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Lattice statistics of branched polymers with specified topologies

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Abstract. We study the numbers of lattice animals with specified topologies. We prove that the growth constant for animals with c cycles and n_k vertices of degree k ($k = 3, \dots, 2d$), weakly embeddable in a d -dimensional hypercubic lattice, is equal to μ , the growth constant for self-avoiding walks. For some particular topologies we derive upper and lower bounds for the corresponding critical exponents and estimate the values of these exponents by deriving and analysing new exact enumeration data. We conjecture that our previous result for trees with b branches (that the exponent is $\gamma + b - 1$, where γ is the self-avoiding walk exponent) is also valid in the more general case in which the cyclomatic index (c) is non-zero; i.e. for $b \geq 1$, the exponent does not depend on c .

We show that our results are consistent with renormalisation group arguments that the universality class of branched polymers is independent of cycle and (non-zero) branching fugacities.

1. Introduction

Although the statistics of branched polymer molecules have been extensively studied since the pioneering paper of Zimm and Stockmayer (1949), it is only quite recently that excluded volume effects have been incorporated by modelling the polymer molecules as lattice animals (i.e. connected graphs weakly embeddable in a regular lattice). This model seems to have been first considered, in this context, by Lubensky and Isaacson (1979). For a general discussion of this problem, with many references, see Gaunt *et al* (1984).

The original renormalisation group calculations (Lubensky and Isaacson 1979, Family 1980) predicted that critical exponents would be independent of branching and cycle fugacities. This led to Monte Carlo and exact enumeration studies of trees (i.e. animals with no cycles) and this work showed that critical exponents were the same for trees and animals (Seitz and Klein 1981, Duarte and Ruskin 1981, Gaunt *et al* 1982). However, if the number of cycles is fixed, rather than the cycle fugacity, then the exponent characterising the number of c -animals depends on the cyclomatic index, c (Whittington *et al* 1983).

The effect of fixing the number of branch points in a tree has also been studied. In particular Lipson and Whittington (1983) have shown that the limiting entropy per

monomer is independent of the number of branch points, provided that the number of branch points does not go to infinity too rapidly, as the size of the tree increases. Gaunt *et al* (1984) have considered lattice trees with specified topologies and have investigated the dependence of the value of the critical exponent characterising the number of such trees on the number of branches.

In this paper we extend this type of treatment and consider connected graphs with a fixed, non-zero, number of cycles and a fixed number of branch points. In § 2 we show that, if $a(n, c; n_3, n_4, \dots, n_{2d})$ is the number of animals with n vertices, c cycles and n_i vertices of degree i ($i = 3, \dots, 2d$) weakly embeddable in a d -dimensional hypercubic lattice, then

$$\lim_{n \rightarrow \infty} n^{-1} \log a(n, c; n_3, \dots, n_{2d}) = \log \mu \quad (1.1)$$

where μ is the growth constant for self-avoiding walks. (The limit in (1.1) is taken with c, n_3, \dots, n_{2d} fixed.)

The set of numbers $\{c, n_3, \dots, n_{2d}\}$ does not uniquely define a topology. For instance, theta graphs and dumbbells (Sykes 1961) both have $c = 2, n_3 = 2, n_4 = \dots = n_{2d} = 0$. These graphs can be distinguished if we define the number (b) of branches as the number of cut edges in the homeomorphically reduced graph. This definition of the number of branches coincides with the definition previously used for the special case of trees (Gaunt *et al* 1984).

Guttmann and Whittington (1978) have investigated the value of the exponent for all the closed connected graphs with $c = 2$. They presented convincing numerical and non-numerical evidence that the exponent for dumbbells ($b = 1$) is identical to that (γ) for self-avoiding walks. Similar non-numerical arguments (based on a counting theorem) can be constructed which indicate that the exponent for tadpoles ($c = 1, b = 1$) is also equal to γ . This suggests that the value of the exponent is determined by the value of b (for $b \geq 1$) and not by the value of c , so that the conjecture of Gaunt *et al* (1984), that the exponent for trees with b branches is $\gamma + b - 1$, may apply to the more general case of a connected graph with b (≥ 1) branches and c cycles.

We investigate this extended conjecture using several techniques. In § 3 we describe several methods by which bounds on the critical exponents may be derived. We concentrate in particular on the numbers of twin-tailed, two-tailed and Y-tailed tadpoles (see figure 1). The first two each have $c = 1, b = 2$, though they differ in the numbers of vertices of degree three and four, and the two-tailed and Y-tailed tadpoles each have $c = 1, n_3 = 2$ but have $b = 2$ and 3, respectively. In § 4 we form numerical estimates of the critical exponents for these three topologies, by enumerating these graphs for small n for the triangular, square and simple cubic lattices, and analysing the resulting series. The results of §§ 3 and 4 are consistent with the above conjecture. We discuss the connection between these results and renormalisation group results in § 5. Our results are summarised and discussed in § 6.

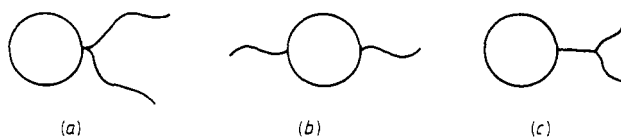


Figure 1. Twin-tailed (a), two-tailed (b) and Y-tailed (c) tadpoles.

2. Growth constants

In this section we shall prove that a graph having fixed cyclomatic index (c) and a fixed number (n_3) of vertices of degree 3, n_4 of degree 4, and so on up to degree $2d$, has a growth constant equal to μ , the growth constant for self-avoiding walks. Let this set of restricted animals be denoted by $A(n, c; n_3, \dots, n_{2d})$ where n is the total number of vertices in the graph, and define the cardinality (per lattice site) of this set to be $a(n, c; n_3, \dots, n_{2d})$. The work which follows concerns graphs weakly embeddable in a d -dimensional hypercubic lattice though extension to other lattices is possible. The vertices of such a lattice are the integer points in a d -dimensional Euclidean space with coordinates (x_1, x_2, \dots, x_d) . The edges of the lattice join vertices which differ by unity in a single coordinate.

