ZINN-JUSTIN AND PRIVMAN-FISHER ESTIMATORS FOR THREE-DIMENSIONAL UNDIRECTED LATTICE ANIMALS

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ABSTRACT — The recent appearance of markedly different non-overlapping ranges for the first correction exponent of undirected lattice animals in 2 and 3 dimensions is examined. One of the earliest estimated ranges (in 2 dimensions) stood for nearly 8 years (the three-dimensional one is 2 years old) and we try to gain a clear perspective on the question using newly extended series data. To the best of the present accuracy we feel the newly-analysed three-dimensional results favour a value closer to 0.64 than to any value below 0.5. (New central estimates of 0.45 from a Monte-Carlo randomization method have been proposed for the radius of gyration of lattice animals in 3 dimensions.)

INTRODUCTION

Lattice animals are by now a classical area of lattice statistics whose studies have influenced an enormous mass of material in most phenomenological subjects relating to cluster growth and kinetics, with a special emphasis on gelation, aggregation, polymers and percolation models. They are, of course, their essential geometrical substrate (in discrete models) and the corpus of exact (and well established) results on topological properties and their influence on critical exponents, growth parameters and dimensional dependence can be used as a testing ground for new developments in series studies, transfer matrix calculations or Monte-Carlo generation procedures.

Real interest in lattice animals, per se, always an overlooked by-product of percolation enumeration in the 1970's, was spurred on by Lubensky's lengthy field theory on animal partitions according to site valence and cyclomatic number [1], which predicted that the upper critical dimensionality was $d_c = 8$ and that the restricted set of lattice animals with no closed loops (or cycles), called 'lattice trees', shared the same critical exponent as the complete set of animals for all dimensions and problems. Family [2], with small-cell renormalization, Seitz and Klein [3], with Monte-Carlo tree generation in 2 and 3 dimensions, and Duarte and Ruskin [4], using series expansions, proved these results on lattice trees. The latter authors have also identified a restricted subset of lattices on which lattice trees collapse into neighbour-avoiding walks (a very different universality class from lattice animals). Ruskin and Duarte [5], have completed the series study for all dimensions using the hypercubic system.

No radius of gyration or generating function exponent predictions appear in [1] for animals with cycles. Also a very troublesome gap in exponent evolution for dimensions higher than 3 hindered any significant refining of the estimated interval for the generating function exponent (quoted as $\Theta = 1.55 \pm 0.10$ in [4] for 3 dimensions). Parisi and Sourlas [6] have established $\Theta = 1$, in 2 dimensions, and $\Theta = 1.5$, in 3 dimensions, as well as $\nu = 0.5$, in 3 dimensions, exactly, while, two years later, Whittington, Torrie and Gaunt [7] have shown that a hierarchy of exponents was hidden in the cycle partition. No statements have been made on the correlation exponent ν and its possible cycle dependence. Numerical results (limited to series expansion evidence) were not outstanding, particularly for the higher cycle values, but a consideration of the equivalent model for directed lattices, [8], where some growth constants are known exactly, lent additional (and better) support to the existence of such an hierarchy of exponents.

Under the influence of all these results, attention has inevitably shifted from the leading exponents to the next correction exponent — the so-called first confluent singularity exponent, [9]. The earliest such attempt, due to Guttmann and Gaunt [10], virtually established a central estimate of 0.86 ± 0.05 in 2 dimensions, which was successively extended to the radius of gyration series [11], to the first moment of the bond distribution [12] and later reobtained by alternative numerical manipulations [13]. Reference [11] also first proposed a value for the confluent exponent in 3 dimensions ($\Omega = 0.64 \pm 0.06$), while trees (from an even shorter series than that available for animals) led to the same radius of gyration interval in 2 dimensions [14].

In the last 12 months, a much heralded breakthrough on series extensions (for lattices that can be divided into two equivalent sublattices – the so-called 'bipartite' or 'loose-packed' lattices) saw its first published results [15], while a successful Monte-Carlo thermal algorithm was put forward by Glaus as an efficient and precise tree-generator, giving growth parameters and generating function exponents as well as ν estimates [16]. On the other hand, the 'incomplete enumeration method' of Dhar and Lam [17], grafting a Monte-Carlo randomization onto the exhaustive series enumeration process, has been tested by Lam [18, 19], on studies of the anisotropy and cycle partition of animals in 2 and 3 dimensions. Lam has also presented studies of the radius of gyration for total animals that show a considerable difference from the accepted confluences of all the other authors, quoting $\Omega = 0.5 \pm 0.05$ and $\Omega = 0.45 \pm 0.10$, in 2 and 3 dimensions respectively. Cycle studies through an equivalent randomization have been independently undertaken by Wilkinson [20].

