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Shape and size of clusters in the Ising model

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Abstract. The cyclomatic number of a cluster is introduced as a measure of its degree of compactness or ramification. Using Monte Carlo data for a two-dimensional Ising model, estimates are given of the average number of spins and the average number of cycles per cluster as a function of temperature. The results are related to the Whitney polynomial studied recently by Temperley and Lieb. An exact calculation by these authors at the critical temperature enables the pattern of behaviour in the critical region to be conjectured.

1. Introduction

The droplet model of condensation was first introduced in the 1930's, and served very effectively as a basis for explaining the phenomena of nucleation and metastability. It was always envisaged that the droplets were spherical in shape, and no attempt was made to take account of other possible shapes of droplet. In an attempt to construct a mimic partition function for a condensing gas, Fisher (1967) allowed for such changes of shape by including a surface entropy term. However, the droplets were still considered to be 'compact', i.e. the surface area s is proportional to n^{σ} for large n where σ is less than 1. One of the present authors (Domb 1976) recently suggested that ramified droplets of a tree-like or sponge-like character for which $\sigma = 1$ should be taken into account, and could play an important part in explaining behaviour in the critical region.

For percolation in random systems (see e.g. Essam 1972) there is good theoretical support for the suggestion that only ramified clusters play a significant role (Domb 1974a, Stauffer 1975). The problem of percolation in Ising systems (i.e. with interactions) has also recently received attention (Müller-Krumbhaar 1974, Coniglio 1975), and the correlation of shapes of clusters with critical behaviour is again of interest.

In a preliminary communication (Domb *et al* 1975) we took advantage of Monte Carlo data obtained with a two-dimensional one-spin-flip Ising model (Glauber model) to obtain statistical estimates of the parameter σ at different temperatures related to T_c. When T/T_c is sufficiently large the interaction can be ignored and the system is one of pure percolation. However the concentration p is equal to $\frac{1}{2}$, which is below the critical concentration for this lattice ($p = 0{\cdot}59$). For all temperatures above T_c the parameter σ was found to be effectively 1, which means that clusters are largely ramified. But even just below T_c typical clusters show evidence of ramification.

The aim of the present paper is to introduce a parameter which represents the degree of compactness or ramification, and hence to quantify the above concepts. We

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were greatly helped in the search for such a parameter by the discussions of Temperley and Lieb (1971) on the Whitney polynomial and its relationship to percolation and the Ising model. This is a polynomial in two variables q and x with attention focused on the cyclomatic numbers of different graphs (for a general introduction to graph theoretical terminology see Essam and Fisher 1970 or Domb 1974b). For $q=1$ the Whitney polynomial is related to the *bond* percolation problem, and for $q=2$ to the Ising problem. The relation between the Potts model (Potts 1952) and the percolation problem was dealt with in the pioneering work of Kasteleyen and Fortuin (1969) and Fortuin and Kasteleyn (1972) and the relation between the Potts model and the Whitney polynomial has been established by Baxter (1973). Temperley and Lieb calculated exactly in the form of a closed form integral the sum of the means of the number of cycles and disconnected components at the critical point for all q; because of a simple relationship between the two at the critical point each of these quantities is known exactly.

Following these ideas we have used the cyclomatic number as a measure of the degree of compactness of a cluster, and we have calculated a number of auxiliary parameters which indicate how the sizes and shapes of clusters change with temperature for the Ising model. Direct comparison with the exact results of Temperley and Lieb is possible only in the Ising case ($q=2$). Data which we have obtained for percolation correspond to *site* percolation, whereas the calculations of Temperley and Lieb are for *bond* percolation; nevertheless one can draw qualitative comparisons between the two problems.

2. Statistical parameters

Consider a cluster of n points and l bonds. The cyclomatic number $c(n, l)$ of the cluster is defined by

$$c(n, l) = l - n + 1, \tag{1}$$

and represents the number of independent cycles in the cluster. For a tree $c=0$, for a simple polygon $c=1$, and ramified clusters correspond to small c. The most compact cluster on a square (SQ) lattice is a square (it is a circle only for a continuum) for which

$$c_{\max} = (n^{1/2} - 1)^2. \tag{2}$$

We therefore define the coefficient of a compactness of a cluster, λ, as

$$\lambda = c/c_{\max} = c/(n^{1/2} - 1)^2. \tag{3}$$

This can go from 0 (completely ramified) to 1 (completely compact).