Recently Lipson and Whittington (1983) have demonstrated that the growth constant for a restricted tree, where the number of branch points is fixed, is μ ; a similar approach will be used here. Thus the upper bound will be obtained by considering the number of connected graphs possible on $n^* = n_1 + n_3 + n_4 + \dots + n_{2d}$ labelled vertices, and a lower bound will be derived by relating $a(n, c; n_3, \dots, n_{2d})$ to the number of embeddings of a certain type of tree.

To derive a lower bound we relate the number of graphs with c cycles to the number with $c - 1$ cycles, thus arriving by recursion at the case of zero cycles (i.e. a restricted tree). The idea is to show that for every set $\{n, c; n_3, \dots, n_{2d}\}$ there exists a corresponding set $\{n', c = 0; n'_3, \dots, n'_{2d}\}$ such that by adding c cycles and adding $n_3 - n'_3, n_4 - n'_4, \dots, n_{2d} - n'_{2d}$ vertices of degree 3, 4, $\dots, 2d$ in a systematic and well defined manner, the restricted tree is converted to an animal having exactly c cycles, n_3 vertices of degree 3, and so on. To do this we require an algorithm for adding vertices of degree 3 and higher to create additional cycles.

We recall that Euler's relation for a connected graph having n vertices, e edges and c elementary cycles is

$$c = e - n + 1 \tag{2.1}$$

where

$$e = \frac{1}{2} \sum_{i=1}^{2d} i n_i \tag{2.2}$$

and hence

$$2c = 2 + \sum_{i=1}^{2d} (i - 2) n_i \tag{2.3}$$

We note that specifying n, c, n_3, \dots, n_{2d} determines n_1 and n_2 .

The graph under consideration consists of a set, S_0 , of vertices. To locate the top vertex first construct the subset $S_1 \subset S_0$ such that the coordinate x_1 of every vertex in S_1 has the maximum value over all vertices in S_0 . Then recursively construct $S_k \subset S_{k-1}$ such that the coordinate x_k of every vertex in S_k has the maximum value over all the vertices in S_{k-1} . Continue this process until the j th subset (S_j) has been constructed, where j is the smallest integer such that S_j has only one member. We call this vertex in S_j the *top vertex* v_t of S_0 . v_t is joined to one or more other vertices, the coordinates of each differing from those of v_t by unity in exactly one coordinate. The *top edge*, e_t , is that which joins v_t to the vertex differing from it in the coordinate of highest number; we call this vertex the *edge vertex*, v_e .

Suppose that we wish to add one or more cycles to this structure. We describe two constructions.

Construction 1. We can add $(i-2)/2$ cycles, converting a vertex of degree 2 to a vertex of degree i , where i is even and greater than 2, as follows. Let the top vertex of the graph be v_t with coordinates $(x_1^t, x_2^t, \dots, x_d^t)$. Define the unit vectors $\hat{u}_1 = (1, 0, 0, \dots, 0)$, $\hat{u}_2 = (0, 1, 0, \dots, 0)$, \dots , $\hat{u}_d = (0, 0, \dots, 1)$. Delete the top edge, adding the vertices $v_t' = v_t + \hat{u}_1$, $v_e' = v_e + \hat{u}_1$ and the edges $(v_t - v_t')$, $(v_e - v_e')$, $(v_t' - v_e')$. (If $v_e = v_t - \hat{u}_1$, as can occur if v_t is of unit degree, a minor gloss is necessary. In this case add the vertices $v_a = v_t + \hat{u}_1$, $v_t' = v_a + \hat{u}_1$, $v_e' = v_t' - \hat{u}_2$ and $v_b = v_e' - \hat{u}_1$, and the edges $(v_t - v_a)$, $(v_a - v_t')$, $(v_t' - v_e')$ and $(v_e' - v_b)$.) A hypercubic lattice in d dimensions is defined by d perpendicular planes, and the set of vertices $\{v_t, v_e, v_t', v_e'\}$ is contained in one plane. Therefore, in order to add the maximum number of cycles, there are $(d-1)$ available planes in which to place the vertices and edges needed to form unit squares (cycles) which contain v_t' as one of their four vertices. So, for example, if i equals four and $d=2$, create a cycle in the plane (\hat{u}_1, \hat{u}_2) by adding the vertices $v_1 = v_t' + \hat{u}_1$, $v_2 = v_t' + \hat{u}_2$, $v_3 = v_1 + \hat{u}_2$, and the edges $(v_t' - v_1)$, $(v_t' - v_2)$, $(v_1 - v_3)$ and $(v_2 - v_3)$. If $d > 2$ then the planes to be utilised will depend on the vector joining v_e' to v_t' . If $v_t' = v_e' + \hat{u}_3$, add the first cycle as above and, if $i=6$, construct the next cycle by adding the vertices $v_4 = v_t' - \hat{u}_2$, $v_5 = v_t' + \hat{u}_3$, $v_6 = v_5 - \hat{u}_2$ and the edges $(v_t' - v_4)$, $(v_t' - v_5)$, $(v_5 - v_6)$ and $(v_4 - v_6)$ (see figure 2). If $v_t' = v_e' + \hat{u}_2$, a cycle can be added in the plane (\hat{u}_1, \hat{u}_3) and a second cycle in the plane (\hat{u}_2, \hat{u}_3) by a similar construction. This process can be continued into higher dimensions, always adding the next cycle in the plane containing unit vectors of lowest possible coordinate until v_t' is of the desired degree i . In figure 2, v_t' is of degree 6 and two cycles have been added. In general, the resulting structure will have $c + (i-2)/2$ cycles and $n + 3(i-2)/2 + 2$ vertices in total, $n_2 + 3(i-2)/2 + 1$ of degree 2 and $n_i + 1$ of degree i , the numbers of vertices of all other degrees being unchanged.

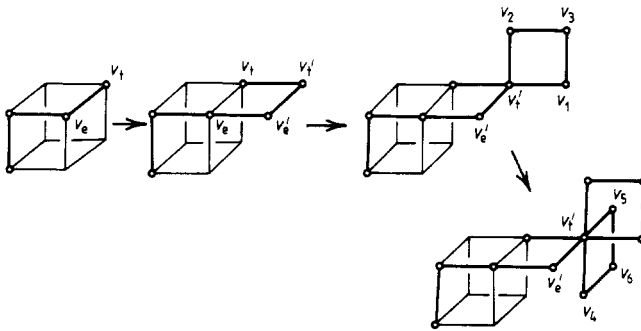


Figure 2. Addition of two cycles through a new vertex of even degree.