Our own approach to the subject [9] has followed the historical mainstream of animal statistics, particularly drawing on a significant amount of published but not analysed data (se also [12]) and it seems fair to assert the importance of such a viewpoint now that the subject is coming close to an explosive loss of overall perspective: references [8], [14] and [16], for example, have virtually no overlapping bibliography and reports on dynamics and growth (where the area is termed 'static lattice animals') emphatically ignore the historical perspective as if lattice animals were freshly born in the past 3 years.

In this paper we undertake an analysis of the generating function for lattice animals in 3 dimensions, using the exact leading singularity exponent, $\Theta = 1.5$, and studying the first moment of the site and bond distributions enumerated in [21] to scan the usual three-dimensional lattices. Our aim is to analyse these numbers in the light of Lam's markedly different exponents for the radius of gyration – Glaus data analyses have always assumed the absence of non-analytical terms while reptation algorithms [3, 22] have not yet specialized to the evaluation of confluent corrections. We also use the extended body-centered cubic evidence [15] to assess the gain represented in practical terms by the code-method developments in 3 dimensions.

ANALYSIS AND DISCUSSION

As stated in the Introduction we report here on the attempt to get the confluent singularity, using the Privman-Fisher and Zinn-Justin estimators, for all series data in 3 dimensions available to us, either on pure or bond- and site-weighted lattice animals [15, 21]. Most of them and particularly the weighted distributions (see appended lists) appeared to be long enough to allow already a safe comment on the bound limits of the sequences.

TABLE 1 — Tabulated values of $\Sigma_b \, bg_{sb}$ (g_{sb} being the number of animals with s sites and b bonds) worked out from refs. [15] and [21]

s	Simple Cubic	Body-centered Cubic	Face-centered Cubic
2	3	4	6
3	30	56	108
4	261	660	1 602
5	2 184	7 400	22 452
6	17 937	81 344	308 118
7	146 160	887 352	4 192 260
8	1 187 049	9 651 836	56 841 252
9	9 631 140	104 896 328	769 801 944
10	78 150 654	1 140 176 604	10 425 240 712
11	634 544 034	12 400 948 880	
12		134 992 129 128	
13		1 470 871 228 200	

For s sites or bonds the asymptotic number of different animals is usually assumed as

$$N_s = As^{-\Theta} \lambda^s \left(1 + Bs^{-\Omega} + g(s) \right)$$

TABLE 2 — Tabulated values of $\Sigma_s \, sg_{sb}$ worked out from ref. [21]

b	Simple Cubic	Face-centered Cubic	Diamond
1	6	12	4
2	45	198	18
3	380	3 712	88
4	3 402	74 217	455
5	31 614	1 542 120	2 448
6	300 980	32 866 554	13 494
7	2 915 160	713 112 984	75 640
8	28 595 115	15 678 677 670	429 255
9	283 236 544		2 459 052
10	2 827 120 098		14 191 320
11			82 387 836
12			480 652 244
13			2 815 642 168

where Θ and Ω are the universal leading and confluent singularities respectively, λ, A and B lattice dependent constants and $g(s)$ more rapidly vanishing confluences. Neglecting such power law correction terms higher than Ω and assuming Θ to be known exactly [6], we took the successive ratios (Privman-Fisher, [13])

$$\lambda_{s,k}(\Omega) = [R_s s - R_{s-k}(s-k)] / [s^w - (s-k)^w]$$

for $k = 1, 2, \ldots << s$, with

$$R_s = [s^{\Theta+\Omega} N_s] / [(s-1)^{\Theta+\Omega} N_{s-1}]$$

and $w = 1 - \Omega$.

We expected to be able to identify the range of the confluent singularity as a region of intersection of the $\lambda_{s,k}$'s close to the values previously predicted for each lattice. The patterns were rather deceptive (even in 2 dimensions) as they failed to predict a confluent singularity below 1 and gave the estimated values of λ in the limit of Ω going to zero instead - probably a sign that such ratios actually overemphasize the relevance of the dominant behaviour.

