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Caliper diameter of branched polymers

V Privman†, F Family‡ and A Margolina§

† Baker Laboratory, Cornell University, Ithaca, NY 14853, USA
‡ Department of Physics, Emory University, Atlanta, GA 30322, USA
§ Department of Chemical Engineering, Princeton University, Princeton, NJ 83544, USA

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Abstract. We report analyses of exact numerical data for the spanning diameter of two-dimensional lattice animals up to size $N = 17$. Estimates of the exponent ν are consistent with previous studies. The leading correction to scaling has an exponent $\sigma \simeq \nu$ which does not result from irrelevant variable effects. Interpretation of this correction as a 'surface' term is proposed.

The scaling form of the radius of gyration, R_N, of N-site lattice animals, which model branched polymers in the dilute limit (Lubensky and Isaacson 1979, Family 1980) is

$$R_N \equiv \langle R_N^2 \rangle^{1/2} = aN^{\nu}(1 + bN^{-\theta} + \ldots), \qquad \text{as } N \to \infty, \tag{1}$$

(see e.g., Stauffer 1978, Peters *et al* 1979). The second term in (1) represents the leading correction to scaling. Higher-order terms are usually higher powers of $1/N$. One has

$$\theta = \nu y, \tag{2}$$

where y is the absolute value of the leading irrelevant-variable renormalisation group eigen-exponent. Several recent numerical estimates of ν and θ in two dimensions (Derrida and DeSeze 1982, Family 1980, 1983, Guttmann 1982, Margolina *et al* 1984a, b, Parisi and Sourlas 1981, Peters *et al* 1979, Privman 1984) can all be plausibly summarised by the ranges

$$\nu = 0.641 \pm 0.005 \tag{3}$$

and

$$\theta = 0.87 \pm 0.07. \tag{4}$$

A different quantity which measures cluster size is the caliper or spanning diameter, $\langle D_N \rangle$, averaged over all N-site animals, defined as a length of a 'projection' of an animal on some fixed axis (Quinn *et al* 1976, Harrison *et al* 1978, see also Redner and Yang 1982). One can also define moments $\langle D_N^2 \rangle$, etc. Asymptotically, for large N, one should have

$$\langle D_N^k \rangle \approx \text{constant} \cdot R_N^k, \qquad k = 1, 2, \ldots \tag{5}$$

(see, e.g., Harrison *et al* 1978), however, *new corrections to scaling* may be present in $\langle D_N^k \rangle$. This property has been noticed by Margolina *et al* (1984a) who studied *directed* lattice animals. The motivation for studying caliper diameter moments is that there is no natural definition of the isotropic radius of gyration for directed problems. Thus more complicated quantities, e.g., caliper diameters, have to be employed. These quantities may have new corrections to the leading scaling relation (5). In this note we report analysis of these corrections in the case of the isotropic, two-dimensional lattice animals.

One may argue that the surface of a cluster (animal) contributes differently to $\langle D_N^k\rangle$ as compared to R_N because the surface structure is averaged in calculating R_N but not in $\langle D_N^k\rangle$ where the external points determine the size of a projection. If one *conjectures*, guided by the analogy with thermodynamic properties (Fisher 1971 and 1973, review by Binder 1983) that this contribution is of a relative magnitude $1/R$, one has

$$\langle D_N^k\rangle = g_k R_N^k + q_k R_N^{k-1} + \ldots, \qquad \text{as } N\to\infty. \tag{6}$$

More detailed scaling arguments for the R_N^{k-n} terms can be proposed (Fisher and Privman, unpublished), however, strong assumptions on the behaviour of scaling functions are needed which cannot be established beyond a level of reasonable conjecture. Thus one cannot exclude the possibility of *non-analytic* power-law corrections. Presence of the R_N^{k-n} terms is also suggested by arbitrariness in defining the spanning diameter by say, a number of sites or bonds, etc. Different definitions of the spanning length, when averaged, will differ by terms of order R_N^{k-1}, $R_N^{k-2}, \ldots$.

We will present numerical evidence (for $k=1,2$) for the presence of the new term, $N^{-\sigma}$, in

$$\langle D_N^k\rangle = A_k N^{k\nu}(1 + B_k N^{-\sigma} + C_k N^{-\theta} + \ldots), \qquad \text{as } N\to\infty, \tag{7}$$

with σ close to ν, see result (12) (relations (6) and (1) imply $\sigma\equiv\nu$).

In table 1 we list results of enumeration of $\langle D_N\rangle$ and $\langle D_N^2\rangle$ for $N\leq 17$, on the square lattice. Results for the number of animals, C_N, are also listed (see Redelmeier (1981) for $C_{18},\ldots, C_{24}$ and Guttmann (1982) for references to earlier enumeration studies). Values of $\langle R_1^2\rangle$ to $\langle R_{15}^2\rangle$ have been calculated by Peters *et al* 1979.

Table 1. Values of $C_N\langle D_N\rangle$, $C_N\langle D_N^2\rangle$ and of C_N, for $N=1,\ldots,17$.

