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Universality in branched polymers on *d*-dimensional hypercubic lattices

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Abstract. We have derived series for weakly and strongly embeddable trees in d-dimensional simple hypercubic lattices for arbitrary integral d. For $d=2, 3, \ldots, 9$ we present series evidence that such trees are in the same universality class as lattice animals. In addition we have derived expansions in inverse powers of $\sigma = 2d-1$ for the growth parameters for bond and site trees and compare these with the corresponding results for animals.

1. Introduction

The statistics of branched polymer molecules with excluded volume have been modelled by lattice animals, i.e. connected clusters embeddable in a regular lattice (Lubensky and Isaacson 1979). There have been several recent studies using field theoretic methods (Lubensky and Isaacson 1979), position space renormalisation group methods (Family 1980), Monte Carlo methods (Redner 1979) and series analysis methods (Duarte and Ruskin 1981) of the importance of cycles in determining the statistics of branched polymers. These studies suggest that lattice embeddable trees (i.e. branched polymers without cycles) are in the same universality class as lattice animals (i.e. branched polymers with no restrictions on the number of cycles). In addition, Seitz and Klein (1981) have used Monte Carlo techniques to estimate the exponent (ν) characterising the asymptotic behaviour of the mean-square radius of gyration for trees and find a value of $\nu = 0.615$ in two dimensions. This should be compared with $\nu = 0.66$ for lattice animals (Stauffer 1978, Herrmann 1979) and $\nu = 0.57 \pm 0.06$ for the particular branching model discussed by Redner (1979). While this numerical evidence is not entirely convincing, it is possible that these three problems are characterised by the same exponent.

In §§ 2 and 3 of this paper, we derive series expansions for the numbers of trees embeddable in the d-dimensional simple hypercubic lattice, for arbitrary integral d. We consider both weakly embeddable (bond) clusters, which are the more natural model of branched polymers, and strongly embeddable (site) clusters which, on general grounds, are expected to be in the same universality class. These series extend through nine sites for both weak and strong embeddings. For the special cases $d = 2$ and 3, Duarte and Ruskin (1981) have derived series for the square-lattice site trees to seventeen sites, the simple cubic site trees to ten sites and the simple cubic bond trees to nine bonds. We have confirmed their results for the square-lattice site trees and extended each of their series for the simple cubic lattice by one term. For the square-lattice bond trees we have extended our general d results from eight bonds to eleven bonds.

Analysis of these series strongly suggests that, for any d, trees and animals are in the same universality class.

If A_n is the number of site animals with n sites, Klarner (1967) has shown that

$$0<\lim_{n\to\infty} n^{-1}\log A_n \equiv \log \Lambda_{\mathrm{a}} < \infty. \tag{1.1}$$

Similarly, if a_n is the number of bond animals, an analogous argument (Whittington and Gaunt 1978) can be constructed giving

$$0<\lim_{n\to\infty} n^{-1}\log a_n \equiv \log \lambda_{\mathrm{a}} < \infty. \tag{1.2}$$

We shall use upper (lower) case letters for the numbers and growth parameters of strongly (weakly) embeddable clusters. An appropriate subscript (in this case 'a' for animal) will be appended when necessary.

Using similar arguments, one can show (Klein 1981) that

$$0<\lim_{n\to\infty} n^{-1}\log t_n \equiv \log \lambda_0 < \infty \tag{1.3}$$

where t_n is the number of weakly embeddable trees with n bonds, and a corresponding result can readily be derived for strongly embeddable trees with n sites. In this case the subscript zero signifies that the maximum number of allowed cycles is zero.

In § 4 we derive expansions in inverse powers of σ $(=2d-1)$ for λ_0 and Λ_0 and comparison with corresponding results (Gaunt *et al* 1976, Gaunt and Ruskin 1978) for λ_{a} and Λ_{a} strongly suggests that $\lambda_0<\lambda_{\mathrm{a}}$ and $\Lambda_0<\Lambda_{\mathrm{a}}$ for all d. These conclusions are supported by the series analysis results.

