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Self-avoiding walks in two to five dimensions: exact enumerations and series study

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Abstract. The method of concatenation (the addition of precomputed shorter chains to the ends of a centrally generated longer chain) has permitted the extension of the exact series for C_N—the number of distinct configurations for self-avoiding walks of length N. We report on the leading exponent γ and x_c (the reciprocal of the connectivity constant) for the 2D Honeycomb lattice (42 terms) 1.3437, 0.541 1968; the 2D square lattice (30 terms) 1.3436, 0.379 0520; the 3D simple cubic lattice (23 terms) 1.161 932, 0.213 4987; the 4D hypercubic (18 terms) $\gamma \simeq 1$, 0.147 60 and the 5D hypercubic lattice (13 terms) $\gamma \leq 1.025$, 0.113 05. In addition we have also evaluated the leading correction terms: honeycomb $\Delta \simeq 1$, square $\Delta \simeq 0.85$, simple cubic $\Delta \simeq 1.0$ and the 4D hypercubic logarithmic correction with $\delta \simeq 0.25$.

1. Introduction

The random walker and its vibrant offspring, the self-avoiding walker, are topics that have received continued attention since the earliest definition of the problem at the turn of the century (Barber and Ninham 1970, Montroll and Schlesinger 1984). The SAW (i.e. the subset of random walks that accidentally avoids self-intersection) has been used to model physical systems from the microscopic scale (polymers, etc) to the macroscopic (clustering of proto-galaxies in the early universe). The SAW can also be defined by the n-vector model in the limit of $n \to 0$ (deGennes 1979), and this may be considered as one of the simplest contenders for testing the predictions of the renormalization group theory. The SAW is also the simplest non-trivial graph determined by exact enumeration which is used in series analysis (see, for example, Fisher and Sykes 1959, Fisher and Gaunt 1964, Martin *et al* 1967, Sykes *et al* 1972, Torrie and Whittington 1975, Guttmann 1978, 1984, 1987, McKenzie 1979a, b, Adler 1983). We surmise that efficient algorithms developed in the past to exactly enumerate all the distinct configurations for a given length, in general, minimized the use of computer memory (a rather scarce commodity in the early days of the computer age) and were as a result more CPU intensive. A typical algorithm (e.g. Grassberger 1982) to enumerate SAWs, also termed chains, on the square lattice may be implemented as follows: the system is initialized by setting each lattice site to zero and the current point to (1, 1). The next step is recursive: check in turn each point in the four directions and if not occupied, set to 1 and make this site the current point. Now solve for $(n-1)$ points. We take advantage of the point group symmetry of the lattice to minimize the generation of SAWs. Thus we consider only walks whose first step is along the positive x axis (a reduction by a factor of 4), and whose second step is either along the positive x axis or the positive y axis (not along the negative y axis and hence a further reduction by a factor of about 3/2). In addition, we check to see whether a distinct walk is created by rotation of 180° about an axis vertical through its centre. We have used these symmetry features to reduce the number of SAWs we must enumerate in order to determine the total number of SAWs of n steps. We refer to this algorithm as the MBF (modified brute force). We present our algorithm in section 2 which is followed by new results for the 2D square and honeycomb lattices, the 3D simple cubic, 4D and 5D hypercubes.

2. The algorithm

In the generation of long chains it appears that we are repeating nearly identical subsearches of shorter segments, and with the adequate storage of the necessary information, it may be possible to increase the speed of the algorithm and hence enumerate longer SAWs. If it is possible to store data for chains of length 6, then this together with the use of the MBF method to generate, for example, chains of length 16, may enable us to extract information on chains of length 28 by adding segments of length 6 to each end. Our method, which could be referred to as 'trimerization', is similar in spirit to the dimerization method proposed by Torrie and Whittington (1975). This example will be used in the remainder of this section. We actually generate and store two independent data structures. The first list contains the (x, y) coordinates of all points of SAWs of length 6, starting at the origin. The second list contains an entry for each point within 6 units of the origin, where a point is defined as being within 6 units of the origin if the sum of the absolute values of its coordinates is less than or equal to 6. An entry is itself a list of which of the 6-unit SAWs go through that point. Having a chain with one end at the origin and knowing which points it occupies within 6 units of the origin, the second list can be used to determine how many chains of length 6 can be tacked on to the origin. This basic idea of concatenating chains, that is, tacking short chains on the ends of longer ones, is used to provide a faster algorithm.

