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LETTER TO THE EDITOR

The collapse of directed animals

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Abstract. Directed animals on a square lattice with attractive nearest-neighbour and next-nearest-neighbour interactions are considered. Using an equivalence between the collapse problem and the directed site bond percolation problem, the bulk free energy per site is calculated exactly in the collapsed phase. It shows no singularity as the transition is approached from the collapsed side. For the three-dimensional directed animals, bulk free energy per site in the collapsed phase is calculated exactly if the interaction weights are related by an algebraic equation.

Branched polymers in dilute solution are known to undergo a collapse transition for sufficiently strong attractive interaction between monomers. For small attraction strength (i.e. when the polymer is in a good solvent) the polymer structure is ramified and the mean size of a polymer with N monomers varies as N^{ν_a} where ν_a is believed to be same as the exponent characterising the size of random animals. For strong attraction (i.e. bad solvent) the polymer collapses to a compact globular shape of size N^{ν_c} where in d-dimensional space $\nu_c = 1/d$. At the transition point, the mean size varies as N^{ν_t}, where ν_t is, in general different from ν_a and ν_c and we have $\nu_a > \nu_t > \nu_c = 1/d$.

The structure of large-branched polymers below and above the collapse transition is the same as that of large percolation clusters above and below the critical percolation threshold. This suggests that the collapse transition may be in the same universality class as the percolation transition. A Flory-like argument by Family (1984) also suggests a similar conclusion. It is, however, not true in general. In two dimensions the exponent ν_t was determined numerically by Derrida and Herrman (1983) and their result is quite different from the exactly known percolation exponent $\nu_p = \frac{48}{91}$. In a Potts-model formulation of the branched polymer problem, Coniglio (1983) found that the percolation and collapse fixed points are distinct, the fixed point describing the collapse transition being more stable. This would imply that the collapse transition will be percolation-like only for very special values of coupling constants.

In this letter, we study the collapse transition of directed animals in two and three dimensions. The problem has been studied using Monte Carlo simulations by Lam and Duarte (1986) and Lam (1987). In this special case, we find that the collapse problem is equivalent to the directed percolation problem. In two dimensions, the bulk free energy per site is determined exactly in the collapsed phase. In three dimensions, the result can be generalised, provided the two-body and three-body coupling constants are related by an equation.

Consider first the two-dimensional directed animals, say on a square lattice. A directed animal is a connected cluster of N sites (including the origin) such that a site

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(i, j) belongs to the cluster only if it is the origin or if at least one of its predecessor sites $(i-1, j)$ and $(i, j-1)$ belongs to the cluster. Let $n_{i,j}$ be the occupation number of the site (i, j) (taking values 0 and 1). For any allowed animal configuration A, we define the energy

$$H(A) = -J_1 \sum_{i,j} n_{i,j}(n_{i+1,j} + n_{i,j+1}) - J_2 \sum_{i,j} n_{i,j} n_{i+1,j-1}. \tag{1}$$

Here J_1 is the attractive interaction strength between nearest-neighbour sites, and J_2 is the interaction between two sites having a common predecessor. The partition function is then defined to be

$$Z(J_1, J_2, N) = \sum_A \exp(-H(A)) \tag{2}$$

where the summation over A extends over all possible directed animal configurations of N sites. The free energy per site is $f(J_1, J_2)$ defined by taking the thermodynamic limit (Dickman and Schieve 1984, 1986)

$$f(J_1, J_2): \lim_{N\to\infty} -(\log Z(J_1, J_2, N))/N. \tag{3}$$

Consider now a directed site bond percolation process on this lattice defined as follows. Each bond is, independently of other bonds or sites, present with a probability p_B. We assume that the origin is 'unblocked' and occupied and each site other than the origin is 'unblocked' with a probability p_S (again independent of others). A site can be occupied only if it is unblocked *and* connected by an occupied bond to at least one of its occupied predecessors. The probability that the origin is connected to a finite cluster A of occupied sites in this process is

$$\text{Prob}(A) = p_S^{N-1} p_B^{n_1} (1 - q_B^2)^{n_2} (1 - p_B p_S)^{n_3} (q_S + p_S q_B^2)^{n_4} \tag{4}$$

where $n_1(n_2)$ is the number of occupied sites with one (two) occupied predecessors, $n_3(n_4)$ is the number of unoccupied (i.e. perimeter) sites with one (two) occupied precedessors and $q_B = 1 - p_B$ and $q_S = 1 - p_S$. These numbers n_1, n_2, n_3 and n_4 are not independent, and can be expressed in terms of three quantities N, N_1, N_2 where N_1 is the number of nearest-neighbour site pairs in the cluster A and N_2 is the number of diagonal pairs having a common predecessor. Simple geometry gives (figure 1)

$$n_1 = 2N - N_1 - 2 \tag{5a}$$

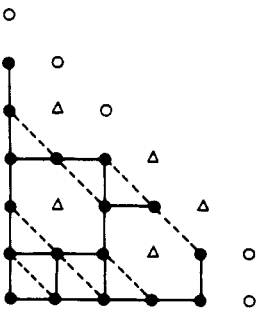

Figure 1. A directed site animal on the square lattice. The occupied sites are shown by full circles. Open circles and triangles denote perimeter sites with one and two occupied predecessors respectively. The nearest-neighbour bonds (full lines) have strength J_1 and diagonal bonds (broken lines) have strength J_2. In the cluster shown $N = 16$, $N_1 = 18$, $N_2 = 8$, $n_1 = 12$, $n_2 = 3$, $n_3 = 4$ and $n_4 = 5$.