Gaunt *et al* (1979) have considered the problem of lattice animals in which the valence of each site is restricted to be less than or equal to some prescribed value (v). This problem is of interest as a model of steric hindrance in branched polymers and polymer gels. It appears that restricted valence animals with $v=3,4,\ldots,Q$, where Q is the lattice coordination number, are in the same universality class, while $v=2$ is in a different universality class (Gaunt *et al* 1979, 1980, Whittington *et al* 1979). In § 5, we derive series for restricted valence site *trees* for the square and simple cubic lattices. Analysis of these series strongly suggests that trees with $v\geqslant 3$ are in the same universality class as unrestricted trees ($v=Q$).

2. Bond clusters

We have derived expressions for the numbers of weakly embeddable trees with n bonds ($n\leqslant 8$) for the hypercubic lattic in d dimensions. These were obtained from the bond perimeter polynomials given by Gaunt and Ruskin (1978) in equation (2.1). To extract this information we note that the coefficient of $q^{2(nd+d-n)}$ in the perimeter polynomial D_n is the number of strongly embeddable trees with n bonds. Similarly the coefficient of $q^{2(nd+d-n)-p}$, $p=1,2,\ldots$, will be the number of trees with 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 trees with n bonds, namely

$$t_1 = \binom{d}{1}$$
$$t_2 = \binom{d}{1} + 4\binom{d}{2}$$
$$t_3 = \binom{d}{1} + 20\binom{d}{2} + 32\binom{d}{3}$$
$$t_4 = \binom{d}{1} + 85\binom{d}{2} + 420\binom{d}{3} + 400\binom{d}{4}$$
$$t_5 = \binom{d}{1} + 362\binom{d}{2} + 4\,140\binom{d}{3} + 10\,368\binom{d}{4} + 6\,912\binom{d}{5}$$
$$t_6 = \binom{d}{1} + 1\,572\binom{d}{2} + 37\,745\binom{d}{3} + 185\,976\binom{d}{4} + 301\,840\binom{d}{5} + 153\,664\binom{d}{6}$$
$$t_7 = \binom{d}{1} + 6\,984\binom{d}{2} + 337\,032\binom{d}{3} + 2\,914\,304\binom{d}{4} + 8\,622\,080\binom{d}{5} + 10\,223\,616\binom{d}{6} + 4\,194\,304\binom{d}{7}$$
$$t_8 = \binom{d}{1} + 31\,579\binom{d}{2} + 3\,009\,273\binom{d}{3} + 43\,043\,049\binom{d}{4} + 206\,473\,320\binom{d}{5} + 427\,217\,328\binom{d}{6} + 396\,809\,280\binom{d}{7} + 136\,048\,896\binom{d}{8} \qquad (2.1)$$

where $\binom{d}{n}$ are binomial coefficients.

In addition we have extended these series for the square and simple cubic lattices and the extended series are given in table 1.

Table 1. Numbers of bond trees $t_n(d)$ and site trees $T_n(d)$ on the square ($d = 2$) and simple cubic ($d = 3$) lattices.

n	$t_n(2)$	$T_n(2)$	$t_n(3)$	$T_n(3)$
1	2	1	3	1
2	6	2	15	3
3	22	6	95	15
4	87	18	678	83
5	364	55	5 229	486
6	1 574	174	42 464	2 967
7	6 986	570	357 987	18 748
8	31 581	1 908	3 104 013	121 725
9	144 880	6 473	27 511 300	807 381
10	672 390	22 202	248 160 162	5 447 203
11	3 150 362	76 886		37 264 974
12		268 352		
13		942 651		
14		3 329 608		
15		11 817 582		
16		42 120 340		
17		150 682 450		

We have analysed all the data above using standard ratio methods (Gaunt and Guttmann 1974). Defining the ratios for the numbers of trees

$$\lambda_0(n) = t_n/t_{n-1} \qquad (2.2)$$

and their linear extrapolants

$$\lambda_0'(n) = n\lambda_0(n) - (n-1)\lambda_0(n-1) \qquad (2.3)$$

we estimate the exponent θ_0 in the expected asymptotic expression

$$t_n \sim n^{-\theta_0}\lambda_0^n \tag{2.4}$$

from the sequence

$$\theta_0(n) = n\{1-[\lambda_0(n)/\lambda_0'(n)]\}. \tag{2.5}$$

For the square lattice the values of $\theta_0(n)$ are shown in figure 1. For comparison we include the estimates of the corresponding exponent (θ) for the total numbers of bond animals. These data provide strong support for the conjecture that $\theta_0 = \theta$. Universality