A more straightforward adaptation of the method introduced in [13] would be to assume both λ and Θ as known, using the values of λ obtained from standard extrapolants that mostly neglect confluent singularities despite the shortness of the series. We thus considered the ratios

$$A_{s,k}\ (\lambda\ ,\ \Omega) = [\, R_s - R_{s-k}\,] \,/\, [\, s^{\Omega} - (\, s - k\,)^{\Omega}\,]$$

with $R_s = s^{\Theta + \Omega}\ \lambda^{-s}\ N_s$ and $k \ll s$, that should display the values of the prefactor constant A for any s, and used them to establish bounds for Ω in a manner essentially dependent upon the trend of each curve. Fortunately, the regions of overlap for the various s values were highly sensitive to the varying values of Ω, inside the quoted ranges, and this led us to reasonable estimates of both A and λ that, for $\Omega = 0.64$, do not conflict with the values pointed out before and even allow for a not overly optimistic narrowing of the error bounds for both values (to be compared with the values fitted in [10] to the ansatz $N_s = As^{-\Theta}\,\lambda^{s}\,\mathrm{esp}\,(\,Bs^{-\Omega}\,)$). The central values of A we found are lower, for most lattices and problems, than the earlier tentative ones of Guttmann and Gaunt [10].

In the light of previous estimates for the bond problems, considerable gain in the evolution of the sequences was brought up during the analysis just by trying a whole shift of the numbers of animals up to their corresponding size in bonds plus (or minus) one, an operation whose effects are negligible for large s. In fact, this implicitly defines new values A′ and B′ such that

$$\begin{aligned} N_s &= As^{-\Theta}\ \lambda^{s}\ [\, 1 + Bs^{-\Omega} + g\,(\,s\,)\,] \\ &= A'\ (\,s + 1\,)^{-\Theta}\ \lambda^{s+1}\ [\, 1 + B'\,(\,s + 1\,)^{-\Omega} + g\,(\,s\,)\,] \end{aligned}$$

with $A' = (\,A \,/\, \lambda\,)\ ((\,s + 1\,) \,/\, s\,)^{\Theta}$ and $B' = B\ ((\,s + 1\,) \,/\, s\,)^{\Omega}$, that go to A/λ and B, respectively, for large s. Our results are summarized on Tables 3 and 4.

From our figures, in general, we think we can safely argue that, again due to the sensitivity of the plots (whose intersection regions are also monotonic as a function of Ω), one may really accept the value of Ω in [11] for the animal generating function (note that the authors proposed it for the radius of gyration) if the published bounds of λ are to be taken as granted. These bounds cover the whole range of allowed values of Ω in the interval there proposed although we do not feel confident enough to narrow this range (see Figs. 1-9).

TABLE 3 — Results of $\Omega = 0.64$ – intersection curves for three dimensional bond animals

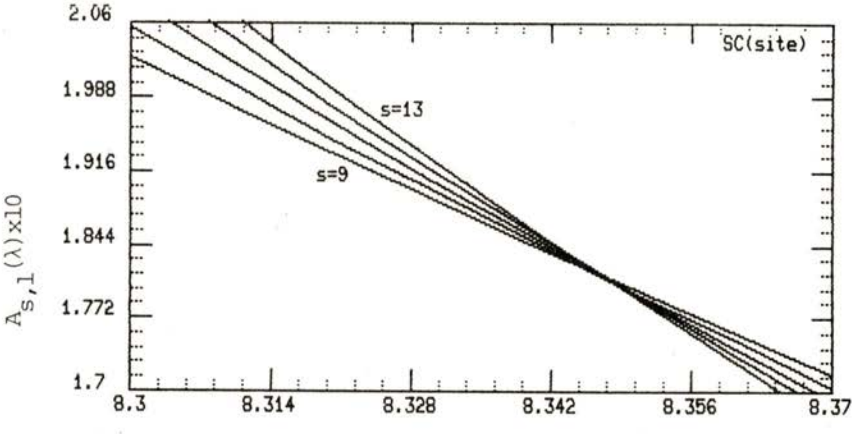
Lattice	λ	A/λ
Body-centered cubic	15.306 ± 0.006	0.0205 ± 0.0002
Site-weighted simple cubic	10.655 ± 0.006	0.0338 ± 0.0003
Site-weighted face-centered cubic	23.984 ± 0.006	0.0114 ± 0.0002
Site-weighted diamond	6.137 ± 0.001	0.0787 ± 0.0004

