LETTER TO THE EDITOR

Lattice animals and percolation

C Domb

Wheatstone Physics Laboratory, King's College, Strand, London WC2R 2LS, UK

Abstract. A brief analysis is undertaken of the statistics of lattice animals (connected clusters) of n cells, and the results are applied to the site percolation problem. Recent proposals by Stauffer and Leath are examined, and an alternative interpretation is offered of the relation between percolation critical exponents and cluster statistics.

A *lattice animal* is a connected cluster formed by unit cells of a lattice with no cut-point. The alternative term *polyomino* as a generalization of domino was introduced by Golomb (1954). Several papers and articles have been written on the statistics of n cell animals (see e.g. Lunnon 1972 for references). It is usual to differentiate between *free* animals in which two clusters which can be derived from one another by a symmetry operation of the lattice are regarded as identical, and *fixed* animals in which they are regarded as different. In physical applications to lattice statistics we are usually concerned with fixed animals.

The most important mathematical result established so far concerns the total number $W(n)$ of fixed n-animals. Klarner (1967) showed that these n-animals are super-multiplicative, and hence deduced that asymptotically

$$W(n) \sim \lambda^n \phi(n) \qquad \left(\lim_{n \to \infty} (\phi(n))^{1/n} = 1 \right). \tag{1}$$

The most extensive exact enumerations of n-animals are due to Sykes and his collaborators in connection with the site percolation problem (see e.g. Sykes and Glen 1976). For this purpose it is important to divide $W(n)$ into sub-classes $g(n, s')$ with site perimeter s' (we use s' to distinguish from the broken-bond surface perimeter s which enters in the Ising problem, see e.g. Domb 1976). From this the *perimeter polynomials* can be formed,

$$D_n(p) = \sum_{s'} g(n, s')(1 - p)^{s'}, \tag{2}$$

and a great deal of useful information can be derived about percolation critical behaviour by manipulating appropriate series expansions (see e.g. Sykes *et al* 1976a, b, c).

Every animal on a lattice corresponds uniquely to a strong embedding of a connected graph on the dual lattice (for graph-theoretical terminology see Essam and Fisher 1970). Hence the total number of n-animals is the total number of strong-embeddings of connected graphs with n vertices. In other enumerative problems of this

kind a successful fit to numerical data has been achieved by assuming that $\phi(n)$ in (1) follows a power-law dependence on n,

$$\phi(n) \sim n^{-\tau}. \tag{3}$$

In a recent investigation of the behaviour of $W(n)$ for simple hypercubical lattices of dimension d, Gaunt *et al* (1976) estimated the value of τ for $d = 2$ to 6; however, the convergence of numerical data to the form (3) was slow, and this was attributed to the presence of a confluent singularity.

The asymptotic behaviour of the function $g(n, s')$ completely determines the cluster statistics in the neighbourhood of the critical percolation concentration p_c. If we define the tth moment of the distribution of n-clusters by

$$m_t(p) = \sum_{n, s'} n^t g(n, s') p^n (1 - p)^{s'} = \sum n^t \langle \nu_n \rangle \tag{4}$$

$m_0(p)$ or $\langle \nu_n \rangle$ represents the mean number of clusters, $m_1(p)$ the mean concentration (which is identically p for $p \leq p_c$), and $m_t(p)$ diverges for $t \geq 2$ with standard percolation critical exponents. Formula (4) is valid for *finite* clusters (i.e. without the percolating cluster) for $p > p_c$.

In a previous article (Domb 1974) a distinction was drawn between compact clusters for which $s' \sim n^\theta$ ($\theta < 1$), and ramified clusters for which $s' \sim n$, and it was argued that only ramified clusters play a significant part in critical percolation. Hence it is convenient to write

$$s'/n = a, \tag{5}$$

$$g(n, s') = h(n, a), \tag{6}$$

and to transform (4) into the form

$$m_t(p) = \sum_{n, a} n^t h(n, a) p^n (1 - p)^{an}. \tag{7}$$

We should emphasize that equation (7) is exact and the only information required to calculate $m_t(p)$ is the form of $h(n, a)$. There is no excluded volume effect to calculate which causes so much complexity in the corresponding Ising problem (Domb 1976).