In analysing the statistics of clusters we must be careful to differentiate between 'per site' and 'per cluster' averages. The following definitions should clarify this point. Consider a lattice of N Ising spins a number of which are overturned; we are interested in the limit of large N. Let $z(n, N)$ be the number of clusters of n points, formed by the overturned spins. We then define $z(n)$, the probability per site of finding an n-cluster, as

$$z(n) = \lim_{N\to\infty} \frac{z(n, N)}{N}. \tag{4}$$

The probability that any given site belongs to an n-cluster of overturned spins is $nz(n)$.

Hence if there is no infinite cluster, the average number of clusters per site is given by

$$\langle C\rangle_{\text{site}} = \sum_n z(n), \tag{5}$$

and the average number of overturned spins per site by

$$\langle P\rangle_{\text{site}} = \sum_n nz(n). \tag{6}$$

The latter is closely related to the magnetization.

In percolation theory we are often interested in statistics in the presence of an infinite cluster; for example, for the Ising model in three dimensions infinite clusters occur for most lattices even when $T < T_c$ (Müller-Krumbhaar 1974). Equation (5) does not have to be modified since the addition of one infinite cluster to $z(n, N)$ makes negligible difference asymptotically as $N \to \infty$. However, equation (6) must be modified to take account of the infinite cluster,

$$\langle P\rangle_{\text{site}} = \sum_n nz(n) + P_\infty, \tag{7}$$

where P_∞ represents the probability per site of belonging to the infinite cluster; for a finite system we define a spanning cluster $S(N)$ as a cluster which extends to the boundaries of the system; if the number of spins belonging to the spanning cluster is $S(N)$ then

$$P_\infty = \lim_{N\to\infty} \frac{S(N)}{N}. \tag{8}$$

We also define the average number of cycles per site as

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

where $\bar{c}(n)$ is the average of $c(n, l)$ over l.

Passing now to cluster averages which characterise cluster sizes and shapes we define the average number of spins per cluster as

$$\langle n\rangle_{\text{cluster}} = \frac{\text{Average number of overturned spins per site}}{\text{Average number of clusters per site}} = \frac{\Sigma\, nz(n)}{\Sigma\, z(n)}. \tag{10}$$

Similarly the average number of cycles per cluster is given by

$$\langle c\rangle_{\text{cluster}} = \frac{\Sigma\, \bar{c}(n) z(n)}{\Sigma\, z(n)}. \tag{11}$$

3. Cluster statistics for the Ising model

In a previous communication (Domb *et al* 1975) we were largely concerned with the behaviour of the number of surface bonds s in a cluster, defined by

$$s = nQ - 2l, \tag{12}$$

where Q is the coordination number of the lattice. Using definition (1) we see that

$$c = n(\tfrac{1}{2}Q - 1) - \tfrac{1}{2}s + 1 \tag{13}$$

so that the $c(n)$ behaviour can be readily obtained from the Monte Carlo cluster surface data. In figure 1 we show the behaviour of $c(n)$ as a function of n for various values of T/T_c. Asymptotically the curves all become linear in n; since by equation (2) c_{max} is asymptotically equal to n, we find that for large clusters, the compactness coefficient is given by

$$\lambda = \lim_{n\to\infty} (\mathrm{d}\bar{c}/\mathrm{d}n). \tag{14}$$

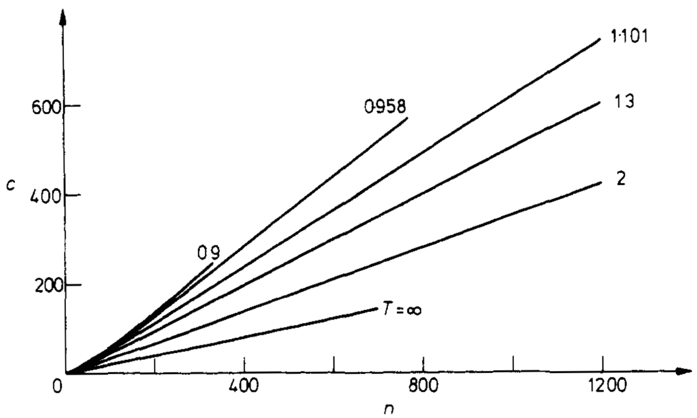

Figure 1. Cyclomatic number c as a function of n at different temperatures. For large n, c becomes linear, and the slope is a measure of the compactness of the cluster. Values of T/T_c are shown on the figure.

