

Home Search Collections Journals About Contact us My IOPscience

Branched polymers with a prescribed number of cycles

This article has been downloaded from IOPscience. Please scroll down to see the full text article. 1983 J. Phys. A: Math. Gen. 16 1695 (http://iopscience.iop.org/0305-4470/16/8/016)

View the table of contents for this issue, or go to the journal homepage for more

Download details: IP Address: 129.252.86.83 The article was downloaded on 30/05/2010 at 17:13

Please note that terms and conditions apply.

# Branched polymers with a prescribed number of cycles

S G Whittington<sup>†</sup>, G M Torrie<sup>‡</sup> and D S Gaunt<sup>§</sup>

<sup>+</sup> Department of Chemistry, University of Toronto, Toronto, Canada M5S 1A1
<sup>‡</sup> Department of Mathematics and Computer Science, Royal Military College, Kingston, Canada K7L 2W3
§ Department of Physics, King's College, Strand, London WC2R 2LS, UK

Received 22 November 1982

Abstract. This paper is concerned with the numbers of lattice animals with exactly c cycles. For weakly embeddable (bond) clusters we show rigorously that the growth constant is independent of c and we derive upper and lower bounds on the critical exponents for each value of c. We use series analysis methods to estimate the critical exponents for c = 1 and 2 in two and three dimensions and find that the critical exponent does depend on the number of cycles. Evidence from series analysis results and from expansions in inverse powers of the dimension suggests that, in the case of strong embeddings (i.e. site clusters) the growth constant is independent of c and the corresponding values of the critical exponents are identical to the values for weak embeddings (i.e. bond clusters). We discuss the relationship of these results to the field theory prediction that the critical exponent is independent of cycle fugacity.

## 1. Introduction

Branched polymer molecules with excluded volume have been modelled as lattice animals (i.e. connected clusters embeddable in a regular lattice) and a number of workers have discussed the importance of cycles on their properties (Lubensky and Isaacson 1979, Family 1980, Daoud and Joanny 1981). These authors have argued that the universality class is independent of cycle fugacity. Direct series evidence that trees and animals are in the same universality class has been presented for a number of lattices in two and three dimensions (Duarte and Ruskin 1981) and for *d*dimensional hypercubic lattices for  $d = 2, 3, \ldots, d_c$  where  $d_c$  (=8) is the upper critical dimension (Gaunt *et al* 1982). The above series evidence was based on estimates of the exponent ( $\theta_0$ ) characterising the number of trees. In addition there is some Monte Carlo work (Seitz and Klein 1981) estimating the value of the exponent ( $\nu$ ) characterising the radius of gyration of trees. Their estimates, in both two and three dimensions, are close to the expected values for animals (Parisi and Sourlas 1981).

In order to investigate the crossover from trees to animals we consider the numbers of clusters with n sites and precisely c cycles. The interesting result which we obtain is that the growth parameter is independent of c but the associated critical exponent varies as c varies.

To be more specific, we define  $a_{nc}$   $(A_{nc})$  as the number, per lattice site, of weakly (strongly) embeddable clusters (i.e. bond and site clusters, respectively) with n sites and cyclomatic index c. We shall refer to clusters with cyclomatic index c as c-animals.

In § 2 we show that the growth parameter

$$\lambda_c = \lim_{n \to \infty} n^{-1} \log a_{nc} \tag{1.1}$$

exists for all finite c, for the d-dimensional hypercubic lattice. In addition we show that

$$\lambda_c = \lambda_0 \qquad \forall c \tag{1.2}$$

where  $\lambda_0$  is the growth parameter for the number of trees  $a_{n0}$  (= $t_n$ , in the notation of Gaunt *et al* (1982)).

In § 3 we enumerate the weakly and strongly embeddable clusters with fixed c for the triangular, square and simple cubic lattices. Assuming the expected asymptotic form

$$a_{nc} \sim n^{-\theta_c} \lambda_c^n \tag{1.3}$$

we estimate  $\theta_c$  and find strong evidence that  $\theta_1 \neq \theta_0$ . Hence trees and animals with precisely one cycle are not in the same universality class.

In the case of strongly embeddable clusters we have been unable to prove the analogous relations to (1.1) and (1.2) but, assuming that

$$A_{nc} \sim n^{-\Theta_c} \Lambda_c^n, \tag{1.4}$$

we find numerical evidence that  $\Theta_1 \neq \Theta_0$  but that  $\Theta_1 = \theta_1$ . (Gaunt *et al* (1982), who used the notation  $A_{n0} \equiv T_n$ , have shown that  $\Theta_0 = \theta_0 = \theta = \Theta$ , where  $\theta$  and  $\Theta$  are the exponents for weak and strong embeddings of animals. According to Parisi and Sourlas (1981),  $\theta = 1$  (d = 2) and  $\theta = 1\frac{1}{2}$  (d = 3).)

In §4 we derive series expansions for the numbers of clusters with precisely c cycles and n sites, which are weakly and strongly embeddable in a d-dimensional simple hypercubic lattice, for arbitrary integral d. These series extend through eight sites for c = 1 and though seven sites for c = 2. We use these series to derive expansions in inverse powers of  $\sigma(=2d-1)$  for  $\lambda_1$  and  $\lambda_2$  and for  $\Lambda_1$  and  $\Lambda_2$ . Comparison of these expansions with the corresponding expansions (Gaunt *et al* 1982) for  $\lambda_0$  and  $\Lambda_0$  shows them to be consistent with  $\lambda_c = \lambda_0$  (proved rigorously in § 2) and  $\Lambda_c = \Lambda_0$  (conjectured on the basis of series analysis results in § 3) for all c.

In § 5 we make contact with the field theoretic treatment of branched polymers which involves a cycle fugacity. We show that our results are consistent with the field theory prediction that the universality class is independent of cycle fugacity.

Our results are summarised and discussed in § 6.