For any given n, possible values of a are discrete and range from a minimum, corresponding to the most compact cluster, to a maximum equal to $(q - 2) + 2/n$, and corresponding to a stiff chain (where q is the coordination number of the lattice). For large n we can reasonably merge these into a continuous distribution $h(n, a) \to k(n, a) \, da$ and replace the sum in a by an integral:

$$m_t(p) \sim \sum_n n^t p^n \int_0^{(q-2)} (1 - p)^{an} k(n, a) \, da. \tag{8}$$

If (1) and (3) are valid it is plausible to postulate for $k(n, a)$ the form

$$k(n, a) \sim (\Lambda(a))^n n^{-\tau_a}, \tag{9}$$

where both $\Lambda(a)$ and τ_a might vary with a; except at critical points we might reasonably expect them to be analytic. It is easy to see using the method of steepest descents that if a_0 corresponds to the maximum of $\Lambda(a)$, $\Lambda'(a_0) = 0$, and

$$\lambda = \Lambda(a_0) \qquad \tau = \tau_{a_0} - \tfrac{1}{2}. \tag{10}$$

Exact solutions are available for percolation problems for a variety of tree and cactus structures (Fisher and Essam 1961). The best known is the Bethe lattice for which

$$\ln \lambda = (q-1) \ln(q-1) - (q-2) \ln(q-2) \qquad \tau = \tfrac{5}{2}. \tag{11}$$

However, a has only a single value $(q-2)$, and $\lambda(a)$ is therefore a δ-function. A better analogy with lattice percolation is provided by the expanded cactus (figure 1) for which a can lie between $\tfrac{1}{3}$ and $\tfrac{1}{2}$. Using the solution of Fisher and Essam we readily find that

$$\ln \Lambda(a) = a[\ln 4 - (a^{-1}-2) \ln(a^{-1}-2) - (3-a^{-1}) \ln(3-a^{-1})] \qquad \tau_a = 3. \tag{12}$$
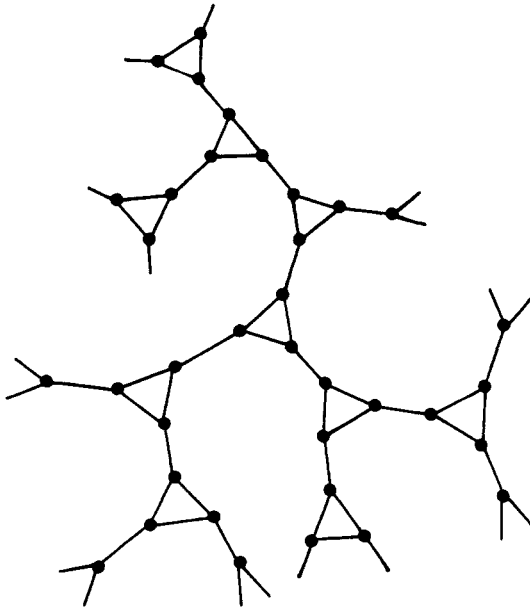

Figure 1. Expanded cactus.

When we come to calculate the integral in (8) we can use the method of steepest descents. For each p there is a unique a which satisfies

$$\Lambda'(a)/\Lambda(a) + \ln(1-p) = 0 \tag{13}$$

and which gives the dominant contribution to the integral. We then examine the sum in n as a function of p; replacing this by an integral there is a unique maximum given by

$$\frac{\partial}{\partial p}[\ln p + a \ln(1-p)] = 0 \qquad a = \frac{1-p}{p}, \tag{14}$$

which gives rise to critical behaviour. Relations (13) and (14) determine the critical values a_c, p_c and there is an additional relation for singular critical behaviour in (8),

$$p_c(1-p_c)^{a_c}\Lambda(a_c) = 1. \tag{15}$$

If this quantity is less than 1 all the moments in (8) are analytic and there is no singular behaviour; if it is greater than 1 even $m_0(p)$ diverges and this represents the number of clusters (per site) which must be finite.

Expanding in the neighbourhood of p_c we find that

$$m_0(p) \sim |p_c - p|^3 \qquad m_1(p) \sim |p_c - p|$$
$$m_2(p) \sim |p_c - p|^{-1} \qquad m_t(p) \sim |p_c - p|^{-2t+3}. \tag{16}$$

The exponents are thus the same as those obtained for a Bethe lattice, and we refer to them as classical exponents.