TABLE 4 — Results of $\Omega = 0.64$ – intersection curves for three dimensional site animals ((¹), (²) are overall estimates and (a), (b), (c), (d) the amplitude ranges consistent with them)

Lattice	λ	A
Simple cubic	8.347 ± 0.005 (¹)	0.180 ± 0.002 (a)
Bond-weighted simple cubic	8.334 ± 0.005 (¹)	0.209 ± 0.001 (b)
Body-centered cubic	11.182 ± 0.006 (²)	0.139 ± 0.001 (c)
Bond-weighted body-centered cubic	11.168 ± 0.005 (²)	0.163 ± 0.001 (d)
Bond-weighted face-centered cubic	13.900 ± 0.005	0.168 ± 0.001

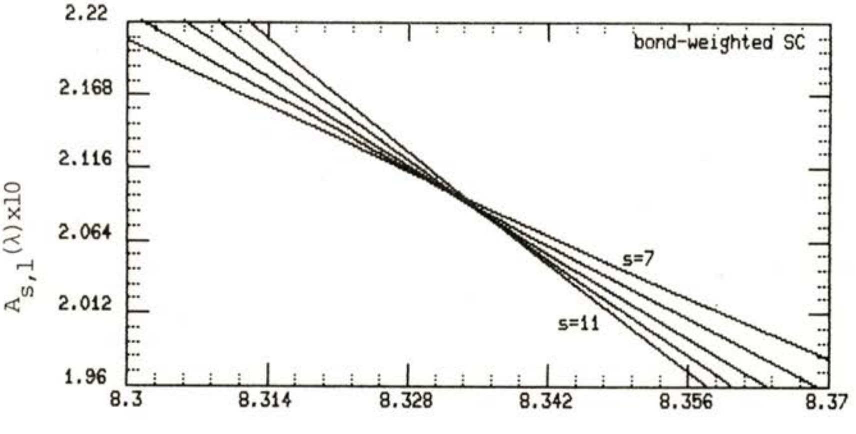
(¹) $\lambda = 8.350 \pm 0.015$ (a) $A = 0.183 \pm 0.005$ (c) $A = 0.141 \pm 0.005$
(²) $\lambda = 11.175 \pm 0.015$ (b) $A = 0.206 \pm 0.005$ (d) $A = 0.161 \pm 0.005$

In a sense we have just stressed the problem of relying on biased parameter estimates, a common practice with short series



λ

Fig. 1 — Intersections of $A_{s,1}$ (λ) for the Simple Cubic site animals for $s = 9, 10, \ldots, 13$ and the input $\Omega = 0.64$.



λ

Fig. 2 — Intersections of $A_{s,1}$ (λ) for the bond-weighted simple cubic lattice animals for $s = 7, 8, \ldots, 11$ and the input $\Omega = 0.64$.

where any induced variations are quickly propagated. The Zinn-Justin estimators [23] are the simplest version of a direct

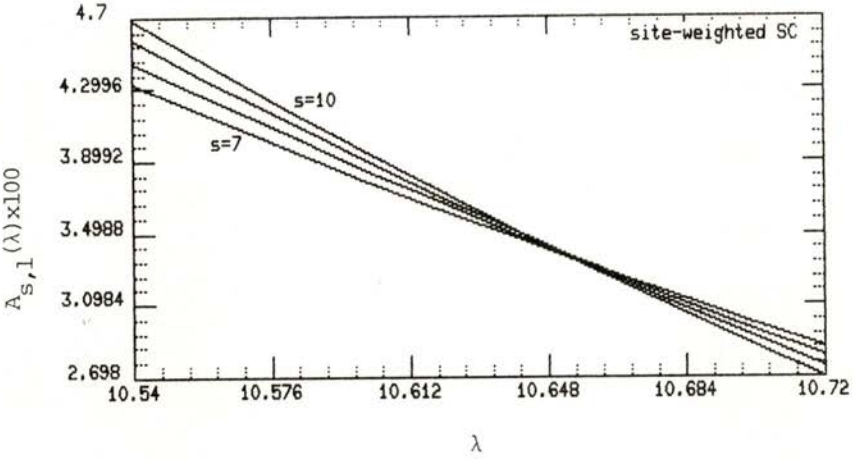


Fig. 3 — Intersections of $A_{s,1}$ (λ) for the site-weighted simple cubic lattice animals for $s = 7, 8, \ldots, 10$ and the input $\Omega = 0.64$.