N	$C_N\langle D_N\rangle$	$C_N\langle D_N^2\rangle$	C_N
1	0	0	1
2	1	1	2
3	6	8	6
4	28	50	19
5	120	266	63
6	498	1 308	216
7	2 040	6 152	760
8	8 299	28 121	2 725
9	33 616	125 962	9 910
10	135 801	555 873	36 446
11	547 698	2 425 500	135 268
12	2 206 620	10 490 282	505 861
13	8 884 486	45 050 386	1 903 890
14	35 757 744	192 354 622	7 204 874
15	143 885 980	817 389 682	27 394 666
16	578 935 561	3 459 473 699	104 592 937
17	2329 387 868	14 591 722 570	400 795 844

We analysed the $\langle D_N \rangle$ and $\langle D_N^2 \rangle$ sequences by the method of Adler *et al* (1982, 1983). This technique has been described in detail by Adler *et al* (1983); $\langle D_N \rangle$ and $\langle D_N^2 \rangle$ are regarded as series expansion coefficients of the generating functions

$$f_k(z) \equiv \sum_{N=2}^{\infty} \langle D_N^k \rangle z^{N-2}, \tag{8}$$

which must be singular at $z = 1$ but analytic for $|z| < 1$. Then ν is estimated for various trial σ values by forming several central Padé approximants, $\nu^{[L/M]}(\sigma)$, to a properly transformed generating function (see Adler *et al* (1983) for details), The curves $\nu^{[L/M]}(\sigma)$ are expected to display a region of 'confluence' near the correct (ν, σ).

In figures 1 and 2 we plot several $\nu^{[L/M]}(\sigma)$ curves for $\langle D_N \rangle$ and $\langle D_N^2 \rangle$, respectively. The series studied here are relatively long; however, due to proliferation of correction terms in $\langle D_N^k \rangle$, the ranges of exponent estimates are relatively broad (see below) and

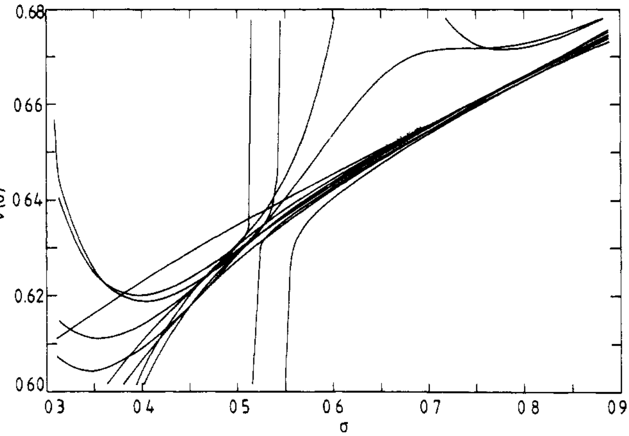

Figure 1. Curves of $\nu^{[L/M]}(\sigma)$ for the $\langle D_N \rangle$ sequence, calculated by using [6/9], [7/8], [8/7], [9/6], [6/8], [7/7], [8/6], [6/7] and [7/6] Padé approximants (see Adler *et al* 1983).

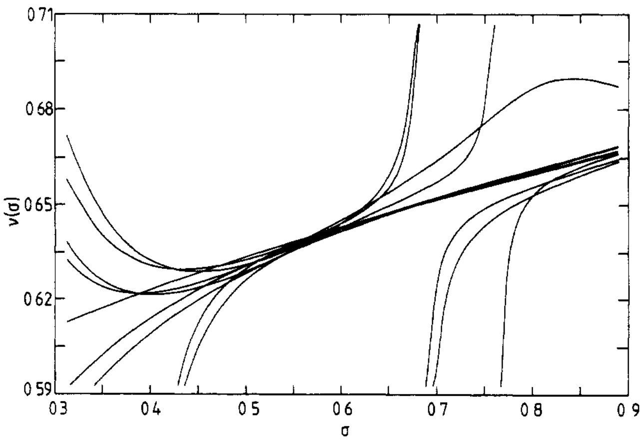

Figure 2. Curves of $\nu^{[L/M]}(\sigma)$ for the $\langle D_N^2 \rangle$ sequence, calculated with the same Padé approximants as in figure 1.

inaccurate as complared to results obtained, e.g., from the (shorter) $\langle R_N^2 \rangle$ series (see Peters *et al* 1980, Margolina *et al* 1984a). In figures 1 and 2 we observe broad confluence regions by considering the size of which one could propose

$$\nu_1 = 0.625 \pm 0.010, \qquad \sigma_1 = 0.49 \pm 0.06, \tag{9}$$

$$\nu_2 = 0.630 \pm 0.015, \qquad \sigma_2 = 0.55 \pm 0.07, \tag{10}$$

where 1 and 2 denote results for $\langle D_N \rangle$ and $\langle D_N^2 \rangle$, respectively. We definitely seem to have $\sigma < \theta$ (see (4)), but the ν estimates are only just consistent with the previous, more accurate results summarised by (3). Therefore the reliability of the error bars in (9) and (10) is rather questionable.

In order to obtain more reliable estimates of σ, we use the ν values given in (3) to bias the estimates: thus we locate the range of values of σ for which the estimates for ν in (7) satisfy

$$0.636 \leqslant \nu^{[L/M]}(\sigma) \leqslant 0.646. \tag{11}$$

The resulting σ estimates are then

$$\sigma_1 = 0.58 \pm 0.07 \qquad \text{and} \qquad \sigma_2 = 0.59 \pm 0.07. \tag{12}$$

These two ranges are consistent and again indicate $\sigma < \theta$. The equality of σ and ν is allowed by the upper limits of the σ ranges here. However, it should be recalled that correction exponent estimates may possess systematic errors arising from the presence of the higher-order terms.

In summary, we have presented numerical evidence for new corrections to scaling in $\langle D_N^k \rangle$, with an exponent close to or actually equal to ν which may be interpreted as a simple 'surface contribution'.

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