#### 2. Growth parameters for weakly embeddable c-animals

We consider the set  $(W_{nc})$  of connected clusters of *n* sites with cyclomatic index *c*, weakly embeddable in a *d*-dimensional hypercubic lattice. If the number of such clusters, per site of the lattice, is  $a_{nc}$ , we shall show that

$$\lim_{n \to \infty} n^{-1} \log a_{nc} = \log \lambda_c \tag{2.1}$$

exists, and is independent of c.

The vertices of the d-dimensional hypercubic lattice are the integer points in a d-dimensional Euclidean space. We shall write the coordinates of a lattice vertex as

 $(x_1, x_2, x_3 \dots x_d)$ . The edges of the lattice join pairs of vertices which differ by unity in precisely one coordinate.

We shall need two definitions. For any set  $S_0$  of vertices we define the *top vertex* as follows. 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 coordinates in  $S_0$ . We 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 vertices in  $S_{k-1}$ . Let j be the smallest integer such that  $S_j$  contains precisely one vertex, and call this vertex t, the top vertex of  $S_0$ .

For any graph  $\Gamma$  (not necessarily connected) with vertex set  $V(\Gamma)$  and non-empty edge set  $E(\Gamma)$  we can define a *top edge*, as follows. First construct the subset  $S_c \subseteq V(\Gamma)$ whose members are all the non-isolated vertices of  $\Gamma$  (i.e. all vertices in  $V(\Gamma)$  on which at least one edge in  $E(\Gamma)$  is incident). The top vertex  $(t_c)$  of  $S_c$  is called the *top* connected vertex of  $\Gamma$  (see for example figure 1). Next, construct the set  $N(t_c)$  whose members are those vertices in  $V(\Gamma)$  which are directly connected to  $t_c$  by an edge in  $E(\Gamma)$ . Let  $t_n$  be the top vertex of  $N(t_c)$ . Then the edge joining  $t_n$  and  $t_c$  is the top edge of  $\Gamma$ .

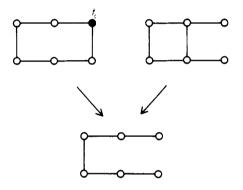


Figure 1. Construction of a tree from different graphs with one cycle. (The top connected vertex of one of these graphs is labelled  $t_{c.}$ )

We now make use of these definitions to prove an upper bound on  $a_{nc}$  for  $c \ge 1$ . Consider any c-animal,  $w \in W_{nc}$   $(c \ge 1)$ . Let the vertex and edge sets of w be V(w) and E(w), respectively. Suppose that  $E^+(w) \subseteq E(w)$  such that edges in  $E^+(w)$  are not cut edges of w. (That is, an edge in E(w) is a member of  $E^+(w)$  if and only if the removal of this edge from w does not decompose w into two or more connected components.)  $E^+(w)$  is necessarily non-void since w has at least one cycle. We now consider the subgraph  $w^+$  of w with edge set  $E(w^+) = E^+(w)$  and vertex set  $V(w^+) = V(w)$ . Let e be the top edge of  $w^+$ . Now consider the graph w' which is obtained by eliminating e from w. Since e was not a cut edge of w, w' is connected. Moreover, w and w' have the same vertices. Hence, using Euler's relation, the cyclomatic index of w' is c - 1 so that  $w' \in W_{n,c-1}$ .

Not all members of  $W_{n,c-1}$  can be obtained from members of  $W_{nc}$  by this construction. (In particular, no member of  $W_{n,c-1}$  which is a section graph (Essam and Fisher 1970) of the lattice can be constructed in this way.) However, some members of  $W_{n,c-1}$  can be constructed in this way from *different* members of  $W_{nc}$ . To be specific, two *c*-animals  $w_1, w_2 \in W_{nc}$ , with identical vertex sets but whose edge sets differ by a single edge, will yield the same member  $w' \in W_{n,c-1}$  if and only if the differing edges

are the top edges of the subgraphs  $w_1^+$  and  $w_2^+$ , defined above (see figure 1 for an example when d = 2). An upper bound on the number of precursors in  $W_{nc}$  of any  $w' \in W_{n,c-1}$  can be obtained by considering the number of ways in which an edge can be added to w'. If we consider the set of graphs obtained from w' by adding an edge in each way at each vertex these 2dn graphs will include all of the precursors of w' in  $W_{nc}$ . Hence

$$a_{nc} \leq 2dna_{n,c-1}, \qquad c \geq 1. \tag{2.2}$$

Now consider any c-animal  $w \in W_{nc}$  and let the top vertex (t) of w have coordinates  $(x_1, x_2, \ldots, x_d)$ . We construct a graph w' by taking w and adding the three vertices  $v_1, v_2, v_3$  with coordinates  $(x_1+1, x_2, x_3, \ldots, x_d)$ ,  $(x_1, x_2+1, x_3, \ldots, x_d)$  and  $(x_1+1, x_2+1, x_3, \ldots, x_d)$  and  $(x_1+1, x_2+1, x_3, \ldots, x_d)$ , respectively, and the four edges  $(t, v_1)$ ,  $(t, v_2)$ ,  $(v_1, v_3)$ ,  $(v_2, v_3)$ . From the definition of top vertex,  $v_1, v_2$  and  $v_3$  are not members of the vertex set of w, so that w' has n+3 vertices. Since w is connected, the four added edges ensure that w' is connected and, because four edges and three vertices have been added, the cyclomatic index of w' is c+1. Hence  $w' \in W_{n+3,c+1}$ . The construction defines an injection from  $W_{nc}$  to  $W_{n+3,c+1}$  (since w' is uniquely determined by w and not all members of  $W_{n+3,c+1}$  can be obtained in this way) so that

$$a_{nc} \leq a_{n+3,c+1}.\tag{2.3}$$

Replacing c by c + 1 in (2.2) and n by n - 3 in (2.3) gives

$$a_{n-3,c} \leq a_{n,c+1} \leq 2dna_{nc}. \tag{2.4}$$

Taking logarithms, dividing by n, and letting n go to infinity shows that if  $\lim_{n\to\infty} n^{-1} \log a_{nc}$  exists and is equal to  $\log \lambda_c$  then  $\lim_{n\to\infty} n^{-1} \log a_{n,c+1}$  exists and is equal to  $\log \lambda_c$ . Klein (1981) has shown that

$$\lim_{n \to \infty} n^{-1} \log a_{n0} \equiv \log \lambda_0 \tag{2.5}$$

exists, so it then follows by induction that

$$\lim_{n \to \infty} n^{-1} \log a_{nc} = \log \lambda_0 \tag{2.6}$$

for any  $c \ge 0$ .