In considering percolation for real lattices we first investigate the form of critical behaviour if we take $\Lambda(a)$ to be analytic but allow τ_a to differ from the classical value. The discussion of the previous section remains valid, relations (13) and (14) determine p_c and a_c as the coordinate of the maximum of the two variable function

$$n \ln p + a \ln(1-p) + \ln \Lambda(a), \tag{17}$$

and relation (15) must be satisfied at the critical point.

We may note incidentally that (14) arises from differentiation with respect to p, and is valid even if $\Lambda(a)$ is non-analytic at a_c. It is therefore worth subjecting this to numerical test; a particularly suitable lattice is the triangular lattice for which p_c is known exactly to be equal to $\frac{1}{2}$ (Sykes and Essam 1964). In figure 2 we have used the data of Sykes and Glen (1976) to calculate $\langle a \rangle$ as a function of n for n-animals at $p = \frac{1}{2}$. It will be seen that successive values converge smoothly to

$$a_c = 1 = (1 - p_c)/p_c. \tag{18}$$

If we now examine the behaviour near $p = p_c$, we find instead of (16) that

$$m_0(p) \sim |p_c - p|^{2\tau_c - 3} \qquad m_1(p) \sim |p_c - p|^{2\tau_c - 5}$$
$$m_2(p) \sim |p_c - p|^{2\tau_c - 7} \qquad m_t(p) \sim |p_c - p|^{2\tau_c - 2t - 3}. \tag{19}$$

In standard exponent terminology

$$\Delta = 2 \tag{20}$$

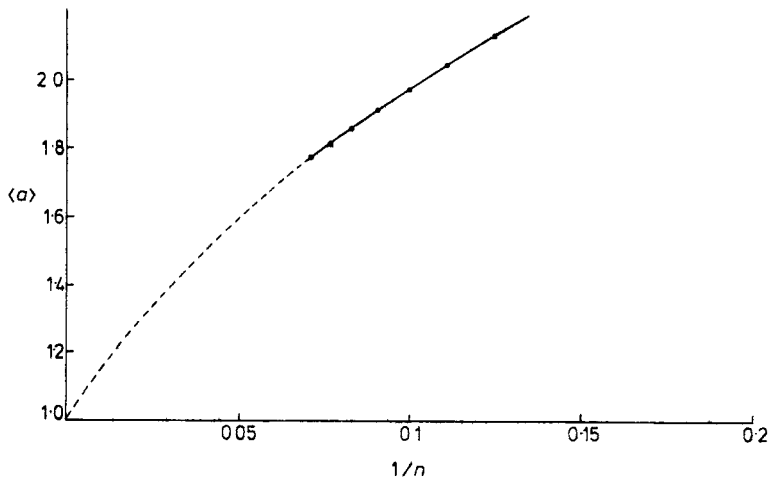and critical exponents depend only on one free parameter $\tau_c \ (= \tau_{a_c})$.

Figure 2. $\langle a \rangle$ at critical percolation density for clusters of size n. Test of $a = (1 - p_c)/p_c$ for site percolation, triangular lattice $(p_c = \frac{1}{2})$.

This suggestion was put forward previously by the present author (Domb 1974) and agreement with numerical data is not unreasonable when $d \geq 3$. However, Stauffer (1975a) pointed out that there is a clear disagreement with numerical data when $d = 2$, and he suggested the following modification in order to introduce a second parameter σ and parallel Fisher's Ising droplet model (Fisher 1967). Assume that

$$s' = an + An^{\sigma}, \tag{21}$$

and

$$\langle \nu_n \rangle \sim \sum_a p^n (1-p)^{an} \Lambda(a)^n \mu(a)^{An^{\sigma}} (1-p)^{An^{\sigma}} n^{-\tau_c} \tag{22}$$

where $\Lambda(a)$ is chosen as above, and $\mu(a)$ is chosen to satisfy

$$\mu(a_c)(1 - p_c) = 1. \tag{23}$$

Near $p = p_c$ the dominant behaviour in (22) is given by

$$\langle \nu_n \rangle \sim n^{-\tau_c} \exp Bn^{\sigma} \qquad B \sim (p_c - p), \tag{24}$$

and critical behaviour parallels that of the Ising droplet model; hence

$$\Delta = 1/\sigma, \tag{25}$$

and as long as $\sigma < \frac{1}{2}$ we can secure agreement with numerical data.

In a subsequent paper (Stauffer 1975b) Monte Carlo data were analysed and found in reasonable agreement with this modification.