By this means the curve in figure 2 has been derived showing the variation of λ with (T_c/T). At $T=\infty$ corresponding to random percolation at 85% of critical concentration, λ is about 0·2. As T decreases, λ increases smoothly and steadily reaching a value of about 0·7 at T_c. Below T_c, λ increases quite rapidly to 1.

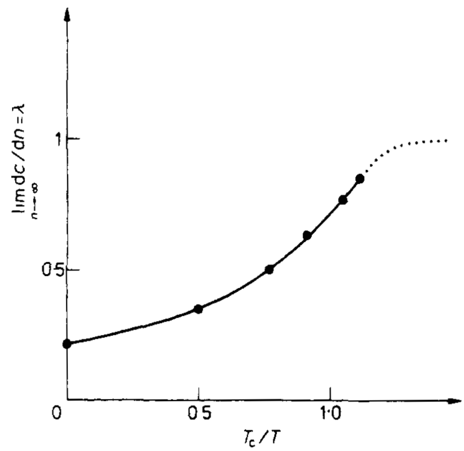

Figure 2. Coefficient of compactness λ of large clusters as a function of temperature.

At T_c the behaviour of $z(n)$ as a function of n is well known from investigations related to Fisher's droplet model

$$z(n) \approx A/n^{2+(1/\delta)}. \tag{15}$$

However, we shall see later that relation (15) can be understood from first principles independently of the assumptions of the droplet model. Because of the long tail of the distribution (15) all moments other than the first become infinite, and care is needed in performing averages. Fortunately in two dimensions we know exactly that $\delta = 15$ and hence the asymptotic contribution of large clusters can be assessed accurately.

Figure 3 shows the variation of the mean number of clusters per site $\langle C \rangle_{\text{site}}$ with temperature. The sudden increase as T goes below T_c seems surprising at first sight; but even though the total number of overturned spins drops very rapidly the fragmentation into small clusters is even more rapid, so that on balance $\langle C \rangle_{\text{site}}$ increases.

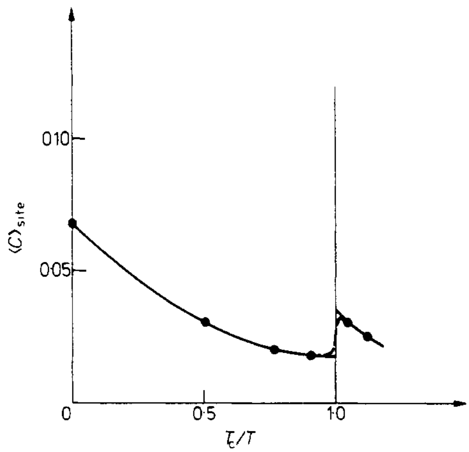

Figure 3. Mean number of clusters per site as a function of temperature. The broken curve represents conjectured behaviour in the critical region.

Turning now to statistics of individual clusters we first calculate the average number of spins per cluster $\langle n \rangle_{\text{cluster}}$ from equation (10). This is shown in figure 4 as a function of T_c/T; the number increases steadily as the temperature is lowered from about 7 at $T = \infty$ to 31 at $T = T_c$. Below T_c the number drops quickly and dramatically to 2 or 3.

We now calculate $\langle c \rangle_{\text{site}}$ from (10) which has a direct relationship to the Whitney polynomial, and show it graphically in figure 5. The maximum value as $T \to T_{c+}$ is about 0·31, whereas for large clusters the value given by the asymptotic slope of $d\bar{c}/dn$ is about 0·36; we thus find that smaller clusters reduce the average of $\langle c \rangle_{\text{site}}$ since they have relatively fewer cycles. The value calculated by Temperley and Lieb at $T = T_c$ is 0·128 (Temperley 1976) and we have marked it on the figure. It is this value which indicates a very rapid continuous variation near T_c, and that the slope at T_c is probably infinite. This calculation has led to the conjectured form of behaviour which we have indicated in the critical region.

We now calculate the average number of cycles per cluster from (11). The result is shown in figure 6, and its behaviour parallels that of $\langle n \rangle_{\text{cluster}}$.