If we now make the usual assumption about the subdominant asymptotic behaviour that

$$a_{nc} \sim n^{-\theta_c} \lambda_c^n \tag{2.7}$$

(2.2), (2.3) and (2.7) imply that

$$\theta_c \ge \theta_{c+1} \ge \theta_c - 1. \tag{2.8}$$

#### 3. Series derivation and analysis

We have derived exact values of  $a_{nc}$  and  $A_{nc}$  for the triangular, square and simple cubic lattices. The data for c = 1 and 2 are given in tables 1-3. Some data for c = 0 have been given by Duarte and Ruskin (1981) and Gaunt *et al* (1982). We have derived additional terms for c = 0, as follows: for the triangular lattice  $a_{10,0}$  and  $a_{11,0}$ ,

and for the square lattice  $a_{13,0}$ ,  $a_{14,0}$  and  $a_{15,0}$ . These data, together with the earlier coefficients, are also given in tables 1-3.

We have analysed the above data using standard series analysis methods (Gaunt and Guttmann 1974). For one-animals weakly embeddable in the square lattice we have plotted against  $n^{-1}$  in figure 2 the ratios  $r_n = a_{n,1}/a_{n-1,1}$ , the linear extrapolants  $r'_n = nr_n - (n-1)r_{n-1}$  and their average  $r''_n = \frac{1}{2}(r_n + r'_n)$ , all of which should approach  $\lambda_1$ as  $n \to \infty$ . The arrow indicates the estimated value of  $\lambda_0$  (Gaunt *et al* 1982) and the data are in good agreement with the result of § 2 that  $\lambda_0 = \lambda_1$ . The corresponding evidence for the triangular and simple cubic lattices is equally satisfactory.

The exponent  $\theta_1$  can be estimated from the sequence of biased estimates

$$\theta_1(n) = n(1 - r_n/\lambda_0) \tag{3.1}$$

$A_{n2}$	$A_{n1}$	$A_{n0}$	<i>a</i> <sub>n2</sub>	$a_{n1}$	$a_{n0}$	n
		1			1	1
		3			3	2
	2	9		2	15	3
3	12	29	3	27	89	4
21	60	99	63	282	576	5
129	281	348	903	2 690	3 930	6
732	1 248	1 260	11 016	24 582	27 782	7
3 795	5 472	4 644	122 754	219 222	201 414	8
19 014	23 662	17 382	1 292 286	1 925 712	1 488 048	9
92 205	101 679	65 822		16 748 178	11 156 061	10
438 264	434 784	251 655			84 622 074	11
2 050 899	1 852 892	969 819				12
9 484 524	7 876 554	3 762 517				13
		14 680 890				14

**Table 1.** Values of  $a_{nc}$  and  $A_{nc}$  for the triangular lattice.

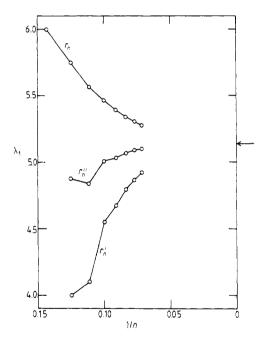
. .

**Table 2.** Values of  $a_{nc}$  and  $A_{nc}$  for the square lattice.

$A_{n2}$	$A_{n1}$	$A_{n0}$	<i>a</i> <sub>n2</sub>	<i>a</i> <sub>n1</sub>	<i>a</i> <sub>n0</sub>	n
· · · · · · · · · · · · · · · · · · ·		1		· · · · · · · · · · · · · · · · · · ·	1	1
		2			2	2
		6			6	3
	1	18		1	22	4
	8	55		8	87	5
2	40	174	2	54	364	6
22	168	570	22	324	1 574	7
134	677	1 908	194	1 863	6 986	8
656	2 708	6 473	1 446	10 372	31 581	9
3 008	10724	22 202	9 928	56 692	144 880	10
13 456	42 012	76 886	64 392	305 796	672 390	11
58 742	163 494	268 352	401 810	1 634 304	3 150 362	12
250 986	633 748	942 651	2 436 762	8 674 612	14 877 317	13
1 056 608	2 448 760	3 329 608		45 806 002	70 726 936	14
4 401 192	9 436 252	11 817 582			338 158 676	15
18 173 796	36 285 432	42 120 340				16
		150 682 450				17

n	a <sub>n0</sub>	<i>a</i> <sub>n1</sub>	$a_{n2}$	$A_{n0}$	$A_{n1}$	$A_{n2}$
1	1			1		
2	3			3		
3	15			15		
4	95	3		83	3	
5	678	48		486	48	
6	5 229	622	18	2 967	496	18
7	42 464	7 308	450	18 748	4 368	378
8	357 987	81 981	7 958	121 725	36 027	4 854
9	3 104 013	895 536	119 520	807 381	288 732	51 030
10	27 511 300	9 627 966	1 640 634	5 447 203	2 280 792	488 976
11	248 160 162			37 264 974	17 866 896	4 463 316

**Table 3.** Values of  $a_{nc}$  and  $A_{nc}$  for the simple cubic lattice.



**Figure 2.** Ratio estimates of  $\lambda_1$  for weak embeddings of one-animals on the square lattice. The arrow indicates the estimated value of  $\lambda_0$ .

where  $\hat{\lambda}_0$  is an estimate of  $\lambda_0$ . (For the square and simple cubic lattices we adopt our previous estimates  $(5.14 \pm 0.01 \text{ and } 10.50 \pm 0.07)$  biased using  $\theta_0 = 1$  and  $\theta_0 = 1\frac{1}{2}$ , respectively, while for the triangular lattice we obtain the biased estimate  $\lambda_0 = 8.41 \pm 0.02$ .)