Construction 2. Cycles may be added by converting two vertices of degree 2 to vertices of degree i and j , with i and j both odd and greater than 2. This can be attained by constructing v_t' and v_e' and then changing them from degree 2 to degrees i and j respectively to produce $[1 + (i+j-6)/2]$ cycles. For an example of this see figure 3. The first cycle is created by adding the vertices $v_1 = v_t' + \hat{u}_1$, $v_2 = v_e' + \hat{u}_1$ and the edges $(v_t' - v_1)$, $(v_e' - v_2)$, $(v_1 - v_2)$. v_t' and v_e' are now both of degree 3. Additional cycles

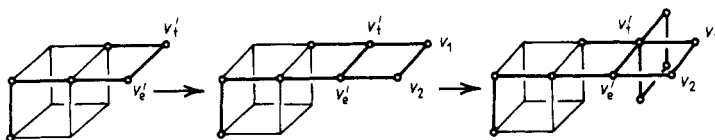


Figure 3. Addition of two cycles through two new vertices of odd degree.

may be added as described above, $(i-3)/2$ joined to v'_i and $(j-3)/2$ to v'_e . The resulting structure has $c + 1 + (i+j-6)/2$ cycles and $n + 4 + \frac{3}{2}(i+j-6)$ vertices in total, $n_2 + 2 + \frac{3}{2}(i+j-6)$ of degree 2, $n_i + 1$ of degree i and $n_j + 1$ of degree j , the numbers of vertices of all other degrees being unchanged.

We now wish to construct a set of graphs which are appropriate 'precursors' to the graph under consideration, and which have either one or no cycles. To do this we look for a set of integers $\{n'_1, n'_3, n'_4, \dots, n'_{2d}\}$ such that

$$n'_k \leq n_k, \quad \forall k \geq 3, \tag{2.4}$$

and

$$n'_1 = n_1. \tag{2.5}$$

If $n_1 \geq 2$, we also require that

$$\sum_{i=1}^{2d} (i-2)n'_i + 2 = 0 \tag{2.6}$$

so that, from (2.3), (2.5) and (2.6),

$$\sum_{i=3}^{2d} (i-2)(n_i - n'_i) = 2c. \tag{2.7}$$

This ensures that the set of vertex degrees $\{n'_1, \dots, n'_{2d}\}$ defines a tree. To be specific, we minimise $n'_{2d}, n'_{2d-1}, \dots$ successively, subject to (2.4) and (2.7).

If $n_1 < 2$ no corresponding tree would exist and so we look for a graph with one cycle by requiring the n'_k to satisfy (2.4), (2.5) and

$$\sum_{i=1}^{2d} (i-2)n'_i = 0. \tag{2.8}$$

This implies that

$$n'_3 = n'_1 \tag{2.9}$$

and

$$n'_k = 0, \quad \forall k > 3. \tag{2.10}$$

If $n_1 = 0$ the set $\{n'_1, n'_3, \dots\}$ corresponds to a polygon.

We concentrate on the case with $n_1 \geq 2$ and consider adding cycles to the tree using constructions 1 and 2 described above.

Using construction 1 we successively add $n_{2d} - n'_{2d}$ vertices of degree $2d$ (forming $(d-1)(n_{2d} - n'_{2d})$ new cycles), $n_{2d-2} - n'_{2d-2}$ vertices of degree $2d-2$ (forming $(d-2)(n_{2d-2} - n'_{2d-2})$ new cycles), etc. For vertices of odd degree we first note that (2.7) implies that

$$\sum_{p=1}^{d-1} (n_{2p+1} - n'_{2p+1}) \equiv 0 \pmod{2} \tag{2.11}$$

so that vertices of odd degree can be added in pairs. We imagine making a list of the vertices of odd degree to be added, starting with those of highest degree, and add them successively from this list, in pairs, using construction 2.

During this process, some vertices of degree 2 will also have been added and each tree with n' vertices, n'_3 of degree 3, \dots , n'_{2d} of degree $2d$ will have given rise to a unique graph having n vertices, n_3 of degree 3, \dots , n_{2d} of degree $2d$, and c cycles. The difference between n and n' will be a (bounded) function of n_3, n_4, \dots etc so that the construction will work for all sufficiently large values of n . Since trees with fixed numbers of branch points (Lipson and Whittington 1983) have a growth constant of μ , it follows from the above that

$$\liminf_{n \rightarrow \infty} n^{-1} \log a(n, c; n_3, \dots, n_{2d}) \geq \log \mu. \tag{2.12}$$

The case with $n_1 = 0$ can be treated in an analogous fashion beginning with a polygon and adding vertices of degree 3 and higher to form an appropriate number of cycles. Since the growth constant for polygons is μ (Hammersley 1961), (2.12) follows.

When $n_1 = 1$ there is no solution except when $n_3 \geq 1$. (The solution is then $n'_1 = n'_3 = 1, n'_4 = \dots = n'_{2d} = 0$, i.e. a tadpole.) To treat this situation we use a polygon as a precursor adding vertices of even degree by construction 1 and pairs of vertices of odd degree (and of degree greater than or equal to 3) by construction 2. This will leave two odd-degree vertices, one of unit degree and one of degree k with $k \geq 3$. We add these vertices by a variant of construction 1. If $k > 3$ we use construction 1 to add a vertex of degree $k - 1$ and then add a single adjacent vertex and the edge joining this pair, with the result that the two vertices are of degree 1 and degree k . If $k = 3$, we form v'_1 and v'_2 and add a single vertex adjacent to v'_1 , and the edge joining them to give two vertices of degree 1 and 3. Each polygon gives a unique graph with fixed c, n_3, \dots by this construction and (2.12) follows.