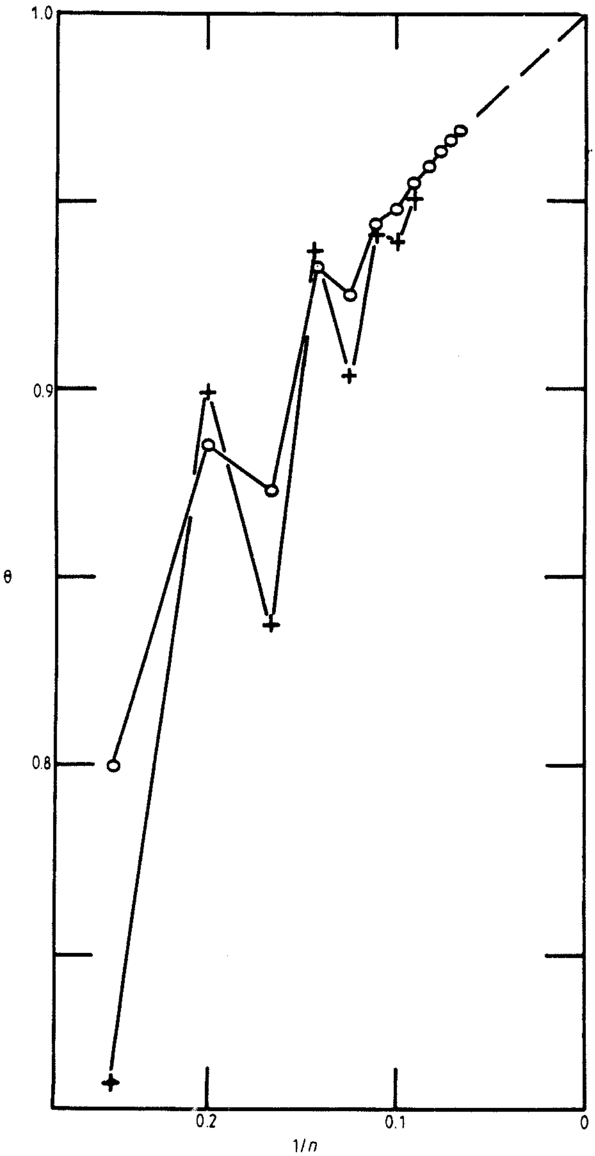

Figure 1. Ratio estimates of the exponent θ for bond trees (+) and bond animals (○) on the square lattice.

arguments coupled with the relationship to the Yang–Lee edge singularity (Parisi and Sourlas 1981) suggest that $\theta = 1$ in two dimensions. Hence it follows that $\theta_0 = 1$. For $d \geqslant 3$, the corresponding results for θ_0 (see table 2) for the hypercubic lattices are in good agreement with previous estimates of θ (Gaunt 1980), and for the higher values of d the plots of the extrapolants for θ and θ_0 essentially coincide.

Table 2. Estimates of exponents and growth parameters for bond clusters. $\Delta\theta_0 = \theta_0 - \hat{\theta}_0$ where $\hat{\theta}_0$ is our central estimate.

d	θ_0	λ_0	$\lambda_0^{(\sigma)}$
2	1.00 ± 0.02	$5.14 \pm 0.01 + 0.26\Delta\theta_0$	4.88
3	1.55 ± 0.05	$10.53 \pm 0.07 + 0.6\Delta\theta_0$	10.98
4	1.9 ± 0.1	$16.2 \pm 0.4 + 1.4\Delta\theta_0$	16.75
5	2.2 ± 0.2	$22.1 \pm 0.9 + 2.0\Delta\theta_0$	22.38
6	2.3 ± 0.2	$27.5 \pm 1.3 + 2.6\Delta\theta_0$	27.94
7	2.4 ± 0.2	$33.0 \pm 1.7 + 3.2\Delta\theta_0$	33.47
8	2.5 ± 0.2	$39.0 \pm 2.2 + 3.9\Delta\theta_0$	38.97
9	2.5 ± 0.3	$44.5 \pm 2.5 + 4.5\Delta\theta_0$	44.46