We also form linear extrapolants

$$\theta_1'(n) = n\theta_1(n) - (n-1)\theta_1(n-1)$$
(3.2)

and the averages

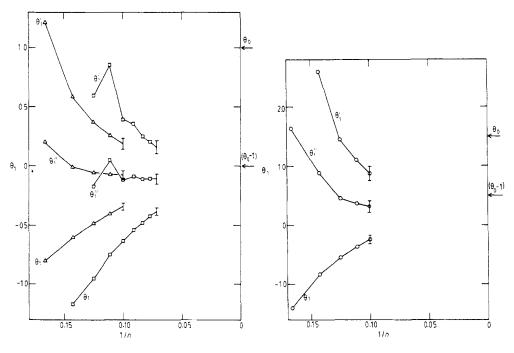
$$\theta_1''(n) = \frac{1}{2} [\theta_1(n) + \theta_1'(n)]$$
(3.3)

and plot  $\theta_1(n)$ ,  $\theta'_1(n)$  and  $\theta''_1(n)$  against  $n^{-1}$  in figures 3 and 4. The expected values of  $\theta_0$  (= $\theta$ ) are indicated by an arrow. Our estimate of  $\theta_1$  is

$$\theta_1 = -0.1 \pm 0.2, \qquad d = 2,$$
 (3.4)

$$= +0.3 \pm 0.4, \qquad d = 3,$$
 (3.5)

so that  $\theta_1$  is clearly not equal to  $\theta_0$ .



**Figure 3.** Biased ratio estimates of  $\theta_1$  for weak embeddings of one-animals on the square ( $\Box$ ) and triangular ( $\triangle$ ) lattices. The error bars reflect the uncertainties induced by the uncertainties in  $\lambda_0$ . The expected values of  $\theta_0$  and  $(\theta_0 - 1)$  are indicated by arrows.

Figure 4. Biased ratio estimates of  $\theta_1$  for weak embeddings of one-animals on the simple cubic lattice. The error bars reflect the uncertainties induced by the uncertainties in  $\lambda_0$ . The expected values of  $\theta_0$  and  $(\theta_0 - 1)$  are indicated by arrows.

It follows from (2.10) that

$$\theta_0 - 1 \le \theta_1 \le \theta_0 \tag{3.6}$$

and, accepting  $\theta_0 = \theta = 1$  for d = 2 (Gaunt *et al* 1982, Parisi and Sourlas 1981), we have

$$0 \le \theta_1 \le 1 \tag{3.7}$$

for d = 2. The results (3.4) and (3.7) strongly suggest that  $\theta_1$  may in fact be exactly equal to zero for d = 2. Further evidence that the lower bound in (3.6) may in fact be an equality is provided by the simple cubic lattice for which (3.6) gives

$$\frac{1}{2} \le \theta_1 \le 1\frac{1}{2},\tag{3.8}$$

assuming  $\theta_0 = \theta = 1\frac{1}{2}$  for d = 3 (Gaunt *et al* 1982, Parisi and Sourlas 1981). The results (3.5) and (3.8) are consistent with  $\theta_1$  being exactly equal to  $\frac{1}{2}$ . Accordingly we make

the conjecture that

$$\theta_1 = \theta_0 - 1 \qquad \forall d. \tag{3.9}$$

We have also confirmed with reasonable numerical precision that, for two-animals weakly embeddable in the same three lattices,  $\lambda_2 = \lambda_0$  as proved in § 2. For the exponent  $\theta_2$ , numerical techniques identical to those used above give the results plotted in figures 5 and 6, while from (2.8) it follows that for arbitrary d

$$\theta_0 - 2 \le \theta_2 \le \theta_0. \tag{3.10}$$

**Figure 5.** Biased ratio estimates of  $\theta_2$  for weak embeddings of two-animals on the square ( $\Box$ ) and triangular ( $\Delta$ ) lattices. The uncertainties induced by the uncertainties in  $\lambda_0$  are not visible on this scale. The expected value of  $(\theta_0 - 2)$  is indicated by an arrow.

**Figure 6.** Biased ratio estimates of  $\theta_2$  for weak embeddings of two-animals on the simple cubic lattice. The uncertainties induced by the uncertainties in  $\lambda_0$  are the size of the points (O). The expected value of  $(\theta_0 - 2)$  is indicated by an arrow.

In two dimensions, we obtain the estimate

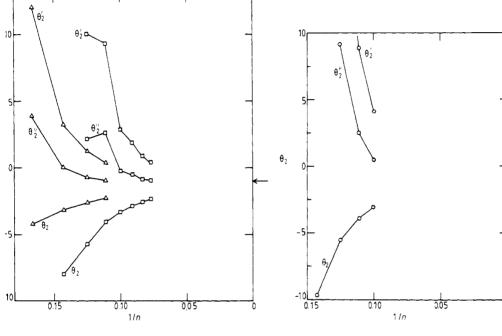
$$\theta_2 = -1 \pm 1, \qquad d = 2, \tag{3.11}$$

from figure 5 and the bounds

$$-1 \le \theta_2 \le 1 \tag{3.12}$$

from (3.10) assuming  $\theta_0 = \theta = 1$  as before. In view of our results for one-animals, these results again suggest that the lower bound in (3.10) might be an equality giving the *conjecture* 

$$\theta_2 = \theta_0 - 2 \qquad \forall d. \tag{3.13}$$



In three dimensions this gives  $\theta_2 = -\frac{1}{2}$  (assuming  $\theta_0 = \theta = 1\frac{1}{2}$ ) which is consistent with the results in figure 6 for the simple cubic lattice.