To obtain an upper bound on $a(n, c; n_3, \dots, n_{2d})$ we first consider an upper bound on the number of ways of connecting the set of $(n_1, n_3, \dots, n_{2d})$ vertices; i.e. we need the number of connected graphs containing n^* labelled vertices, and c cycles, where

$$n^* = n_1 + n_3 + n_4 + \dots + n_{2d}. \tag{2.13}$$

An upper bound on this quantity is given by the number of graphs on n^* labelled vertices, which is $2^{\binom{n^*}{2}}$. The edges in this graph are now replaced by the N simple chains contained in each member of $A(n, c; n_3, \dots, n_{2d})$, N being given by

$$N = 1 - c + 2n_3 + 3n_4 + \dots + (2d - 1)n_{2d}. \tag{2.14}$$

Making up these N chains are $m = n + c - 1$ edges, and each chain has between one and $m - (N - 1)$ edges. Recall that the number of embeddings of a simple chain having m edges is $\exp[m\kappa + o(m)]$ where $\kappa = \log \mu$. From the above

$$a(n, c; n_3, \dots, n_{2d}) \leq 2^{\binom{n^*}{2}} \sum_{m_1} \sum_{m_2} \dots \sum_{m_N} \exp[m_1\kappa + o(m_1) + m_2\kappa + o(m_2) + \dots], \tag{2.15}$$

where m_l is the number of edges in the l th simple chain and the sums are taken over

$\{m_l\}$ subject to the conditions

$$m_l > 0, \quad \sum_{l=1}^N m_l \equiv m = c + n - 1. \tag{2.16}$$

The sum on the right-hand side of (2.15) includes configurations with self-avoiding but not mutually avoiding chains. Performing the summations, and noticing that $m_l \leq m$ for all l gives

$$a(n, c; n_3, n_4, \dots, n_{2d}) \leq 2^{\binom{c}{2}} m^N \exp[m\kappa + o(m)] \tag{2.17}$$

and from (2.13), (2.14) and (2.17)

$$a(n, c; n_3, n_4, \dots, n_{2d}) \leq \exp[n\kappa + o(n)] \tag{2.18}$$

where c and n_3, n_4, \dots, n_{2d} are fixed. Then from (2.12) and (2.18)

$$\lim_{n \rightarrow \infty} n^{-1} \log a(n, c; n_3, \dots, n_{2d}) = \log \mu = \kappa. \tag{2.19}$$

Therefore an animal with a fixed number of cycles and a fixed number of branch points has the same growth constant, or limiting entropy per monomer, as that of a self-avoiding walk.

3. Bounds on exponents

In this section we derive exponent bounds for three particular topologies, the twin-tailed, two-tailed and Y-tailed tadpoles (see figure 1). These are simple examples of graphs with fixed numbers of cycles and branch points and these results play an important role in our discussions concerning a possible form for the dependence of the value of the exponent on certain characteristics of the topology.

To simplify the notation we shall write $t_n^{(1)}$, $t_n^{(2)}$ and $t_n^{(3)}$ for the numbers, per site, of weak embeddings of twin-tailed, two-tailed and Y-tailed tadpoles, with n edges. Notice that all of these graphs are undirected and unrooted. Similarly, we write t_n and p_n for the numbers of undirected, unrooted tadpoles and polygons and c_n for the number of *directed* self-avoiding walks. We shall assume the usual asymptotic forms

$$c_n \sim n^{\gamma-1} \mu^n, \tag{3.1}$$

$$p_n \sim n^{\alpha-3} \mu^n, \tag{3.2}$$

and, by analogy

$$t_n^{(k)} \sim n^{\gamma(k)-1} \mu^n \quad (k = 1, 2, 3). \tag{3.3}$$

We first consider an upper bound for the number of two-tailed tadpoles. We write n_1, n_2, n_3 for the numbers of edges in the circuit and in the two simple chains. With these numbers fixed we can concatenate a polygon with two self-avoiding walks, with the walks attached by a unit degree vertex to the polygon at each pair of polygon vertices in turn. The resulting graphs will include all two-tailed tadpoles with this distribution of edges and, summing over n_1, n_2, n_3 subject to $n_1 + n_2 + n_3 = n$, we have

$$t_n^{(2)} \leq \sum_{\substack{n_1, n_2, n_3 \\ n_1 + n_2 + n_3 = n}} p_{n_1} c_{n_2} c_{n_3} n_1^2 \leq A \sum n_1^{\alpha-3} n_2^{\gamma-1} n_3^{\gamma-1} n_1^2 \mu^n \tag{3.4}$$

for some positive constant A . From the assumed form (3.1) and the result of Hammersley and Morton (1954) on the direction of approach to the limit, it follows that $\gamma - 1 \geq 0$, so that

$$\gamma(2) \leq \max[2\gamma + 1, 2\gamma + \alpha]. \tag{3.5}$$

Similar arguments for Y-tailed tadpoles yield $\gamma(3) \leq \max[2\gamma + 2, 2\gamma + \alpha]$ and for twin-tailed tadpoles, $\gamma(1) \leq \max[\gamma + 2, \gamma + \alpha]$. Numerical evidence indicates that $0 < \alpha < 1$.

The bounds for $\gamma(3)$ and $\gamma(1)$ can, however, be improved somewhat. If we consider each Y-tailed tadpole and remove an edge in the circuit, incident on the vertex of degree 3 in the circuit, the resulting graph is a Y (i.e. a star with three branches) having $n - 1$ edges. If we write y_n for the number of Y's with n edges and assume

$$y_n \sim n^{\phi-1} \mu^n, \tag{3.6}$$

we have

$$t_n^{(3)} \leq A y_{n-1} \tag{3.7}$$

for some constant A and hence

$$\gamma(3) \leq \phi. \tag{3.8}$$

Gaunt *et al* (1984) have shown that $\phi \leq 2\gamma + 1$ so that

$$\gamma(3) \leq 2\gamma + 1. \tag{3.9}$$

A similar argument for two-tailed tadpoles gives $\gamma(2) \leq 2\gamma + 1$.