$$n_2 = N_1 - N + 1 \tag{5b}$$

$$n_3 = N_1 - 2N_2 + 2 \tag{5c}$$

$$n_4 = N + N_2 - N_1 - 1. \tag{5d}$$

The thermodynamic weight of the cluster A under the Hamiltonian H is $\exp(N_1 J_1 + N_2 J_2)$, which is the same form as in equation (4). Thus the relative weights between different animal configurations of size N under the Hamiltonian H are exactly the same as in the directed site bond percolation process if we put

$$\exp(J_1) = (1+q_B)(1-p_B p_S)/(q_S + p_S q_B) \tag{6a}$$

$$\exp(J_2) = (q_S + p_S q_B^2)/(1-p_B p_S^2)^2. \tag{6b}$$

In the percolation problem, the probability that the cluster containing the origin has precisely N sites is obtained by summing equation (4) for all configurations A containing N sites. We thus get

$$\text{Prob}(|A| = N) = \frac{(1+q_B)(1-p_B p_S)^2}{p_B p_S (q_S + p_S q_B^2)} \left(\frac{p_S p_B (q_S + p_S q_B^2)}{(1+q_B)} \right)^N Z(J_1, J_2, N). \tag{7}$$

Taking logarithms, and the thermodynamic limit $N \to \infty$, we get

$$f(J_1, J_2) = \log\left(\frac{p_S p_B (q_S + p_S q_B^2)}{(1+q_B)} \right) + \lim_{N\to\infty} (1/N) \log \text{Prob}(|A| = N). \tag{8}$$

For p_B and p_S sufficiently large (above percolation threshold) it is known that the probability of large finite clusters of N sites decreases as $\exp(-N^{1-1/d})$ for N tending to infinity (Kunz and Suillard 1978, Stauffer 1979). The second term on the right-hand side of equation (8) is thus zero, and we get in the collapsed phase

$$f(J_1, J_2) = \log\left(\frac{p_S p_B (q_S + p_S q_B^2)}{1+q_B} \right) \tag{9}$$

where p_S and p_B can be determined in terms of J_1, J_2 from equation (6). The right-hand side of equation (9) is a smooth function of p_S and p_B, and remains so as p_S or p_B are decreased below the critical percolation threshold. Thus the bulk free energy per site $f(J_1, J_2)$ shows no singularity as the transition is approached from the collapsed phase side. The onset of the transition is signalled by the vanishing of the surface free energy term (the term proportional to $N^{1-1/d}$ in $\log Z$). The average density of occupied sites in the bulk equals $P_\infty(p_S, p_B)$, the probability that a randomly chosen site in the corresponding percolation problem belongs to the infinite cluster.

The variables p_S and p_B may be eliminated from equation (9), and the result expressed in terms of J_1 and J_2 explicitly. The explicit expression is rather messy, and is omitted here. It simplifies considerably in special cases.

(i) $J_2 = 0$. This case corresponds to a pure bond percolation process with $p_S = 1$, $q_B = (e^{J_1} - 1)^{-1}$ and we get

$$f(J_1, J_2 = 0) = \log(e^{J_1} - 2/(e^{J_1} - 1)^2). \tag{10}$$

The free energy is non-singular for all $\exp(J_1) > 2$. But the critical threshold for the bond percolation problems is known from numerical studies (Kinzel and Yeomans 1981) to be approximately $q_{BC} = 0.3553$, which corresponds to $\exp(J_{1C}) \simeq 3.814$. This agrees well with the Monte Carlo simulations of Lam and Duarte (1986).

Equation (10) may be expanded in powers of e^{-J_1}. The radius of convergence of the resulting series is clearly $\frac{1}{2}$, which is not equal to the critical value. This behaviour is quite unexpected (see, for example, Dickman and Schieve 1984).

(ii) $J_1 = 0$. This corresponds to a directed site percolation process with $p_B = 1$, $q_S = \exp(-J_2)$. The free energy per site is easily seen to be

$$f(J_1 = 0, J_2) = \log[e^{-J_2}(1 - e^{-J_2})] \tag{11}$$

which is again valued only for e^{-J_2} less than its critical value $e^{-J_{2c}}$.

The arguments given above can be easily generalised to three dimensions. Consider a directed animal on the cubic lattice with Hamiltonian given by

$$H = -J_2 N_2 - J_3 N_3 \tag{12}$$

where J_2 and J_3 are interaction strengths, and N_2 and N_3 are the number of sites having two and three occupied predecessors respectively. The thermodynamic weight of this animal in the partition function is $\exp(N_2 J_2 + N_3 J_3)$.

For a directed bond percolation process on this lattice having bond concentration p, it is easy to check that the probability of occurrence of a cluster of N sites having N_2 sites with two predecessors and N_3 sites with three predecessors is

$$q^3 (pq^2)^{N - N_2 - N_3 - 1} (q - q^3)^{N_2} (1 - q^3)^{N_3}. \tag{13}$$

The two problems are thus equivalent if

$$(1 + q)/q = e^{J_2} \tag{14a}$$

$$(1 + q + q^2)/q^2 = e^{J_3}. \tag{14b}$$

Eliminating q, we get the condition for the equivalence to hold is

$$e^{J_3} = e^{2J_2} - e^{J_2} + 1 \tag{15}$$

and the free energy per site in the collapsed phase is

$$f = \log(pq^2) = \log(e^{J_2} - 2/(e^{J_2} - 1)^3). \tag{16}$$

Equation (15) is a special case of the disorder condition or the cellular automation condition. For values of coupling constants satisfying this condition it is found that the partition function can be evaluated quite simply, and is an algebraic function of the Boltzmann weights. For a recent review, and earlier references on this topic, the reader is referred to a recent paper by Rujan (1987).

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