We have analysed the corresponding data for strongly embeddable clusters in exactly the same way. Although we have been unable to prove rigorously the analogue of (1.2), namely

$$\Lambda_c = \Lambda_0 \qquad \forall c, \tag{3.14}$$

this relation is supported by (or, at worst, is not inconsistent with) the numerical results for both one- and two-clusters given in figures 7, 8 and 9 for the triangular, square and simple cubic lattices, respectively. The arrows indicate the estimated values of  $\Lambda_0$ . (For the square and simple cubic lattices we adopt the values given by Gaunt *et al* (1982), while for the triangular lattice we have obtained the biased estimate  $\Lambda_0 = 4.196 \pm 0.007$ .) The conjecture (3.14) is also consistent with the results of  $1/\sigma$  expansions obtained in § 4.

Results for the exponent  $\Theta_1$  are shown in figures 10 and 11 and for  $\Theta_2$  in figures 12 and 13. The hypothesis of universal critical exponents for both weak and strong embeddings suggests that the existing conjectures (Gaunt *et al* 1982, Gaunt 1980)

$$\Theta_0 = \theta_0 = \theta = \Theta \tag{3.15}$$

should be supplemented by

$$\Theta_1 = \theta_1, \qquad \Theta_2 = \theta_2. \tag{3.16}$$

Thus, we expect from (3.9), (3.13) and (3.15), using  $\theta = 1$  (d = 2) and  $\theta = 1\frac{1}{2}$  (d = 3)

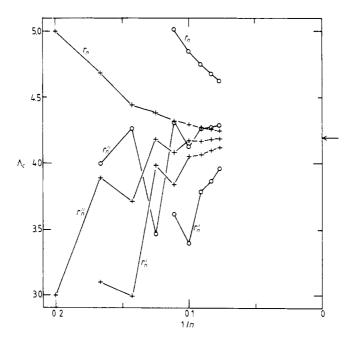


Figure 7. Ratio estimates of  $\Lambda_c$  for strong embeddings of one-animals (+) and two-animals (O) on the triangular lattice. The arrow indicates the estimated value of  $\Lambda_0$ .

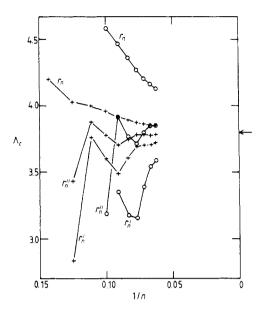


Figure 8. Ratio estimates of  $\Lambda_c$  for strong embeddings of one-animals (+) and two-animals ( $\bigcirc$ ) on the square lattice. The arrow indicates the estimated value of  $\Lambda_0$ .

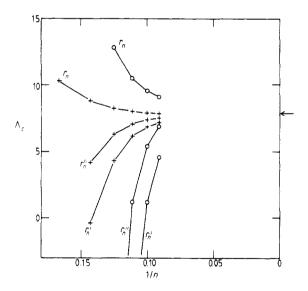
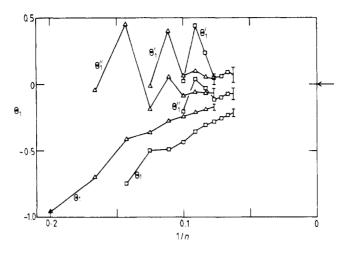


Figure 9. Ratio estimates of  $\Lambda_c$  for strong embeddings of one-animals (+) and two-animals ( $\bigcirc$ ) on the simple cubic lattice. The arrow indicates the estimated value of  $\Lambda_0$ .

(Parisi and Sourlas 1981), that

$$\Theta_1 = 0 \ (d = 2), \qquad \Theta_1 = \frac{1}{2} \ (d = 3), \\ \Theta_2 = -1 \ (d = 2), \qquad \Theta_2 = -\frac{1}{2} \ (d = 3).$$
 (3.17)

These predictions are well supported by the numerical evidence. For one-clusters we



**Figure 10.** Biased ratio estimates of  $\Theta_1$  for strong embeddings of one-animals on the square  $(\Box)$  and triangular  $(\Delta)$  lattices. The error bars reflect the uncertainties induced by the uncertainties in  $\Lambda_0$ . The expected value of  $(\Theta_0 - 1)$  is indicated by an arrow.

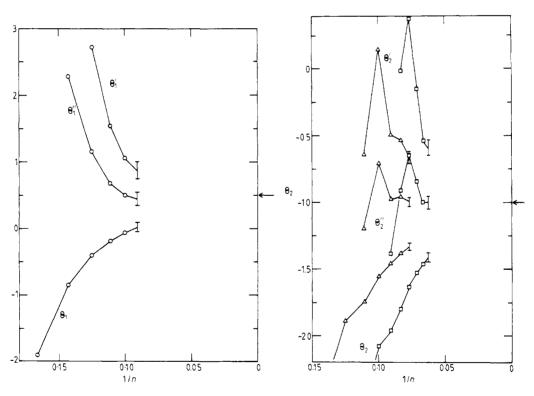


Figure 11. Biased ratio estimates of  $\Theta_1$  for strong embeddings of one-animals on the simple cubic lattice. The error bars reflect the uncertainties induced by the uncertainties in  $\Lambda_0$ . The expected value of  $(\Theta_0 - 1)$  is indicated by an arrow.

**Figure 12.** Biased ratio estimates of  $\Theta_2$  for strong embeddings of two-animals on the square ( $\Box$ ) and triangular ( $\Delta$ ) lattices. The error bars reflect the uncertainties induced by the uncertainties in  $\Lambda_0$ . The expected value of ( $\Theta_0 - 2$ ) is indicated by an arrow.