In order to improve the bound on $\gamma(1)$ we make use of an idea due to Guttmann and Whittington (1978), and we consider only the square lattice though similar arguments can be constructed for any simple hypercubic lattice. Each twin-tailed tadpole contains a single vertex of degree 4 (which we label O) connected to four vertices which we label N, E, S and W, in an obvious notation. Two of these vertices are connected to one another by a simple chain not containing O and the other two are each connected by a simple chain to a vertex of unit degree. The set of twin-tailed tadpoles can be divided into six subsets, characterised by the pair of vertices from N, E, S and W which form part of a circuit, and examples of members of the subsets NS, WS and NW are shown in figure 4. Clearly, by symmetry, the number of members of NS is equal to the number of members of WE, and the number of members of NW, NE, SE and SW are all equal.

We consider a twin-tailed tadpole, t , which is *not* a member of SW or NE. The graph is rooted at O. Suppose there are s_n such graphs, with n edges. Clearly,

$$s_n \leq t_n^{(1)} \leq 2s_n, \tag{3.10}$$

so that (3.3) and (3.10) imply that

$$s_n \sim n^{\gamma(1)-1} \mu^n. \tag{3.11}$$

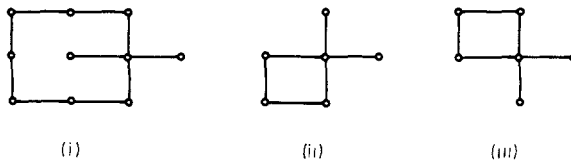


Figure 4. Twin-tailed tadpoles in (i) the NS class, (ii) the SW class and (iii) the NW class.

For each such graph we define an operation (T) in which the edges ON and OE are removed and replaced by $O'N$ and $O'E$ where O' is the fourth point of the square defined by ON and OE , as in figure 5. Now we have several possibilities to consider.

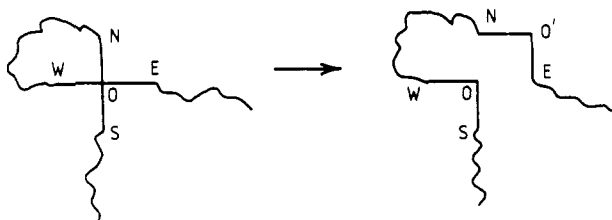


Figure 5. The operation in which ON and OE are replaced by $O'N$ and $O'E$. In this case the resulting graph is a simple chain.

If O' is not a vertex of t then Tt is a simple chain (or undirected self-avoiding walk) rooted at O . If O' is a member of t and either $O'N$ or $O'E$ is an edge of t , then Tt will contain a double edge and deletion of this edge will yield an $(n - 2)$ -edge simple chain rooted at O . If O' is a member of t but neither $O'N$ nor $O'E$ is an edge of t , then O' can be either of degree 1 or of degree 2 in t and hence of degree 3 or 4 in Tt . In the former case Tt is a tadpole with n edges, rooted at O . In the latter case Tt will be a twin-tailed tadpole (and it is easy to see that Tt cannot be of type SW or NE). In this case we iterate, forming T^2t, T^3t , etc until a simple chain, a simple chain with an added double edge or a tadpole is produced. Clearly one of these events must eventually occur since the root remains at O and as successive twin-tailed tadpoles are formed the vertex of degree 4 moves in a north easterly direction at each iteration and would otherwise eventually leave the original graph. Hence

$$s_n \leq (n - 2)c_{n-2} + nc_n + nt_n. \tag{3.12}$$

For every tadpole, removing an edge of the circuit, incident on the vertex of degree 3, produces a simple chain, so that

$$t_n \leq c_{n-1} \tag{3.13}$$

and hence

$$s_n \leq 3nc_n. \tag{3.14}$$

Then from (3.1), (3.11) and (3.14)

$$\gamma(1) \leq \gamma + 1. \tag{3.15}$$

We now show that $\gamma(1), \gamma(2)$ and $\gamma(3)$ are each greater than or equal to γ .

We consider each n -edge self-avoiding walk weakly embeddable in the d -dimensional simple hypercubic lattice. We define the top vertex, edge vertex and top edge in the usual way (see § 2, for instance). For a particular walk let the top vertex (v_t) have coordinates $(x_1^t, x_2^t, \dots, x_d^t)$, and let the edge vertex (v_e) have coordinates $(x_1^e, x_2^e, \dots, x_d^e)$. The vertices v_t and v_e can be of degree 1 or 2. We first carry out a construction which produces a self-avoiding walk with both the top and edge vertices of degree 2. To do this we remove the top edge $(v_t - v_e)$, add the vertices $v'_t = v_t + \hat{u}_1$ and $v'_e = v_e + \hat{u}_1$ and the edges $(v'_t - v'_e), (v_t - v'_t)$ and $(v_e - v'_e)$. The resulting graph is

a self-avoiding walk with $n + 2$ edges with top vertex v'_t and edge vertex v'_e . (If $x_1^e = x_1^t - 1$, as can occur if the top vertex is of degree 1, a minor gloss is necessary similar to that described in § 2.)

In order to form twin-tailed, two-tailed and Y-tailed tadpoles we now carry out the following three constructions: (i) add the vertices $v_1 = v'_t + \hat{u}_1$, $v_2 = v'_t + \hat{u}_2$ and $v_3 = v_2 + \hat{u}_1$ and the four edges $(v'_t - v_1)$, $(v'_t - v_2)$, $(v_1 - v_3)$ and $(v_2 - v_3)$ giving a twin-tailed tadpole with $n + 6$ edges; (ii) add the two vertices $v_1 = v'_t + \hat{u}_1$ and $v_2 = v'_e + \hat{u}_1$ and the three edges $(v'_t - v_1)$, $(v'_e - v_2)$ and $(v_1 - v_2)$, giving a two-tailed tadpole with $n + 5$ edges; (iii) add the vertices $v_1 = v'_t + \hat{u}_1$, $v_2 = v_1 + \hat{u}_1$, $v_3 = v_2 + \hat{u}_2$ and $v_4 = v_1 + \hat{u}_2$ and the five edges $(v'_t - v_1)$, $(v_1 - v_2)$, $(v_2 - v_3)$, $(v_3 - v_4)$, $(v_1 - v_4)$, giving a Y-tailed tadpole with $n + 7$ edges.