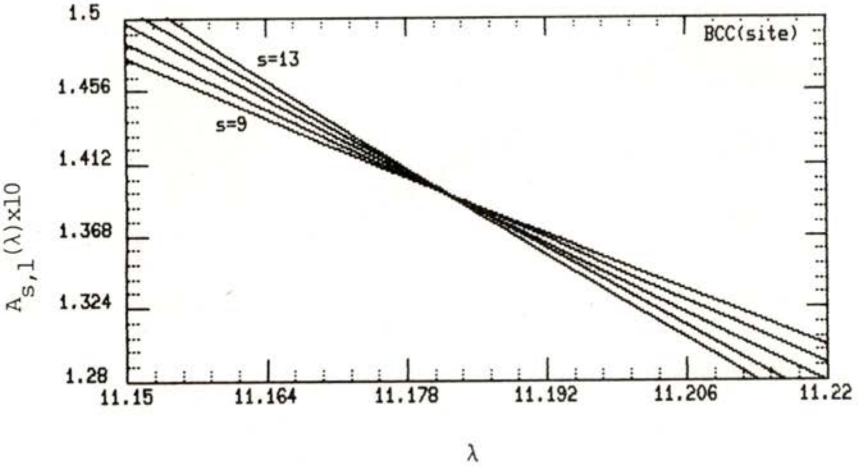


Fig. 4 — Intersections of $A_{s,1}$ (λ) for the body-centered cubic site animals for $s = 9, 10 \ldots, 13$ and the input $\Omega = 0.64$.

evaluation of the confluent singularity (up to corrections of order O (1/s)), provided we can use a reasonably good estimate

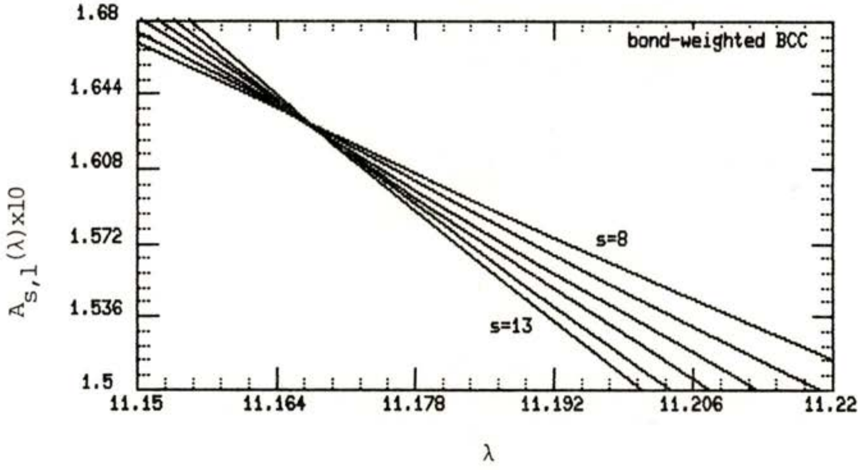


Fig. 5 — Intersections of $A_{s,1}$ (λ) for the bond-weighted body-centered cubic lattice animals for s = 8, 9, ..., 13 and the input Ω = 0.64.

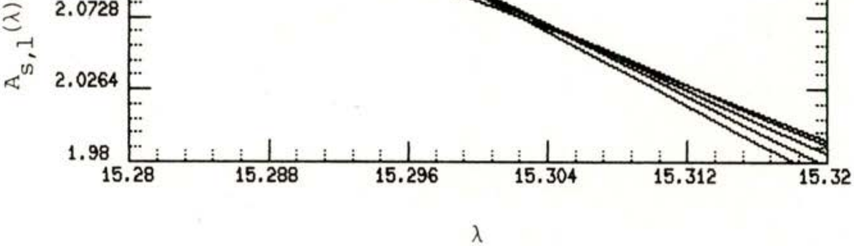


Fig. 6 — Intersections of $A_{s,1}$ (λ) for the body-centered cubic bond animals for s = 10, 11, ..., 14 and the input Ω = 0.64.