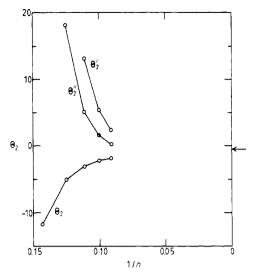


Figure 13. Biased ratio estimates of  $\Theta_2$  for strong embeddings of two-animals on the simple cubic lattice. The uncertainties induced by the uncertainties in  $\Lambda_0$  are not visible on this scale. The expected value of  $(\Theta_0 - 2)$  is indicated by an arrow.

estimate

$$\Theta_1 = -0.075 \pm 0.1, \qquad d = 2,$$
 (3.18)

$$= 0.4 \pm 0.3, \qquad d = 3, \qquad (3.19)$$

from figures 10 and 11, respectively, and for two-clusters

$$\Theta_2 = -1.0 \pm 0.25, \qquad d = 2,$$
 (3.20)

from figure 12. The results for the simple cubic lattice shown in figure 13 are consistent with a value of  $\Theta_2 = -\frac{1}{2}$  as given in (3.17).

## 4. Expansions for hypercubical lattices

First we derive expressions for the numbers of clusters with precisely c (=1, 2) cycles and m bonds, both weakly and strongly embeddable in a simple hypercubic lattice in d dimensions. These are obtained from the bond perimeter polynomials (see e.g. Sykes *et al* 1981) given by Gaunt and Ruskin (1978) in equation (2.1). To extract this information we note that the coefficient of  $q^{2(m+1)d-2m-2cd}$  in the perimeter polynomial  $D_m$  is the number of strongly embeddable clusters with m bonds, c cycles and hence n = m + 1 - c sites. Thus,

$$A_{11} = A_{21} = A_{31} = 0, \qquad A_{41} = 1 \binom{d}{2},$$

$$A_{51} = 8 \binom{d}{2} + 24 \binom{d}{3}, \qquad A_{61} = 40 \binom{d}{2} + 376 \binom{d}{3} + 576 \binom{d}{4},$$

$$A_{71} = 168 \binom{d}{2} + 3864 \binom{d}{3} + 15840 \binom{d}{4} + 15680 \binom{d}{5},$$

$$A_{81} = 677 \binom{d}{2} + 33996 \binom{d}{3} + 282216 \binom{d}{4} + 688640 \binom{d}{5} + 491520 \binom{d}{6},$$

$$(4.1)$$

and

$$A_{12} = A_{22} = A_{32} = A_{42} = A_{52} = 0, \qquad A_{62} = 2\binom{d}{2} + 12\binom{d}{3},$$
  
$$A_{72} = 22\binom{d}{2} + 312\binom{d}{3} + 624\binom{d}{4},$$
  
(4.2)

where  $\binom{d}{n}$  are binomial coefficients. Furthermore, the coefficient of  $q^{2(m+1)d-2m-2cd-p}$ , p = 1, 2, ... in  $D_m$  is the number of clusters with m bonds, c cycles and precisely p neighbouring contacts, i.e. pairs of neighbouring sites not joined by a bond. Summing these contributions gives the total number of weakly embeddable clusters with c cycles and n = m + 1 - c sites, namely

$$a_{11} = a_{21} = a_{31} = 0, \qquad a_{41} = 1 \begin{pmatrix} d \\ 2 \end{pmatrix}, \qquad a_{51} = 8 \begin{pmatrix} d \\ 2 \end{pmatrix} + 24 \begin{pmatrix} d \\ 3 \end{pmatrix},$$

$$a_{61} = 54 \begin{pmatrix} d \\ 2 \end{pmatrix} + 460 \begin{pmatrix} d \\ 3 \end{pmatrix} + 576 \begin{pmatrix} d \\ 4 \end{pmatrix},$$

$$a_{71} = 324 \begin{pmatrix} d \\ 2 \end{pmatrix} + 6 336 \begin{pmatrix} d \\ 3 \end{pmatrix} + 20 256 \begin{pmatrix} d \\ 4 \end{pmatrix} + 15 680 \begin{pmatrix} d \\ 5 \end{pmatrix},$$

$$a_{81} = 1 863 \begin{pmatrix} d \\ 2 \end{pmatrix} + 76 392 \begin{pmatrix} d \\ 3 \end{pmatrix} + 474 024 \begin{pmatrix} d \\ 4 \end{pmatrix} + 880 640 \begin{pmatrix} d \\ 5 \end{pmatrix} + 491 520 \begin{pmatrix} d \\ 6 \end{pmatrix},$$
and

and

$$a_{12} = a_{22} = a_{32} = a_{42} = a_{52} = 0, \qquad a_{62} = 2\binom{d}{2} + 12\binom{d}{3},$$
$$a_{72} = 22\binom{d}{2} + 384\binom{d}{3} + 624\binom{d}{4}.$$
(4.4)

For the special cases d = 2 and 3 we have extended each of these series as given in tables 2 and 3, respectively.