Since, by these constructions, each walk yields a unique twin-tailed, two-tailed or Y-tailed tadpole (except for the walk direction) we have

$$\frac{1}{2}c_n \leq t_{n+6}^{(1)}, \quad \frac{1}{2}c_n \leq t_{n+5}^{(2)}, \quad \frac{1}{2}c_n \leq t_{n+7}^{(3)}, \tag{3.16}$$

so that each of the exponents $\gamma(1)$, $\gamma(2)$ and $\gamma(3)$ is greater than or equal to γ . We summarise the results of this section as

$$\gamma \leq \gamma(1) \leq \gamma + 1, \quad \gamma \leq \gamma(2) \leq 2\gamma + 1, \quad \gamma \leq \gamma(3) \leq 2\gamma + 1. \tag{3.17}$$

These bounds are consistent with the conjectured exponent $\gamma + b - 1$ discussed in § 1. Using the presumably exact value (Nienhuis 1982) of $\gamma = 1\frac{11}{32}$ in two dimensions and the renormalisation group estimate (Baker *et al* 1978, le Guillou and Zinn-Justin 1980) $\gamma = 1.1615$ in three dimensions, we give the corresponding numerical values of the upper bounds in (3.17) in table 1.

Table 1. Series estimates of critical exponents for $d = 2$ and 3 dimensions. The conjectured exponent ($\gamma + b - 1$) and numerical values of the upper bounds are given for comparison purposes.

Tadpole topology	$d = 2$			$d = 3$		
	Upper bound	$\gamma + b - 1$	Series estimates	Upper bound	$\gamma + b - 1$	Series estimates
One-tailed	1.343 75	1.343 75	1.35 ± 0.05	1.1615	1.1615	1.2 ± 0.1
Twin-tailed	2.343 75	2.343 75	2.5 ± 0.2	2.1615	2.1615	2.3 ± 0.5
Two-tailed	3.6875	2.343 75	2.8 ± 0.7	3.323	2.1615	2.0 ± 1.5
Y-tailed	3.6875	3.343 75	3.0 ± 1.5	3.323	3.1615	—

— No estimate possible with available data.

4. Series derivation and analysis

As in previous sections, we focus attention primarily on weak embeddings of twin-tailed, two-tailed and Y-tailed tadpoles. Data are presented in the appendix for the square (sq), triangular (τ) and simple cubic (sc) lattices and are classified by the total number (n) of bonds. For twin-tailed tadpoles, $t_n^{(1)}$ extends through $n = 21, 16, 16$ for the sq, τ and sc lattices, respectively; for two-tailed and Y-tailed tadpoles, $t_n^{(2)}$ and $t_n^{(3)}$ extend through $n = 14, 13, 12$ and $n = 14, 11, 12$, respectively. In certain cases this represents

a significant extension of existing data (Domb 1960, McKenzie 1967, Guttmann and Nymeyer 1977).

Several methods were used to obtain the new data. The most direct method was computer enumeration of each realisation of a given topology followed by summation over all realisations. Since the number of realisations to be considered increases asymptotically like n^{l-1} (l is the number of lines in the topology), this method rapidly becomes impractical. For $t_n^{(1)}$, we have been able to generate somewhat longer series by viewing these embeddings as random walks having no immediate reversals and precisely one self-intersection at a vertex of degree 4, and adapting the 'dimerisation' method of Torrie and Whittington (1975) to this case. The remaining method involved enumerating *all* lattice animals with n bonds ($n = 1, 2, 3, \dots$) and classifying them according to the set $(c; n_3, n_4, \dots, n_q)$. Clearly this classification does not specify the topology uniquely. For example, $t_n^{(2)}$ and $t_n^{(3)}$ are produced as a sum $(t_n^{(2)} + t_n^{(3)})$. It is, however, possible to 'separate' these topologies using published data and the following counting theorem first derived by McKenzie (1967):

$$2t_n^{(3)} + 4t_n^{(2)} = (n-2)(\sigma-1)c_{n-1} - 2 \sum_i (i-1)t_{i,n} - 2t_n^{(1)} + 3\sigma s_{n-1}^{(3)} - 3s_n^{(3)}. \quad (4.1)$$

Here c_n denotes the number of undirected self-avoiding walks with n steps, $t_{i,n}$ denotes the number of simple (or one-tailed) tadpoles with i bonds in the 'head' and n in total (Guttmann and Sykes 1973), $s_n^{(3)}$ denotes the number of stars with three branches and n bonds in total (Gaunt *et al* 1984) and $\sigma + 1$ is the lattice coordination number.

We have analysed the data in the appendix using the standard series analysis methods (Gaunt and Guttmann 1974) employed by Gaunt *et al* (1984). For example, the exponent $\gamma(1)$ can be estimated from the sequence $\gamma_n(1) = 1 + n[(r_n/\hat{\mu}) - 1]$, where the ratio $r_n = t_n^{(1)}/t_{n-1}^{(1)}$ and $\hat{\mu}$ is an estimate of μ for which we have used the unbiased estimates of Watts (1975). We also form linear extrapolants $\gamma'_n(1) = [n\gamma_n(1) - (n-m)\gamma_{n-m}(1)]/m$ from adjacent points ($m = 1$) for the τ lattice, or alternate points ($m = 2$) for the sq and sc lattices, and the averages $\gamma''_n(1) = \frac{1}{2}[\gamma_n(1) + \gamma'_n(1)]$.

Plots against $1/n$ of $\gamma_n(1)$, $\gamma'_n(1)$ and $\gamma''_n(1)$ are given in figure 6 for the sq and τ lattices. The corresponding plots for the sc lattice are shown in figure 7. Our best estimates of $\gamma(1)$ are

$$\gamma(1) = 2.5 \pm 0.2 \quad (d = 2) \quad (4.2)$$

$$= 2.3 \pm 0.5 \quad (d = 3). \quad (4.3)$$

We have analysed in a similar fashion all the data given in the appendix. The series for the two-tailed and Y-tailed tadpoles are less well behaved than those for the twin-tailed tadpole and we give some typical results in figure 8. Our estimates of the exponents are given in table 1. We have also analysed the data available in the literature (Guttmann and Sykes 1973, Hioe 1967) for simple (one-tailed) tadpoles and our exponent estimates are also given in table 1.

