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LETTER TO THE EDITOR

The shapes of domains occurring in the droplet model of phase transitions

H N V Temperley†
Cavendish Laboratory, Madingley Road, Cambridge CB3 0HE, UK

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Abstract. A proper treatment of the droplet model of phase transitions needs some knowledge of the degree of compactness of random clusters. It is pointed out that some numerical evidence on this is already available for both site and bond clusters on the plane square lattice. The domains occurring in a Monte Carlo solution of the percolation problem are found to be highly ramified, those for the Ising and Potts problems less so.

Domb (1974, 1976) has recently examined the use of the droplet approximation for the study of dilute ferromagnets and of the analytic nature of phase transitions. He concluded that it is not enough to consider domains of 'conventional' droplet shape (in a two-dimensional model perimeter proportional to the square root of the area), but that one must also consider contributions to the free energy from 'ramified' domains or droplets (perimeter proportional to the area). He showed that certain difficulties in the original form of the droplet model disappear if this is done. Domb *et al* (1975) report the results of some Monte Carlo studies, which show that the relevant domains in the percolation problem are indeed ramified. Stauffer (1975) suggested that the consistent use of the droplet model may require fairly precise estimates of domain numbers of a given area and perimeter. He also suggested that the domains that dominate in the Onsager–Ising problem are not necessarily less ramified than those that dominate in the percolation problem.

In this letter, we shall point out that definite numerical information with a bearing on these matters is already available for both 'site' and 'bond' types of domain, and that more could be obtained with relatively little effort.

We now consider the enumeration of single connected domains of sites on the plane square lattice: 'site clusters'. This problem (the 'animal' problem) is still unsolved despite a great deal of work. Temperley (1956) showed that a restricted form of it, namely the enumeration of these connected domains without gaps in the columns (so that each column consists of a continuous line of sites, gaps in the rows being allowed) has a closed algebraic generating function

$$G=\frac{x^2z(1-z)^3}{1-(x^2+4)z+(x^2+6)z^2-(x^4-x^2+4)z^3+(1-x^2)z^4} \tag{1}$$

†On leave from Department of Applied Mathematics, University College, Swansea.

where the coefficient of $z^N x^{2L}$ is the number of such domains containing N sites and L columns. For N and L large, we have, as usual

$$N \propto z \frac{\partial}{\partial z}(\ln G) \qquad L \propto \tfrac{1}{2} x \frac{\partial}{\partial x}(\ln G) \tag{2}$$

and we obtain the expected value of L for a given N by putting $x = 1$ in (2). For N large and $x = 1$, the relevant root of the denominator is $z \sim 0{\cdot}316$ (not $\frac{1}{4}$ as wrongly stated in the paper).

Inserting these values, we conclude that for a large domain $N/L \approx 2{\cdot}4$, that is to say that the majority of large domains *are* ramified, the number of sites in each column being only about 2·4. This particular subset of domains may not have gaps in the columns. The completely general 'animal' or 'site cluster' may have gaps in the columns and internal 'lakes', so may be expected to be, on the average, even more ramified than this subset.

Temperley (1956) also considered the problem of enumerating domains of this restricted type by perimeter as well as by area. He obtained a set of difference equations for this more general problem but was only able to obtain the generating function in special cases. The difference equations should provide the desired information about the asymptotic distribution of number of domains as a function of perimeter and area.

We next consider bond clusters, and the percolation and Potts problems. We state the 'bond percolation problem' as follows. Select at random a fraction p of the bonds on the plane square lattice. What is the expected number of connected domains formed by the bonds? (We make the convention that an isolated site, to which none of the chosen bonds are incident, is counted as a domain.) We state the Potts problem thus: each point on the lattice can be coloured with one of q colours. There is an interaction energy $-J$ for each pair of neighbouring points coloured alike. (The interaction for unlike pairs is taken as zero.) In other words, we weight each configuration with a factor $\exp(J/kT)$ for each like pair of neighbours. We then ask 'how does the expected equilibrium number of like pairs of neighbours vary with J/kT?'

The solutions of these problems are at present known analytically only *at* the critical values of p or T, but we shall show that they give considerable information about the degree of ramification of 'bond clusters'. The critical cases are the cases of most physical interest and the ones that are the most difficult to handle by series expansion methods.

Temperley and Lieb (1971) and Baxter (1973) proved two distinct results for these problems. Firstly, they can both be transformed into particular cases of the problem of evaluating the Whitney–Tutte polynomial for the plane square lattice. This polynomial is defined as the following sum over all sub-graphs of the lattice, the sub-graphs being formed by removing bonds from the lattice but leaving all the sites. We define the polynomial in the form tabulated by Temperley and Lieb (1971) tables 4 and 6:

$$W(q, x) = \sum q^{\frac{1}{2}(C+S)} x^l \tag{3}$$

where, in each sub-graph, C is the number of connected clusters of bonds plus the number of isolated sites, S is its nullity or cyclomatic number and l is the total number of bonds. We can eliminate any one of these quantities from (3) by using Euler's relation $C = L - l + S$ where L is the total number of points in the lattice. For example, we can eliminate S and express (3) in the form

$$W(q, x) = q^{-\frac{1}{2}L} \sum q^C (xq^{\frac{1}{2}})^l \tag{4}$$

which is the form used by Baxter (1973), who showed that the Potts problem is equivalent to evaluating (4) for q integral and $q^{\frac{1}{2}}x = \exp(J/kT) - 1$. The percolation problem is equivalent to evaluating the expected value of C as a function of x for q in the neighbourhood of unity. (W is trivial if $q = 1$ what we want is $\bar{C} = \lim_{q\to 1} \partial(\ln W)/\partial q$.) The case $q = 2$ corresponds to the Onsager–Ising problem without magnetic field, and, for this case, W is simply related to Onsager's (1944) solution and can be obtained for *all* values of x. At critical $(x = 1)L^{-1}$ $\ln W$ is found to be $\ln(1+2^{-\frac{1}{2}}) + (2G/\pi)$ where G is Catalan's constant. This is in satisfactory agreement with the numerical values obtained by Cooper and tabulated by Temperley and Lieb (1971) in their table 6.