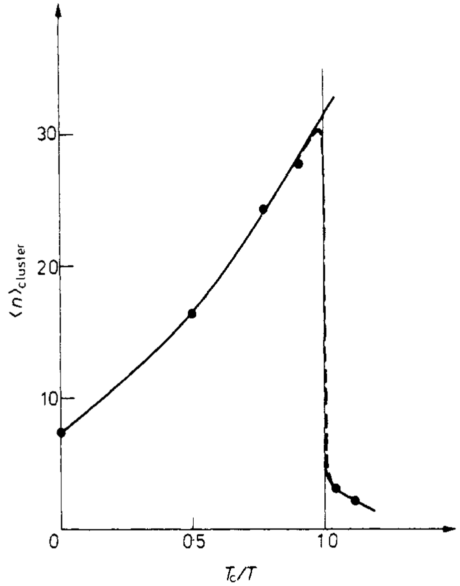

Figure 4. Mean number of spins per cluster as a function of temperature.

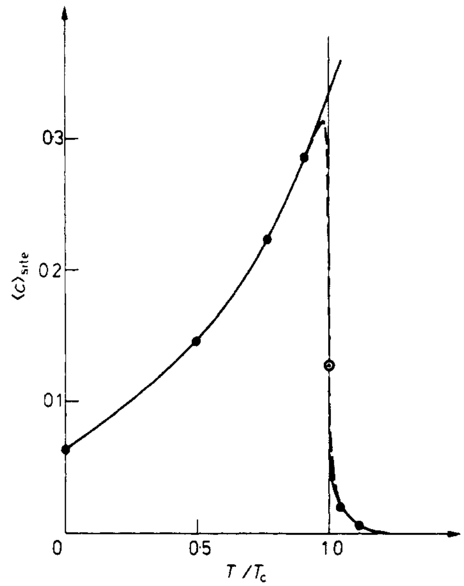

Figure 5. Mean number of cycles per site as a function of temperature. ⊙ represents the exact calculation of Temperley and Lieb at $T = T_c$.

4. Theoretical discussion

In a previous communication (Domb *et al* 1975) attention was drawn to the difference between physical clusters which represent real physical droplets and are of relevance to the Ising problem for $T < T_c$, and geometrical clusters which arise in the percolation

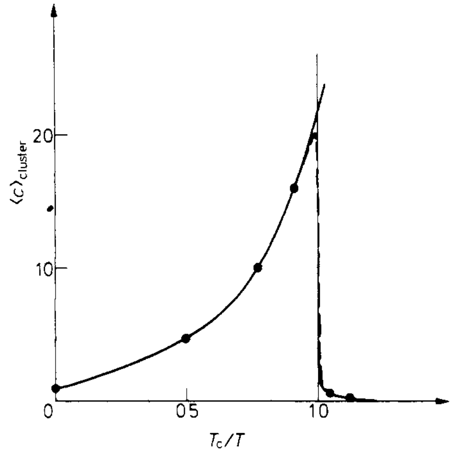

Figure 6. Mean number of cycles per cluster as a function of temperature.

problem and in the two-dimensional Ising problem for $T > T_c$. Some doubts were expressed as to whether the latter have any relevance to critical behaviour.

However the Whitney polynomial (Temperley and Lieb 1971, Essam 1971, Baxter 1973) which serves as a bridge between the percolation and Ising problems does focus attention on such geometrical clusters. It would be interesting to examine cluster statistics for the pure percolation problem to find whether they parallel the statistics of the Ising model described in the previous sections. The same Monte Carlo system can be used as previously to obtain percolation statistics, but the magnetic field must be varied at sufficiently high temperatures so as to change the concentration. A computer has been programmed to gather such data, and we hope to undertake an analysis in a subsequent communication. We also hope to deal with cluster statistics for finite values of T/T_c (>1) where both percolation and Ising interaction effects are present.

In regard to the Fisher droplet model we remarked that the parameters σ and τ did not have the significance which Fisher originally assigned to them. Nevertheless since scaling seems to hold for percolation as well as Ising systems (Essam and Gwilym 1971), one might expect that the distribution of clusters near the critical point will depend on only two parameters. We therefore look for an alternative interpretation of these parameters which can apply in both problems.