The series estimates of the exponents for one-tailed and twin-tailed tadpoles are slightly higher than the numerical values of the upper bounds. In view of this, and the manner of convergence displayed in figure 6, for example, we suggest that the exponents may be exactly γ and $\gamma + 1$, respectively. Since the number of branches (b) is 1 and 2, respectively, these results support our conjecture that the value of the exponent is given by $\gamma + b - 1$. The numerical estimates given in table 1 for the other topologies are also consistent with this conjecture.

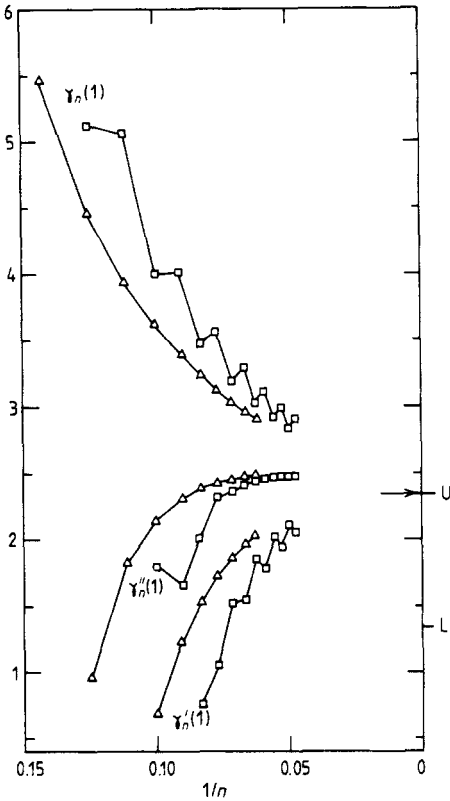


Figure 6. Plots against $1/n$ of biased ratio estimates of $\gamma(1)$ for weak embeddings of twin-tailed tadpoles on the square (\square) and triangular (Δ) lattices. The conjectured exponent $(\gamma + 1)$ is indicated by an arrow and the upper and lower bounds by U and L, respectively.

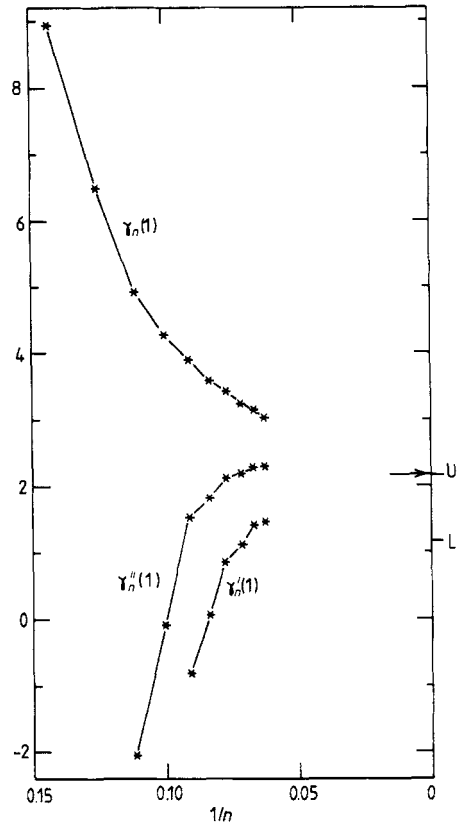


Figure 7. Plots against $1/n$ of biased ratio estimates of $\gamma(1)$ for weak embeddings of twin-tailed tadpoles on the simple cubic lattice. The conjectured exponent $(\gamma + 1)$ is indicated by an arrow and the upper and lower bounds by U and L, respectively.

5. Connection with renormalisation group results

In this section we use arguments similar to those of Whittington *et al* (1983) and Gaunt *et al* (1984) to reconcile our result that the exponent depends on b but not on c , with the renormalisation group prediction (Lubensky and Isaacson 1979, Family 1980) that the exponent is independent of branching and cycle fugacities. The conjectured form, $\gamma + b - 1$, for this exponent plays a central role in this reconciliation.

Let us define fugacities z_b and z_c associated with branches and cycles, respectively. The generating function for all lattice animals is

$$G(n, z_b, z_c) = \sum_c \sum_b a_{n,b,c} z_b^b z_c^c \tag{5.1}$$

where $a_{n,b,c}$ is the number of embeddings of lattice animals having n bonds, b branches and c cycles. In general, this is a sum over many topologies. The coefficient of z_c^c in (5.1) is

$$G_c(n, z_b) = \sum_b a_{n,b,c} z_b^b \tag{5.2}$$

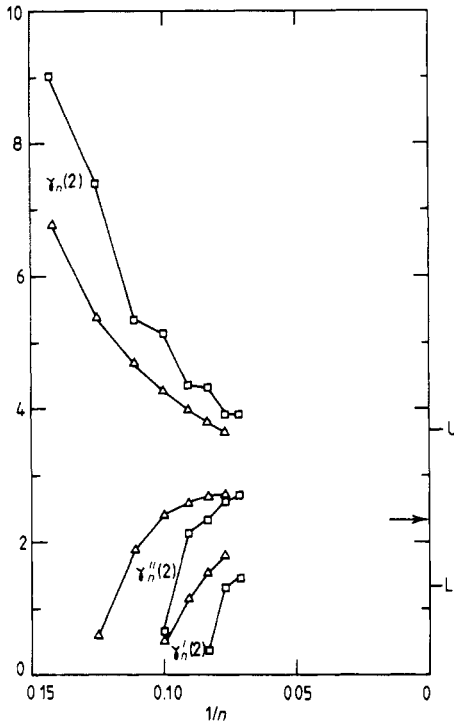


Figure 8. Plots against $1/n$ of biased ratio estimates of $\gamma(2)$ for weak embeddings of two-tailed tadpoles on the square (\square) and triangular (\triangle) lattices. The conjectured exponent ($\gamma + 1$) is indicated by an arrow and the upper and lower bounds by U and L , respectively.