However, if we examine this suggestion more closely a number of difficulties appear. Firstly in regard to the interpretation of the parameter σ, Stauffer suggested that it represents the 'surface' contribution to the cluster; but this is geometrically impossible since $\sigma < \frac{1}{2}$. In the Ising droplet model it is possible to argue (Fisher 1971) that σ is an 'effective exponent' which takes account of excluded volume effects; but there are no excluded volume effects in percolation clusters, the exclusion being completely taken into account by the $(1-p)^{s'}$ factor in (4).

Again the suggested form (24) gives the result (25) only when $p > p_c$ (paralleling $T < T_c$ in the Fisher model). For $p < p_c$ we must introduce the decay term

$$\langle \nu_n \rangle \sim n^{-\tau} \exp[n^{\sigma}(p_c - p) - n(p_c - p)^2], \tag{26}$$

and critical exponents correspond to the maximum of the exponent in (26) as a function of n. Instead of (25) we now find

$$\Delta = 1/(1-\sigma), \tag{27}$$

and the symmetry between $p > p_c$ and $p < p_c$ is destroyed.

It is well known of course that the Fisher droplet model is only satisfactory for $T < T_c$ (see e.g. Domb 1973). Attempts to adapt it to $T > T_c$ (e.g. Reatto and Rastelli 1972) are based on approximations to the excluded volume which, as mentioned above, does not arise in percolation clusters. Hence the attempt by Stauffer (1975b) to use the formula of Reatto and Rastelli can be regarded as only empirical.

More recently Leath (1976) has attempted to fit the function $g(n, s')$ from Monte Carlo data. He suggested that the dependence on a near a_c is of the form

$$\Lambda(a)^n n^{-\tau_c} \exp -Dn^{2\phi}[a - a_c - (E/n^{\psi})]^2 \tag{28}$$

where

$$\ln \Lambda(a) = -a \ln a + (a+1)\ln(a+1). \tag{29}$$

The choice of (29) was motivated by theoretical considerations of fractional dimensions. The exponent ϕ plays the same role as σ in Stauffer's formula (22), and the exponent ψ is dismissed as giving rise to lower order terms. Some details of the derivation have been criticized in a recent preprint by Stauffer (1976) concerning the distribution of cluster size and perimeter for two-dimensional percolation.

A more serious criticism of assumption (29) is that it fails to provide a unique a_c, p_c from equations (13) and (14) since both of these equations give rise to the same relation (14); likewise relation (15) is satisfied for all a, p.

However, the Monte Carlo data to which Leath fitted his formula are presumably reliable, and we should like to suggest the following alternative interpretation of his results; the exponent 2ϕ should really be 1, the true $\Lambda(a)$ being given by

$$\ln \Lambda(a) = -a \ln a + (a+1)\ln(a+1) - D(a-a_c)^2. \tag{30}$$

(Leath's actual estimate for 2ϕ was $0\cdot80\pm0\cdot08$.) The important new feature in Leath's formula would then be the shift term E/n^ψ. This feature is present in exact enumerations, as shown by figure 3, in which the histogram plots of the data of Sykes and Glen for the simple quadratic lattice with $n = 10$ and $n = 17$ have been smoothed to give continuous curves.
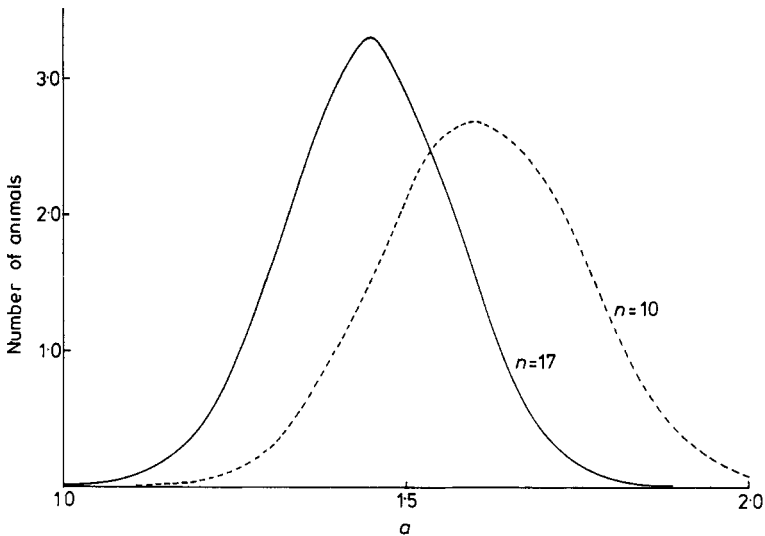

Figure 3. Distribution of animals on the simple quadratic lattice. $a = $ surface sites/bulk sites.