The critical point in both problems is characterised by a slow decay of large clusters of the form

$$z(n) \approx A/n^{2+\tau}. \tag{16}$$

This has been established recently for percolation by Monte Carlo analysis (Quinn *et al* 1976) and by exact enumeration (Gaunt and Sykes 1976), and estimates of τ have been obtained. For the Ising problem in a field H the magnetisation is given by

$$m = 1 - 2 \sum_{n=1}^{\infty} nz(n) \exp(-n\beta H). \tag{17}$$

If we assume that for sufficiently small H the distribution (16) is not significantly affected, we obtain from (17) the relation

$$m \sim H^{1/\tau}, \tag{18}$$

so that τ is simply related to the critical exponent δ. Since we know that $\delta = 15$ exactly in two dimensions, we also know that

$$\tau = \tfrac{1}{15}. \qquad (19)$$

It is more difficult to find a suitable interpretation for the second parameter (which we shall call σ^* to differentiate from Fisher's original σ). In the simple Fisher model the parameter σ was related to the surface exponent, and described the distribution of clusters away from T_c as

$$z(n) \sim n^{-\tau} \exp(-An^{\sigma}(T_c - T)). \qquad (20)$$

This formula cannot be correct for $T > T_c$ since it corresponds to an exponential increase with increasing n. In fact the model fails to give physically sensible results for $T > T_c$ (Gaunt and Baker 1970) since it ignores the volume exclusion of different droplets, and this plays a very significant role in the critical region (Domb 1976). Attempts have been made to take account of the volume exclusion empirically (e.g. Reatto 1970), but using scaling ideas only one could assume instead of (20) that

$$z(n) \sim n^{-\tau} F(n^{\sigma^*}(T_c - T)) \qquad (21)$$

with $F(u)$ an arbitrary scaling function. From the relation (17) in zero field below T_c one then finds that the spontaneous magnetisation is given by

$$m_0 \sim 1 - 2\int_1^{\infty} x^{1-\tau} F(x^{\sigma^*}(T_c - T))\, dx \qquad (22)$$

and hence that the exponent β is equal to $1/\sigma^*\delta$. Thus

$$\sigma^* = 1/\beta\delta$$

and is exactly $\tfrac{8}{15}$ in two dimensions.

Monte Carlo data for T near T_c in two dimensions fit reasonably well to a formula of type (21) (Müller-Krumbhaar and Stoll 1976). Unfortunately in three dimensions the problem is complicated by the presence of infinite percolating clusters below T_c (Müller-Krumbhaar 1974) and no such simple interpretation is possible. Binder (1976) has attempted to re-define the concept of cluster thereby introducing a new scaling exponent. His ideas are quite sophisticated and have been used by Müller-Krumbhaar and Stoll (1976) in an attempt to fit three-dimensional Monte Carlo cluster data. However no clear prescription has yet been given for dealing with the infinite percolating cluster.

Using similar ideas Stauffer (1976) has proposed differentiating between the internal and external surfaces of a cluster; he suggests that the internal surfaces give rise to the asymptotic value $\sigma = 1$ quoted in the introduction, whereas external surfaces are responsible for the true exponent σ^*. Applying the concept to percolating clusters Stauffer suggests (as does Binder) that ramification does not play a significant part in critical behaviour.

Whilst these interesting ideas offer a partial explanation of observed numerical data, they have some features which are untenable. For example, the value 0·4 of σ^* derived for percolation clusters is geometrically impossible (the same property of σ in three dimensions was already noted by Fisher (1967) in the original droplet model).

In our view the theory given by Stauffer is an oversimplification, and a rigid differentiation between internal and external surfaces is no longer helpful in the critical region. We also feel that the picture of the external surface of a percolation cluster near the critical concentration as a slightly imperfect sphere is inadequate. We suggest that further insight into the physical significance of σ^* may be obtained from studying the statistics of percolating clusters, and of the transition from the percolation to the Ising critical point. We hope to undertake such studies shortly.

5. Conclusions

The introduction of the cyclomatic number has enabled us to provide a numerical measure of the degree of compactness λ of a cluster. Using Monte Carlo data obtained in a one-spin-flip simulation of the Ising model we have computed the variation of λ with temperature, as well as various other statistical parameters connected with the distribution of clusters. Some of these parameters are related to the Whitney polynomial which has been the subject of recent exact investigations.

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