In view of the above results we form biased estimates of λ_0,

$$\lambda_0''(n) = n\lambda_0(n)/(n-\theta) \tag{2.6}$$

where we use the best available estimates (Gaunt 1980) of the bond animal exponent θ, except that for $d = 2$ and 3 we use the values given by Parisi and Sourlas (1981), and for $d \geqslant 8$ we use the mean field value of θ. These estimates approach λ_0 from above while the sequence given by equation (2.3) approaches λ_0 from below. We form the sequence

$$\lambda'''(n) = \tfrac{1}{2}[\lambda_0'(n) + \lambda_0''(n)] \tag{2.7}$$

which, it transpires, is only very weakly dependent on n. The final estimates of λ_0 formed in this way are given in table 2. The error estimates given differentiate between the inherent uncertainty and the uncertainty induced by errors in the estimate of θ. In two dimensions the inherent error bars of the estimates of λ_a (Gaunt 1980) and λ_0 (table 2) do not overlap, which strongly suggests that λ_0 is *strictly* less than λ_a. In higher dimensions the error bars do overlap. Nevertheless, we strongly suspect that $\lambda_0 < \lambda_a$ for all d and we present some evidence for this in § 4.

It is possible, using an extension of the methods used by Whittington and Gaunt (1978), to show that

$$\log \lambda_0 \geqslant m^{-1} \log(dt_m) \tag{2.8}$$

for any m for a d-dimensional hypercubic lattice. For $d=2$, using $m = 11$ we obtain $\lambda_0 \geqslant 4.1507\ldots$ while for $d = 3$ using $m = 10$ gives $\lambda_0 \geqslant 7.7123\ldots$. Although these bounds are rather weak (cf table 2) they are sufficient to prove rigorously that $\lambda_0 > \mu$, where μ is the self-avoiding walk limit, i.e. the exponential of the connective constant of the lattice.

3. Site clusters

The numbers (T_s) of trees with s sites strongly embeddable in the d-dimensional hypercubic lattice (site trees) can be obtained from the bond perimeter polynomial $D_{s-1}(q)$ given by Gaunt and Ruskin (1978), as the coefficient of the highest power of q. The results are given below for $s \leqslant 9$.

$$T_1 = 1$$
$$T_2 = \binom{d}{1}$$
$$T_3 = \binom{d}{1} + 4\binom{d}{2}$$
$$T_4 = \binom{d}{1} + 16\binom{d}{2} + 32\binom{d}{3}$$
$$T_5 = \binom{d}{1} + 53\binom{d}{2} + 324\binom{d}{3} + 400\binom{d}{4}$$
$$T_6 = \binom{d}{1} + 172\binom{d}{2} + 2\,448\binom{d}{3} + 8\,064\binom{d}{4} + 6\,912\binom{d}{5}$$
$$T_7 = \binom{d}{1} + 568\binom{d}{2} + 17\,041\binom{d}{3} + 112\,824\binom{d}{4} + 239\,120\binom{d}{5} + 153\,664\binom{d}{6}$$
$$T_8 = \binom{d}{1} + 1\,906\binom{d}{2} + 116\,004\binom{d}{3} + 1\,382\,400\binom{d}{4} + 5\,445\,120\binom{d}{5} + 8\,257\,536\binom{d}{6} + 4\,194\,304\binom{d}{7}$$
$$T_9 = \binom{d}{1} + 6\,471\binom{d}{2} + 787\,965\binom{d}{3} + 15\,998\,985\binom{d}{4} + 104\,454\,120\binom{d}{5} + 280\,717\,488\binom{d}{6} + 326\,265\,408\binom{d}{7} + 136\,048\,896\binom{d}{8}. \quad (3.1)$$

We have extended these series for $d = 2$ and 3 to $s = 17$ and $s = 11$, respectively, and the results are given in table 1. Using the methods described in § 2 we have analysed all of the above series and the results are given in table 3.