With respect to our example of a 28-unit SAW, we would generate all the configurations of 16-unit SAWs and tack 6-unit chains on to each end, thereby determining the total number of 28-unit SAWs. The 16-unit base SAW, starting at the origin, is generated using the MBF algorithm, but extra information is maintained during the recursive searching. This information is in the form of a list of the number of points of intersection between each 6-unit SAW and the current configuration of the sites within 6 units of the origin. If the entry in this intersection list for a particular 6-unit SAW is 2, then that means that tacking the 6-unit SAW on to the origin point would result in a self-overlap of 2 points. The number of chains that can be concatenated to the base chain (the number of 0s in this list) is updated as points are added and deleted in the 16-unit base SAW, using the second data structure mentioned in the last paragraph. If a point added to the SAW is within 6 units of the origin, then the intersection list must be updated by incrementing by 1 all entries which correspond to 6-unit SAWs which go through the new point. The entries are decremented when the point is deleted from the base SAW. At the termination of constructing each 16-unit base SAW, we have a list of 6-unit SAWs which can be added to the beginning without self-overlap. Now the end of the base SAW is examined in a similar manner to determine which subset of 6-unit SAWs may be added to the end. Now, knowing the allowable subset to be tacked on at the beginning and the allowable subset to be tacked on at the end, we cannot simply multiply the sizes of the two sets, since adding a particular SAW to the beginning may preclude adding certain ones to the end. This happens when the endpoints of the base SAW are within $2*6=12$ units, which is often. Here, we have to look at each 6-unit SAW at, say, the end, and check which 6-unit SAWs can still be added to the origin.

All SAWs of length 16 are generated using the standard MBF recursive algorithm, then for each of these base SAWs one determines how many SAWs of length 28 have this base SAW as their middle 16 units. There are several symmetry relations to be taken advantage of when building the 16-unit base SAW. These include four-point symmetry about the origin, mirror symmetry about the x axis (because the first step is always along the x axis), and two-way reverse symmetry, which is symmetry obtained by placing the origin of the SAW at its endpoint, and the end at the origin. These provide a speed-up of roughly 4, 2 and 2 times, respectively, which is to say that it requires enumeration of only 1/16 of all SAWs of length 16, on the square lattice. Similar economics can be realized on other lattices.

We summarize the essential features of our algorithm:

(i) Precompute an array $A[i]$, where i ranges from 1 to the number of chains of a fixed length, l (in our example 6), and each element of the array is a list of the (x, y) points of a particular chain.

(ii) Precompute an array $B[p]$ which, for a given point, p, lists which SAWs of length l go through that point, and therefore cannot be added to the origin if that point is already occupied.

(iii) Use the basic recursive algorithm to build base SAWs of length b (in our case 16). Use the array B to maintain the list of which SAWs of length l can be added to the origin. For each b-unit SAW generated, use the array B at the end of the b-unit SAW to create a list of which SAWs of length l can be added to the end. Use the array A to append each SAW from this list to the end, and use B to update the list of valid SAWs for the origin. Sum the number that can be added to the origin after attaching each applicable SAW to the end. This sum is the number of chains of length $2*l+b$ which have the particular base SAW as its middle b segments. We note that this algorithm does not reduce the complexity of the calculation, but by calculating information about the ends and storing it we have reduced the actual CPU time for the enumeration of chains of a given length. Because of the concatenation process a lower bound to the time required to enumerate chains of length n will grow exponentially as $n-2b$ rather than as n for the MBF algorithm. The time required to enumerate C_{30} on the SQ lattice on a SUN 386i workstation was approximately $4\frac{1}{2}$ days.

The end-to-end distance could be calculated if the array B is replaced with array A. Thus the array A is used for adding precomputed chains to both ends of the base chain. This would slow the algorithm but not significantly. We intend to use this modified form of the algorithm to determine the end-to-end distance for chains in three-dimensions.

3. Enumeration of SAWs

This algorithm is used to extend the enumeration C_n of SAWs of length n on the 2D honeycomb (HC) lattice and on the family of cubic lattices in two, three, four and five dimensions: namely the square (SQ), simple cubic (SC) and the loose-packed hypercubic lattices which we denote $C4$ and $C5$. Table 1 shows the number of terms we have generated and the longest previous enumeration in each of the cases.

Table 1. Maximum number of steps in SAWs enumerated and comparison with previous work.

D	Lattice	n	Previous	Reference
2	HC	42	34	†
	SQ	30	27	‡
3	SC	23	20	‡
4	$C4$	18	13	§
5	$C5$	13	11	¶

† Sykes *et al* (1972).
‡ Guttmann (1987).
§ Guttmann (1978).
¶ Fisher and Gaunt (1964).

The C_n for these lattices are tabulated in table 2. Our results agree with previously published results and we have added 8, 3, 3, 5 and 2 to the respective series as tabulated. Our new terms up to $n = 28$ on the SQ and $n = 20$ for the SC were reported in STATPHYS 16 in Boston (MacDonald *et al* 1986). The values agreed with Guttmann's (1986, 1987) calculations to order 27 on the SQ and also to order $n = 20$ on the SC which were also reported at that conference. An additional three terms on the SC were reported at STATPHYS 17 in Rio de Janeiro (Hunter *et al* 1989).