We now use these results to derive expansions for  $\Lambda_c$  and  $\lambda_c$  for c = 1 and 2 in inverse powers of  $\sigma = 2d - 1$ . The data in (4.1) may be written in the general form

$$A_{n1}(d) = \sum_{\xi=2}^{n-2} A_{n1}^{\xi} \binom{d}{n-\xi}.$$
(4.5)

For  $\xi = 2$  and 3 we have been able to calculate  $A_{n1}^{\xi}$  as functions of *n*,

$$A_{n1}(d) = 2^{n-3}n^{n-5}(n-2)(n-3)\binom{d}{n-2} + 2^{n-5}n^{n-7}(n-3)(n-4)$$
$$\times (2n^3 - 9n^2 + 5n + 50)\binom{d}{n-3} + \dots \qquad (n \ge 3).$$
(4.6)

This result may be obtained by first observing that strongly embeddable clusters with n sites and three or more cycles cannot 'stretch' into (n-3) dimensions or higher. Hence, the coefficients of the  $\binom{d}{n-\xi}$  ( $\xi = 1, 2, 3$ ) in  $N_n$ , the total number of strongly embeddable clusters with n sites, contain only contributions from  $A_{n0}$ ,  $A_{n1}$  and  $A_{n2}$ . The expansion of  $N_n$  is given by Gaunt *et al* (1976) in equation (2.4), and subtracting the expansions of  $A_{n0}$  and  $A_{n2}$  given by Gaunt *et al* (1982, equation (4.6)) and (4.9) below, respectively, gives (4.6). The leading term in (4.6) is in fact identical to the second contribution to  $\alpha_2^b$  given in equation (2.4) of Gaunt and Ruskin (1978), who also explain its origin in graph-theoretic terms.

Following the approach outlined by Gaunt *et al* (1976), we expand the binomial coefficients in (4.6) in inverse powers of  $\sigma$ , giving

$$A_{n1}(d) = \frac{1}{2} \frac{n^{n-5} \sigma^{n-2}}{(n-4)!} \left( 1 - \frac{5(n-4)(n^2 - n - 10)}{2n^2} \sigma^{-1} + \ldots \right).$$
(4.7)

Hence,

$$\ln \Lambda_1(d) = \lim_{n \to \infty} n^{-1} \ln A_{n1}(d) = \ln \sigma + 1 - 2\frac{1}{2}\sigma^{-1} + O(\sigma^{-2}),$$
(4.8)

which is term-by-term identical with the analogous expansion for  $\ln \Lambda_0$  (Gaunt *et al* 1982, equation (4.7)), at least to this order. This is consistent with  $\Lambda_1 = \Lambda_0$  as conjectured in (3.14).

For the case c = 2, we have only managed to calculate the leading coefficient  $A_{n2}^3$  in the analogue of (4.5), namely

$$A_{n2}(d) = \sum_{\xi=3}^{n-2} A_{n2}^{\xi} \binom{d}{n-\xi}$$
  
=  $2^{n-6} n^{n-7} (n-3)(n-4)(n-5)(n+6) \binom{d}{n-3} + \dots \qquad (n \ge 3).$  (4.9)

This coefficient is easily checked against the data in (4.2) but its derivation is rather difficult. In terms of the underlying graphs it contains contributions from the  $\theta$ -graph  $(3,1,3)_{\theta}$  decorated with (n-6) 'tails' and the 'dumbbells'  $(4,i,4)_D$  with  $i = 0, 1, 2, \ldots, (n-7)$ , and decorated with (n-7-i) 'tails'. No other graphs can stretch into (n-3) dimensions. (For the graph terminology, see Sykes (1961) and Sykes *et al* (1966).) If we again expand the binomial coefficient in  $1/\sigma$  we obtain

$$A_{n2}(d) = \frac{1}{8}n^{n-7} \frac{(n+6)}{(n-6)!} \sigma^{n-3} [1 + \mathcal{O}(\sigma^{-1})]$$
(4.10)

which yields

$$\ln \Lambda_2(d) = \lim_{n \to \infty} n^{-1} \ln A_{n2}(d) = \ln \sigma + 1 + O(\sigma^{-1}).$$
(4.11)

This expansion too coincides, as far as it goes, with the corresponding expansion for  $\ln \Lambda_0$  and is therefore consistent with  $\Lambda_2 = \Lambda_0$  as in (3.14).

We have performed similar calculations for the weak embeddings but only to zeroth order for both the c = 1 and 2 cases. For clusters which stretch into the maximum possible number of dimensions, there is no difference between weak and strong embeddings. Thus, the coefficients of  $\binom{d}{n-2}$  in (4.3) and (4.1) are identical, as are the coefficients of  $\binom{d}{n-3}$  in (4.4) and (4.2). Hence, from (4.6) and (4.9) we may write

$$a_{n1}(d) = 2^{n-3} n^{n-5} (n-2)(n-3) {d \choose n-2} + \dots \qquad (n \ge 2), \qquad (4.12)$$

$$a_{n2}(d) = 2^{n-6} n^{n-7} (n-3)(n-4)(n-5)(n+6) {d \choose n-3} + \dots \qquad (n \ge 3), \tag{4.13}$$

respectively. These expressions for  $a_{n1}$  and  $a_{n2}$ , like the expression for  $A_{n2}$ , are of

the form  $2^{n-p}n^{n-q}P(n) \binom{d}{n-r}$  where p, q and r are fixed integers and  $\lim_{n\to\infty} P(n)^{1/n} = 1$ . For any such function, expanding the binomial coefficients and proceeding as before will yield an expression of the form (4.11). To calculate the coefficient of  $\sigma^{-1}$  would require further terms in (4.9), (4.12) and (4.13), the calculation of which is highly non-trivial.

## 5. Connection with field theory results

Much of the work which has appeared on the importance of cycles in the modelling of branched polymer molecules by lattice animals has focused on the relationship between trees and animals with unrestricted cyclomatic index. The evidence suggests that these two classes of graphs have different growth constants but the same critical exponent (Duarte and Ruskin 1981, Gaunt *et al* 1982). In addition, renormalisation group arguments (Lubensky and Isaacson 1979, Family 1980) suggest that varying the cycle fugacity does not change the universality class.