Table 3. Estimates of exponents and growth parameters for site clusters. $\Delta\theta_0 = \theta_0 - \hat{\theta}_0$ where $\hat{\theta}_0$ is our central estimate of θ_0.

d	θ_0	Λ_0	$\Lambda_0^{(\sigma)}$
2	1.0 ± 0.1	$3.795 \pm 0.007 + 0.15\Delta\theta_0$	2.25
3	1.5 ± 0.1	$7.85 \pm 0.05 + 0.4\Delta\theta_0$	7.32
4	1.9 ± 0.1	$12.7 \pm 0.3 + 0.9\Delta\theta_0$	12.61
5	2.15 ± 0.15	$17.9 \pm 0.5 + 1.4\Delta\theta_0$	17.96
6	2.3 ± 0.2	$23.3 \pm 0.7 + 1.8\Delta\theta_0$	23.34
7	2.4 ± 0.2	$28.8 \pm 1.0 + 2.3\Delta\theta_0$	28.74
8	2.5 ± 0.3	$34.0 \pm 1.2 + 2.8\Delta\theta_0$	34.15
9	2.5 ± 0.3	$39.5 \pm 1.5 + 3.2\Delta\theta_0$	39.57

The agreement between these estimates of θ_0 and the corresponding estimates for bond trees (table 2), bond animals and site animals (Gaunt 1980) is excellent. If we compare the estimates of Λ_0 with the estimates of Λ_a given by Gaunt (1980) we see that the central estimates of Λ_0 are always less than the central estimates of Λ_a. In addition, for $d \leqslant 4$, the inherent error bars (i.e. not including uncertainties in the value of the exponent) of Λ_0 and Λ_a do not overlap which strongly suggests that $\Lambda_0 < \Lambda_a$.

Following the arguments of Whittington and Gaunt (1978) it is easy to show that

$$\log \Lambda_0 \geqslant m^{-1} \log(dT_m). \quad (3.2)$$

Using the last available series coefficient in (3.2) gives $\Lambda_0 \geqslant 3.1533\ldots$ for $d=2$ and $\Lambda_0 \geqslant 5.3910\ldots$ for $d=3$. In fact, repeating this procedure for $d=4,5,6\ldots$ (3.2) shows that $\Lambda_0 > (2d-1) > \mu$.

4. Expansions in inverse powers of dimension

In this section we derive expansions for λ_0 and Λ_0 in inverse powers of $\sigma = Q-1 = 2d-1$.

Equation (2.1) can be written as

$$t_n(d) = 2^n(n+1)^{n-2}\binom{d}{n} + 2^{n-2}(n+1)^{n-4}(n-1)(n+1)(2n-1)\binom{d}{n-1} + 2^{n-4}(n+1)^{n-6}(n-2)(n+1)\tfrac{1}{6}(12n^4-20n^3-33n^2-46n+195)\binom{d}{n-2} + \ldots + \binom{d}{1}. \quad (4.1)$$

This can be obtained from equation (2.4) of Gaunt and Ruskin (1978), which is the corresponding result for bond animals, by omitting terms corresponding to contributions from clusters containing cycles.

Following the general procedure outlined by Gaunt and Ruskin (1978) we expand the binomial coefficients in inverse powers of σ giving

$$t_n(d) = \frac{(n+1)^{n-2}\sigma^n}{n!}\left(1 - \frac{n(n-5)}{2(n+1)}\sigma^{-1} + \frac{n(n-1)(n-2)(3n^2-82n+155)}{24(n+1)^3}\sigma^{-2} + \ldots\right). \quad (4.2)$$

Hence

$$\ln \lambda_0(d) = \lim_{n\to\infty} n^{-1} \ln t_n(d) = \ln\sigma + 1 - \tfrac{1}{2}\sigma^{-1} - 2\tfrac{2}{3}\sigma^{-2} - \ldots. \quad (4.3)$$

This can be written as

$$\lambda_0(d) = B(\sigma)(1 - 2\tfrac{1}{2}\sigma^{-2} + \ldots) \quad (4.4)$$

where

$$B(\sigma) = \sigma^\sigma/(\sigma-1)^{\sigma-1} \quad (4.5)$$

the Bethe approximation to the number of lattice animals.