If we replace $a_{n,b,c}$ by its conjectured asymptotic form $A_{b,c}n^{\gamma+b-2}\mu^n$ for $b \geq 1$, and write $a_{n,0,c} \sim A_{0,c}n^{\phi(c)}\mu^n$ for animals with $b = 0$, then

$$G_c(n, z_b) \sim n^{\gamma-2}\mu^n \sum_{b \geq 1} A_{b,c}(nz_b)^b + A_{0,c}n^{\phi(c)}\mu^n \sim n^{\gamma-2}\mu^n B_c(nz_b) + A_{0,c}n^{\phi(c)}\mu^n, \tag{5.3}$$

where

$$B_c(w) = \sum_{b=1}^{\infty} A_{b,c}w^b \tag{5.4}$$

is the generating function of the amplitudes $A_{b,c}$.

From (5.2) we see that $G_c(n, 1) = a_{nc}$, the number of c -animals with n bonds (and c cycles). If we assume (Whittington *et al* 1983) that

$$a_{nc} \sim A_c n^{-\theta_0+c} \lambda_0^n, \tag{5.5}$$

then it follows that

$$B_c(w) \sim A_c w^{2+c-\theta_0-\gamma} (\lambda_0/\mu)^w - A_{0,c} w^{\phi(c)+2-\gamma}. \tag{5.6}$$

Substituting this equation into (5.3) we obtain, at least for z_b close to the c -animal limit ($z_b = 1$),

$$G_c(n, z_b) \sim (A_c z_b^{2+c-\theta_0-\gamma}) n^{-\theta_0+c} (\lambda_0^z \mu^{1-z_b})^n, \tag{5.7}$$

where we have kept only the dominant term. Setting $c = 0$ essentially reproduces (5.13) in Gaunt *et al* (1984), the minor differences arising from different definitions of fugacity.

Inserting (5.7) into (5.1) we obtain

$$G(n, z_b, z_c) \sim \sum_c (A_c z_b^{2+c-\theta_0-\gamma}) n^{-\theta_0+c} (\lambda_0^{z_b} \mu^{1-z_b})^n z_c^c \sim (z_b^{2-\theta_0-\gamma}) n^{-\theta_0} (\lambda_0^{z_b} \mu^{1-z_b})^n C(v), \tag{5.8}$$

where

$$C(v) = \sum_c A_c v^c \quad (v = n z_b z_c) \tag{5.9}$$

is the generating function for the amplitudes A_c . From (5.1) we see that $G(n, 1, 1) = a_n$, the total number of lattice animals with n bonds. If we assume (Duarte and Ruskin 1981, Gaunt *et al* 1982)

$$a_n \sim A n^{-\theta_0} \lambda^n, \tag{5.10}$$

then

$$C(v) \sim A(\lambda/\lambda_0)^v, \tag{5.11}$$

so that, at least close to the animal limit ($z_b = z_c = 1$),

$$G(n, z_b, z_c) \sim (A z_b^{2-\theta_0-\gamma}) n^{-\theta_0} (\mu^{1-z_b} \lambda_0^{z_b(1-z_c)} \lambda^{z_b z_c})^n. \tag{5.12}$$

As expected, the amplitude and growth parameter are fugacity dependent whereas the critical exponent is not. Thus the critical exponent for branched polymers with cycles is independent of the branching and cycle fugacities.

6. Discussion

In this paper we have considered branched polymers with a specified topology. We have proved (in § 2) that the growth constant for an animal with c cycles and n_k vertices of degree k ($k = 3, \dots, 2d$) is equal to μ , the growth constant for self-avoiding walks. We have derived bounds on critical exponents (in § 3) and have estimated the values of these exponents using series analysis (in § 4), for several particular topologies. These results are consistent with the exponent being $\gamma + b - 1$ ($b \neq 0$), as conjectured for trees by Gaunt *et al* (1984). An interesting feature of this extended conjecture is that the exponent is independent of c . This is consistent with previous results on dumbbells (Guttman and Whittington 1978) and tadpoles (Whittington *et al* 1975). We note that the conjecture is not intended to apply to graphs with $b = 0$. Several examples with $b = 0$ have been studied (e.g. Martin *et al* 1967, Guttman and Whittington 1978) and the exponents clearly depend on the cyclomatic index, c .

In § 5 we have discussed the connection between our results and those obtained using renormalisation group methods. We have presented an heuristic argument, using our conjectured form for the exponent, that the universality class of branched polymers is independent of branching and cycle fugacities. However, if the numbers of branches (b) and cycles (c) are fixed, rather than being controlled by fugacities, the critical exponent does depend on b but not on c .

We have concentrated in this paper on weak embeddings but we expect that analogous results will hold for strong embeddings. This would be consistent with

general universality considerations and with previous work on related problems (Gaunt *et al* 1982, 1984, Whittington *et al* 1983).

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Appendix. Exact enumeration data (new data are indicated by †).

Table A1. Twin-tailed tadpoles, $t_n^{(1)}$.

n	T	SQ	SC
5	36		
6	342	4	72
7	2328	24	720
8	13 860	96	5688
9	76 368	368	38 328
10	400 056	1264	238 728
11	2023 446	4252	1412 844
12	9972 846†	13 532	8046 660
13	48 185 460†	42 756†	44 724 012†
14	229 185 732†	130 496†	242 991 144†
15	1076 273 700†	397 064†	1301 776 272†
16	5001 229 908†	1180 420†	6870 013 452†
17		3502 916†	
18		10 226 316†	
19		29 817 072†	
20		85 890 408†	
21		247 191 136†	

Table A2. Two-tailed tadpoles, $t_n^{(2)}$.

n	T	SQ	SC
5	90		
6	999	24	288
7	7572	136†	2808
8	48 750	646†	24 582
9	285 654	2532†	170 100
10	1575 174	9452†	1132 080
11	8321 868	32 584†	6891 288
12	42 595 239†	109 962†	41 163 150
13	212 761 356†	354 928†	
14		1132 726†	

Table A3. Y-tailed tadpoles, $t_n^{(3)}$.

n	T	SQ	SC
6	192		
7	2712	24†	480
8	24 732	184†	6624
9	184 116	1044†	66 984
10	1217 400	4796†	551 976
11	7440 702	20 000†	4100 040
12		77 084†	28 123 152
13		282 464†	
14		993 088†	

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