In order to make contact with the field theoretic treatments, we present the following heuristic argument for weakly embeddable clusters (although analogous results appear to hold for strongly embeddable clusters). Consider the generating function

$$G(n, z) = \sum_{c \ge 0} a_{nc} z^{c}$$
(5.1)

where z is the cycle fugacity. Let us write

$$a_{nc} \simeq b_c n^{-\theta_c} \lambda_c^n \tag{5.2}$$

where  $b_c$  is the appropriate amplitude and use the exact result  $\lambda_c = \lambda_0$  (as implied by (2.6)) and the conjecture  $\theta_c = \theta_0 - c$  (which is the natural extension of the conjectures (3.9) and (3.13) and is discussed fully in § 6, equation (6.2) *et seq.*). Thus we obtain

$$G(n,z) = n^{-\theta_0} \lambda_0^n \sum_{c=0}^{c_{\max}} b_c n^c z^c \sim n^{-\theta_0} \lambda_0^n F(nz), \qquad n \to \infty,$$
(5.3)

where

$$F(w) = \sum_{c=0}^{\infty} b_c w^c$$
(5.4)

is the generating function of the amplitudes. Since  $G(n, 1) = a_n$ , the number of weakly embeddable animals with *n* sites, and  $\lim_{n \to \infty} a_n^{1/n}$  exists (Klarner 1967), it follows that

$$F(w) = \exp[O(w)], \qquad w \to \infty.$$
(5.5)

We find that  $\ln F(w)$  can be mimicked, over its whole range, by a [2/1] Padé approximant (Gaunt and Guttmann 1974). From (5.3), it is clear that this form for  $\ln F(w)$ , or indeed any [m+1/m] Padé approximant, is consistent with the growth constant being a function of z but with the exponent being independent of z and, in particular, with  $\theta_0 = \theta$ . Additive logarithmic correction terms ( $\phi \ln w$ ) to the Padé approximant form proposed for  $\ln F(w)$  appear to be ruled out since they would imply  $\theta = \theta_0 - \phi$  rather than  $\theta = \theta_0$ .

# 6. Discussion

In this paper we have considered the problem of animals with fixed cyclomatic index (*c*-animals). In § 2 we have shown rigorously that, for bond animals on the simple hypercubic lattice, the growth constant  $(\lambda_c)$  of *c*-animals is independent of the cyclomatic index (*c*), i.e.  $\lambda_c = \lambda_0$  for all *c*. Making the usual assumption that, asymptotically, the number  $(a_{nc})$  of *c*-animals with *n* sites can be written

$$a_{nc} \sim n^{-\theta_c} \lambda_c^n, \qquad n \to \infty \tag{6.1}$$

we have shown that  $\theta_c \ge \theta_{c+1} \ge \theta_c - 1$ . In § 3 we have used series analysis methods to estimate  $\lambda_c$  and  $\theta_c$  for c = 1, 2 and have found that the series evidence is consistent with  $\theta_c = \theta_{c-1} - 1$  for c = 1, 2. We have suggested that this may be true for all c.

For strong embeddings, the series analysis results suggest that the growth constants  $(\Lambda_c)$  are independent of c, i.e.  $\Lambda_c = \Lambda_0$  for all c, though we have been unable to prove this conjecture. In § 4 we have derived expansions of  $\Lambda_1$  and  $\Lambda_2$  in inverse powers of  $\sigma = 2d - 1$ , for d-dimensional hypercubic lattices, and these expansions are consistent with  $\Lambda_0 = \Lambda_1 = \Lambda_2$ . We have used series analysis techniques to estimate the corresponding exponents  $\Theta_1$  and  $\Theta_2$  and we suggest that  $\Theta_c = \Theta_{c-1} - 1$ . Together with the previous evidence that  $\theta_0 = \Theta_0$  (Duarte and Ruskin 1981, Gaunt *et al* 1982), this would imply that

$$\Theta_c = \theta_c = \theta_0 - c \tag{6.2}$$

for all c. Of course, (6.2) is only a conjecture, based on series evidence for c = 0, 1, 2. However, (2.8) implies the weaker result

$$\theta_c \ge \theta_0 - c. \tag{6.3}$$

In § 5 we considered the relationship between our results (especially that  $\theta_c$  depends on c) and the field theory arguments which suggest that the exponent is independent of cycle fugacity. We show that the particular expression which we propose for the c dependence of  $\theta_c$ , and the functional form for the generating function of the amplitudes indicated by our numerical data, are consistent with the field theory prediction.

#### Acknowledgments

It is a pleasure to thank Dr M F Sykes for helpful conversations and for communicating to us an unpublished theorem which enabled us to derive equation (4.9). In addition, his unpublished cluster data provided a useful check on some of our enumerations.

This research was financially supported in part by NSERC of Canada and NATO.

## References

Daoud M and Joanny J F 1981 J. Physique 42 1359 Duarte J A M S and Ruskin H J 1981 J. Physique 42 1585 Essam J W and Fisher M E 1970 Rev. Mod. Phys. 42 271 Family F 1980 J. Phys. A: Math. Gen. 13 L325 Gaunt D S 1980 J. Phys. A: Math. Gen. 13 L97

- Gaunt D S and Guttmann A J 1974 Phase Transitions and Critical Phenomena vol 3, ed C Domb and M S Green (New York: Academic) p 181
- Gaunt D S and Ruskin H J 1978 J. Phys. A: Math. Gen. 11 1369
- Gaunt D S, Sykes M F and Ruskin H J 1976 J. Phys. A: Math. Gen. 9 1899
- Gaunt D S, Sykes M F, Torrie G M and Whittington S G 1982 J. Phys. A: Math. Gen. 15 3209
- Klarner D A 1967 Can. J. Math. 19 851
- Klein D J 1981 J. Chem. Phys. 75 5186
- Lubensky T C and Isaacson J 1979 Phys. Rev. A 20 2130
- Parisi G and Sourlas N 1981 Phys. Rev. Lett. 46 871
- Seitz W A and Klein D J 1981 J. Chem. Phys. 75 5190
- Sykes M F 1961 J. Math. Phys. 2 52
- Sykes M F, Essam J W, Heap B R and Hiley B J 1966 J. Math. Phys. 7 1557
- Sykes M F, Gaunt D S and Glen M 1981 J. Phys. A: Math. Gen. 14 287