *Phys. Rev. Lett.* **40** 133–5
—— 1978b *J. Stat. Phys.* **19** 77–106
Leath P L and Reich G R J 1978 *J. Phys. C: Solid St. Phys.* **11** 4017–36
Müller-Krumbhaar H and Stoll E 1976 *J. Chem. Phys.* **65** 4294–302
Odagaki T, Ogita N and Matsuda H 1975 *J. Phys. Soc. Japan* **39** 618–24
Reynolds P J, Stanley H E and Klein W 1978 *J. Phys. A: Math. Gen.* **11** L199–207
Schwartz M 1978 *Phys. Rev.* B **18** 2364–6
Stauffer D 1978a *J. Stat. Phys.* **18** 125–36
—— 1978b *Phys. Rev. Lett.* **41** 1333–6
—— 1978c *Preprint*
Stoll E and Domb C 1978 *J. Phys. A: Math. Gen.* **11** L57–61
Stoll E, Domb C and Schneider T 1978 *Proc. 13th IUPAP Conf. on Statistical Physics, Ann. Isr. Phys. Soc.* vol 2 (Bristol: Adam Hilger) pp 303–7
Sykes M F, Gaunt D S and Glen M 1976 *J. Phys. A: Math. Gen.* 725–30
Temperley H N V and Lieb E H 1971 *Proc. R. Soc.* A **322** 251–80