The origin of this shift lies in the compactness of the clusters. When clusters are grouped according to the value of a, true ramification is reached only for sufficiently large n; for example a completely compact square cluster of 16 spins will be included in the $a = 1$ group.

If we recalculate the behaviour in the critical region with this modification, we will be led to a formula similar to Stauffer's in (28) with the second exponent ψ paralleling the second exponent σ.

If we now return to our original postulate (9) and try to take account of the n-shift of the maximum, we might replace it by

$$k(n, a) \sim [\Lambda(a) - (\mu(a)/n^\theta)]^n n^{-\tau_a}. \tag{31}$$

This means that for the total number of n-animals, formula (3) must be replaced by

$$\phi(n) \sim n^{-\tau} \exp - Fn^{1-\theta}. \tag{32}$$

The exponential factor may then explain the slow convergence observed by Gaunt *et al* (1976).

Since the distribution of clusters at the critical concentration is well established as being of the form $n^{-\tau_c}$ (Quinn *et al* 1976, Gaunt and Sykes 1976) we must assume that

$$\mu(a_c) = 0. \tag{33}$$

We are then led to a result equivalent to that of Leath.

However, the difficulty of the violation of scaling discussed in § 5 is not resolved. So far no convincing argument has been given for scaling in percolation processes besides the analogy with critical behaviour in Ising and Heisenberg systems. Perhaps it is worth examining the numerical data again more critically.

If scaling is to be preserved the most obvious fault to be remedied in the above treatment is that of analyticity in $\Lambda(a)$ at a_c. If instead of (28) we take a dependence of the form

$$\Lambda(a)^n \dot{n}^{-\tau_c} \exp -n|a - a_c - (E/n^\psi)|^\chi, \tag{34}$$

by suitably relating χ to ψ it is possible to restore scaling. But before pursuing such a postulate further we think it advisable to have more detailed numerical data and (if possible) better theoretical information about $k(n, a)$.

References

Domb C 1973 *J. Phys. C: Solid St. Phys.* **6** 39–42
—— 1974 *J. Phys. C: Solid St. Phys.* **7** 2677–80
—— 1976 *J. Phys. A: Math. Gen.* **9** 283–99
Essam J W and Fisher M E 1970 *Rev. Mod. Phys.* **42** 271–88
Fisher M E 1967 *Physics* **3** 255–83
—— 1971 *Critical Phenomena—Proc. Int. School Phys. Enrico Fermi* vol. 51 ed. M S Green (New York: Academic Press) p 52
Fisher M E and Essam J W 1961 *J. Math. Phys.* **2** 609–19
Gaunt D S and Sykes M F 1976 *J. Phys. A: Math. Gen.* **9** 1109–16
Gaunt D S, Sykes M F and Ruskin H 1976 *J. Phys. A: Math. Gen.* **9** 1899–911
Golomb S 1954 *Am. Math. Monthly* **61** 672–82
Klarner D A 1967 *Can. J. Math.* **19** 851–63
Leath P L 1976 *Phys. Rev. Lett.* **36** 921–4
Lunnon W F 1972 *Graph Theory and Computing* ed. R Read (New York and London: Academic Press) pp 87–108
Quinn G D, Bishop G H and Harrison R J 1976 *J. Phys. A: Math. Gen.* **9** L9–14
Reatto L and Rastelli E 1972 *J. Phys. C: Solid St. Phys.* **5** 2785–804
Stauffer D 1975a *J. Phys. C: Solid St. Phys.* **8** L172–7

—— 1975b *Phys. Rev. Lett.* **35** 394–7

—— 1976 *Preprint*

Sykes M F and Essam J W 1964 *J. Math. Phys.* **5** 117–27

Sykes M F and Glen M 1976 *J. Phys. A: Math. Gen.* **9** 87–95

Sykes M F, Gaunt D S and Glen M 1976a *J. Phys. A: Math. Gen.* **9** 97–103

—— 1976b *J. Phys. A: Math. Gen.* **9** 715–24

—— 1976c *J. Phys. A: Math. Gen.* **9** 725–30