For other values of q (apart from 0 and 1) and equal horizontal and vertical interactions, W is known only *at* the critical value of x (which is unity for all q), and this is the function tabulated by Temperley and Lieb (1971). For all these critical cases, any bond is present with a probability $x/(1+x) = \frac{1}{2}$, the expected number of bonds is always half the total of $2L$ and Euler's relation then shows that the expected values of C and S are equal.

The Potts problem *at* critical thus reduces to a generalization of the bond percolation problem, each sub-graph being weighted with the power $\frac{1}{2}(C+S)$ of q. We could, for any value of x, solve it by a Monte Carlo method—choose bonds on the lattice at random, and record $(C+S)$ for a representative selection of sub-graphs of each size. (Of course, other ways are known by which the percolation, Ising and Potts problems can be reduced to the enumeration of graphs on the lattice.)

We now use the data in table 6 of Temperley and Lieb (1971) to show that, for the bond percolation problem, the average graph that would occur in such a Monte Carlo calculation is highly ramified even at critical. We shall also estimate how the degree of ramification changes when q increases up to 4. It is clear from (3) that, as q increases, we are giving greater weight to graphs with large C (that is, we are increasing the number of components of the average graph) and with large S (that is, we are increasing the number of circuits and therefore the compactness). (It is also clear from Euler's relationship that, for fixed numbers of sites and bonds, C and S must increase together.)

We first do the calculations for $q = 1$, i.e. $Z = 1$ in Temperley and Lieb's (1971) table 6. The expected number of connected components and isolated sites was found (table 5) to be

$$0{\cdot}09807L \tag{5}$$

and this value was shown to be consistent with an estimate from a 'perimeter' type series expansion. However, this includes isolated sites, the expected number of which is known exactly from the perimeter argument (Sykes and Essam 1964). The probability that a given site is isolated is precisely equal to the probability that all four lines incident on it are absent that is to say $1/2^4$ at critical. Subtracting this out from (5), we estimate that the number of clusters, each containing at least one line is

$$0{\cdot}03557L. \tag{6}$$

(We could go into even more detail if we wished, since the perimeter argument gives separately the numbers of clusters containing 1, 2, 3, ... lines.) The expected number of bonds at critical is L and these have to be distributed among the number of clusters of lines given by (6), so each such cluster contains, on average, about 28 lines. The expected number of independent circuits is also given by (5) and the fact that the square lattice is self-dual means that $L/16$ of these circuits are expected to be elementary squares on the lattice.

The specification of the typical connected cluster of bonds which would occur in a Monte Carlo treatment of the percolation problem: about 28 bonds, enclosing, on an average, about 1·7 single squares and one longer cycle.

It is, therefore, correct to describe the average bond cluster as highly ramified. 28 bonds can enclose as many as 10 independent cycles on the plane square lattice. Domb and Stoll (1976) found a figure of about 80% ramification for the percolation problem, which is in good agreement with the above figures. They used the cyclomatic number as a measure of compactness.

Since the expected numbers of components and circuits are the same, we can deduce from (5) that the expected number of circuits per line of the average graph is 0·09807 since the expected number of lines is L. (For a large and very compact graph on the square lattice, the number of circuits per line would approach 0·5.)

For the Ising model $q = 2$, and the relevant value of Z in table 6 of Temperley and Lieb (1971) is $2^{\frac{1}{4}}$. We estimate from the table $Z\partial \ln W/\partial Z \approx 0{\cdot}256L$ which means that the estimated number of bond clusters and isolated sites is approximately $0{\cdot}128L$. This is also the expected number of circuits. We cannot specify the typical cluster as precisely as in the case $q = 1$, because we can no longer calculate the expected number of isolated points. The perimeter argument of Sykes and Essam (1964) fails for $q \neq 1$. We can develop a series expansion by introducing an extra variable into (3) to count the number of isolated points and then differentiate logarithmically. The convergence of the expansion turns out to be poor and this is not surprising, because $x = 1$ at critical and this is almost certainly the limit of convergence.

We therefore content ourselves with recording the expected number of circuits per bond for the three cases $q = 1, 2, 4$ and these show clearly that, as expected from the arguments above, and in agreement with the Monte Carlo work of Domb and Stoll (1976), that the ramification decreases as q increases. The expected numbers of circuits per bond are:

$$0{\cdot}098\ (q = 1), \qquad 0{\cdot}128\ (q = 2), \qquad 0{\cdot}170\ (q = 4).$$

In conclusion, we have shown that definite numerical evidence about the expected shapes of both site and bond clusters already exists, and that more could be obtained with relatively little effort. This should help the further development of the droplet model of phase transitions. As pointed out by Domb (1976), study of this model is extremely important in view of the fact that it has proved very difficult to obtain even asymptotic information about the behaviour of large cluster integrals in the rigorous Mayer approach.

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