of the leading exponent (ideally it should be exactly known). It involves considering, for large s, the consecutive differences

$$\Omega_s = (R_s - R_{s-1})^{-1} - 2$$

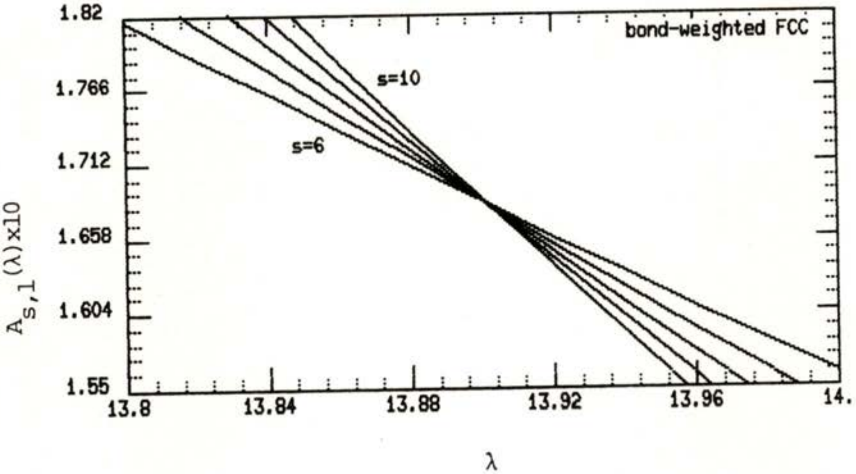


Fig. 7 — Intersections of $A_{s,1}$ (λ) for the bond-weighted face-centered cubic lattice animals for $s = 6, 7, \ldots, 10$ and the input $\Omega = 0.64$.

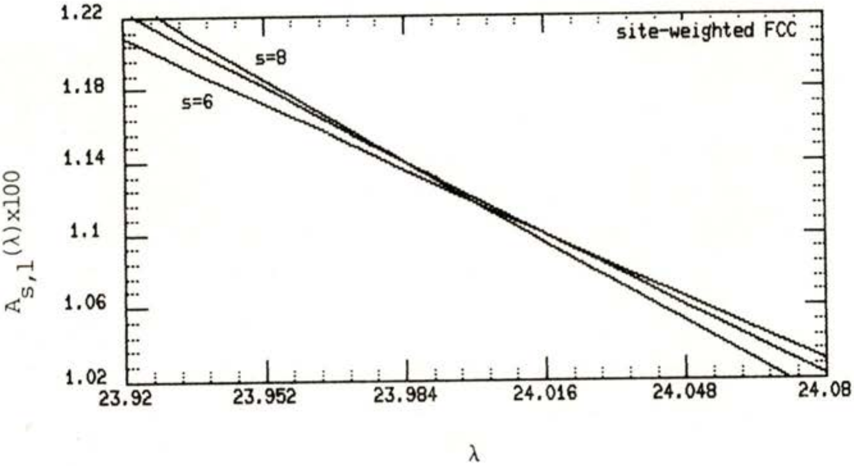


Fig. 8 — Intersections of $A_{s,1}$ (λ) for the site-weighted face-centered cubic lattice animals for $s = 6, 7, 8$, and the input $\Omega = 0.64$.