For the corresponding site problem it can be shown that

$$T_s(d) = 2^{s-1}s^{s-3}\binom{d}{s-1} + 2^{s-3}s^{s-5}(s-2)(2s^2-7s+12)\binom{d}{s-2} + 2^{s-5}s^{s-7}(s-3)\tfrac{1}{6}(12s^5-116s^4+459s^3-916s^2+1044s-720)\binom{d}{s-3} + \ldots + \binom{d}{1} \quad (4.6)$$

and hence that

$$\ln \Lambda_0(d) = \ln\sigma + 1 - 2\tfrac{1}{2}\sigma^{-1} - 2\tfrac{1}{6}\sigma^{-2} - \ldots \quad (4.7)$$

or, alternatively,

$$\Lambda_0(d) = B(\sigma)[1 - 2\sigma^{-1} + O(\sigma^{-3})]. \quad (4.8)$$

Although these series are probably asymptotic, comparison of (4.4) and (4.8) suggests that $\Lambda_0(d) < \lambda_0(d)$ for all d. Similarly, comparison of (4.4) and (4.8) with the corresponding expansions for λ_a (Gaunt and Ruskin 1978) and Λ_a (Gaunt *et al* 1976) suggests that the rigorous results $\lambda_0 \leq \lambda_a$ and $\Lambda_0 \leq \Lambda_a$ are in fact *strict* inequalities for all d.

For $d = 2, 3, \ldots, 9$ we have estimated λ_0 and Λ_0 by truncating (4.4) and (4.8) after the last term given, and the resulting estimates, $\lambda_0^{(\sigma)}$ and $\Lambda_0^{(\sigma)}$, are presented in tables 2 and 3 respectively. These estimates agree with the series estimates, to within the inherent uncertainties in the latter, when $d \geq 5$ for bond trees and when $d \geq 4$ for site trees. As expected, the agreement improves as d increases.

5. Restricted valence site trees

In this section we investigate whether restricting the maximum allowed valence of sites in a tree changes the universality class.

We have enumerated site trees with maximum valence $v = 2, 3, \ldots, Q$ for the square and simple cubic lattices. For $v = 2$ the resulting trees are the neighbour avoiding walks (Whittington *et al* 1979, Gaunt *et al* 1980). We give the results for $3 \leq v < Q$ in table 4.

Table 4. Numbers of restricted valence site trees on the square and simple cubic lattices.

	Square	Simple cubic		
n	$v = 3$	$v = 3$	$v = 4$	$v = 5$
1	1	1	1	1
2	2	3	3	3
3	6	15	15	15
4	18	83	83	83
5	54	471	486	486
6	170	2 805	2 961	2 967
7	552	17 271	18 693	18 747
8	1 828	109 167	121 257	121 719
9	6 132	704 331	803 526	807 336
10	20 796	4 619 459	5 415 905	5 446 847
11	71 212	30 709 443	37 014 099	37 262 148
12	245 744			
13	853 500			
14	2 980 892			
15	10 461 630			
16	36 871 562			

Standard series analysis methods yield for the square lattice

$$\lambda_0(v = 3) = 3.75 \pm 0.02 \tag{5.1}$$

and, for the simple cubic lattice

$$\begin{aligned} \lambda_0(v = 3) &= 7.62 \pm 0.08 \\ \lambda_0(v = 4) &= 7.835 \pm 0.035 \\ \lambda_0(v = 5) &= 7.845 \pm 0.05. \end{aligned} \tag{5.2}$$

The estimates of the corresponding exponent are 1.00 ± 0.07 for the square lattice and 1.5 ± 0.1 for the simple cubic lattice, for $v = 3, 4$ and 5. Thus, restricted valence trees for $v \geq 3$ appear to be in the same universality class as unrestricted trees and both valence restricted and unrestricted animals. However, trees with $v = 2$ are in the same universality class as self-avoiding walks, for which the exponents are approximately $-\frac{1}{3}$ in two dimensions and $-\frac{1}{6}$ in three dimensions (Watson 1970, Torrie and Whittington 1977, Gaunt *et al* 1980).

6. Summary

The primary result of this paper is that, for hypercubic lattices from two dimensions up to and including the upper critical dimension, both site and bond trees are in the same universality class as both site and bond animals. This strongly supports the proposal (Lubensky and Isaacson 1979) that in branched polymers the universality class is independent of cycle fugacity.

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