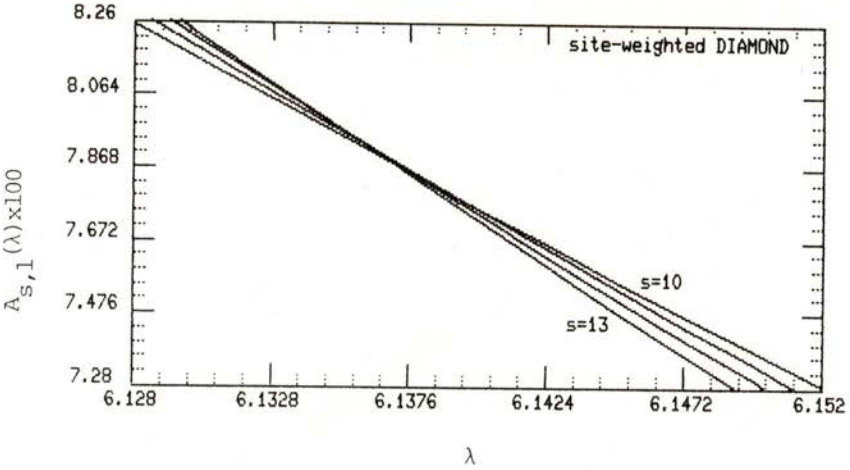


Fig. 9 — Intersections of $A_{s,1}$ (λ) for the site-weighted diamond lattice animals for $s = 10, 11, \ldots, 13$ and the input $\Omega = 0.64$.

from the log-ratios

$$R_s = (\ln T_s / T_{s-1})^{-1} \simeq -[(\Omega + 2)\ln(s-1)/s]^{-1} \simeq s/(\Omega + 2)$$

where

$$T_s = \ln(W_s W_{s-2} / W_{s-1}^2) \simeq B\,\Omega\,(\Omega + 1) / s^{\Omega + 2}$$

and $W_s = s^{\Theta} N_s$. In other words, the T_s's are successive discrete logarithm derivatives,

$$T_s = (\ln W_s - \ln W_{s-1}) / (s - (s-1)) - (\ln W_{s-1} - \ln W_{s-2}) / ((s-1) - (s-2))$$

which makes them less than ideal for short series. Finally, an averaging of two consecutive Ω_s's may be required in order to damp any oscillations. They have been plotted against $1/s$ in Fig. 10 where only bond-weighted body- and face-centered cubic sequences remain above 1 but with acceptably fast descending slopes. Their spreading makes it hard to believe that the picture will be drastically altered by adding a few more terms, however tempting a clue this might provide for the presence of more distant singularities, although the simple cubic site data show a troublesome final slope (line *e*, fig. 10).

In summary and to conclude we note that we have sampled two kinds of estimators in the search for a decisive position of the series approach concerning the disparity of values proposed for the first confluent exponent of lattice animals in 3 dimensions. Falling into a band between 0.6 and 1.1, our results for the confluence of the generating function support the higher range ($\Omega = 0.64 \pm 0.06$) and certainly do not put in doubt the reliability and control of the methods used to locate singularities. For the Zinn-Justin estimators the extended series of [15] mainly confirm the trends one already obtains with data from [21] while in the Privman-Fisher version the last body-centered cubic figures added improve the tendency to a more favourable overlapping region.

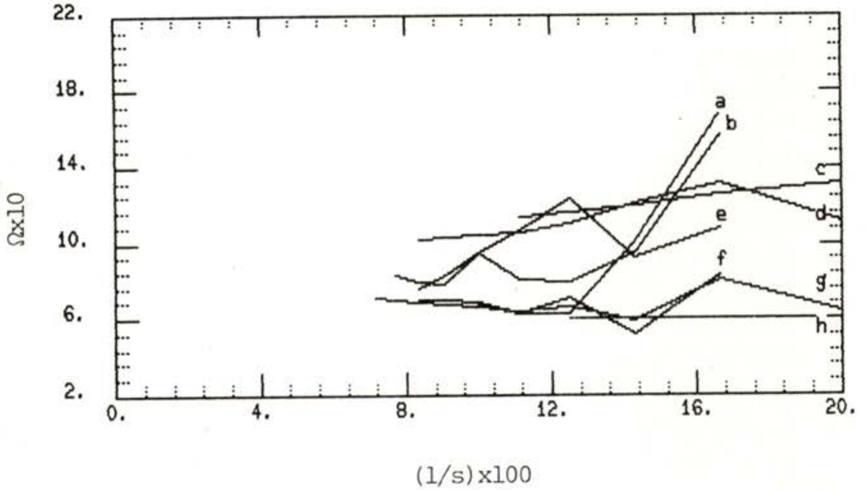


Fig. 10 — Estimates of the confluent singularity exponent for the *a*: body-centered cubic site, *b*: site-weighted diamond, *c*: bond-weighted face-centered cubic, *d*: bond-weighted body-centered cubic, *e*: simple cubic site, *f*: site-weighted simple cubic, *g*: body-centered cubic bond and *h*: site-weighted face-centered cubic animals.

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