3.1. 2D SAWs

The SAW generating function

$$f(x) = \sum_{n=0} C_n x^n \sim A(1-\mu x)^{-\gamma}[1+B(1-\mu x)^{\Delta}+\ldots] \qquad (1)$$

which implies $C_n \sim \mu^n n^{\gamma-1}$ has been analysed for the HC and the SQ lattices by both the conventional methods (Hunter and Baker 1973, Gaunt and Guttmann 1974) to detect the dominant singularity and by other methods to detect the correction-to-scaling behaviour. For the HC lattice we have the distinct advantage that we know $\mu = 1/x_c = \sqrt{(2+\sqrt{(2)})}$ exactly ($=1.847\,759\,065\ldots$). Unbiased estimates of μ and γ from the roots and residues of Padé approximants to the derivative of the logarithm of the generating function (Dlog Padés) were well converged and agreed very well with the known μ and with Nienhuis's (1982) prediction that $\gamma = 43/32 = 1.343\,75$. Our conclusion based on the unbiased Dlog Padés is summarized in the first line of table 3.

Because of the period 4 oscillations in the ratios for the HC series, we performed a Euler transformation to move the interfering singularities further away in the complex plane. This did little to the unbiased Padé estimates except to provide a marginal improvement in the degree of convergence. However, after the transformation we obtained unbiased ratio method estimates (line 2, table 3) which, although not as accurate, are consistent with the Padé results.

Using first-order non-homogeneous integral approximants (Hunter and Baker 1979, Fisher and Au-Yang 1979) we obtained the unbiased estimates recorded in line 3 of table 3. These are in remarkable agreement with the exact results for μ and with Nienhuis's γ. We have used the approximants as defined by Hunter and Baker which are similar, but not identical, to those used by Guttmann.

Table 2. Number of SAWs, C_n, of n steps on various lattices in $D = 2, 3, 4, 5$.

2D HC lattice SAWs: C_n		2D SQ lattice SAWs: C_n		3D SC lattice SAWs: C_n		4D cubic lattice SAWs: C_n		5D cubic lattice SAWs: C_n	
1	0	1	0	1	0	1	0	1	0
3	1	4	1	6	1	8	1	10	1
6	2	12	2	30	2	56	2	90	2
12	3	36	3	150	3	392	3	810	3
24	4	100	4	726	4	2 696	4	7 210	4
48	5	284	5	3 534	5	18 584	5	64 250	5
90	6	780	6	16 926	6	127 160	6	570 330	6
174	7	2 172	7	81 390	7	871 256	7	5 065 530	7
336	8	5 916	8	337 966	8	5 946 200	8	44 906 970	8
648	9	16 268	9	1 853 886	9	40 613 816	9	398 227 610	9
1 218	10	44 100	10	3 809 878	10	276 750 536	10	3 527 691 690	10
2 328	11	120 292	11	41 934 150	11	1 886 784 200	11	31 255 491 850	11
4 416	12	324 932	12	198 842 742	12	12 843 449 288	12	276 741 169 130	12
8 388	13	881 500	13	943 974 510	13	87 456 597 656	13	2 450 591 960 890	13
15 780	14	2 374 444	14	4 468 911 678	14	594 876 193 016	14		
29 892	15	6 416 596	15	21 175 146 054	15	4 047 352 264 616	15		
56 268	16	17 245 332	16	100 121 875 974	16	27 514 497 698 984	16		
106 200	17	46 466 676	17	473 730 252 102	17	187 083 712 725 224	17		
199 350	18	124 658 732	18	2 237 723 684 094	18	1 271 271 096 363 128	18		
375 504	19	335 116 620	19	10 576 033 219 614	19				
704 304	20	897 697 164	20	49 917 327 838 734	20				
1 323 996	21	2 408 806 028	21	235 710 090 502 158	21				
2 479 692	22	6 444 560 484	22	1 111 781 983 442 406	22				
4 654 464	23	17 266 613 812	23	5 245 988 215 191 414	23				
8 710 212	24	46 146 397 316	24						
16 328 220	25	123 481 354 908	25						
30 526 374	26	329 712 786 220	26						
57 161 568	27	881 317 491 628	27						
106 794 084	28	2 351 378 582 244	28						
199 788 408	29	6 279 396 229 332	29						
372 996 450	30	16 741 957 935 348	30						
697 217 994	31								
1 300 954 248	32								
2 430 053 136	33								
4 531 816 950	34								
8 459 583 678	35								
15 769 091 448	36								
29 419 727 280	37								
54 816 035 922	38								
102 216 080 286	39								
190 380 602 052	40								
354 843 312 276	41								
660 671 299 170	42								

Table 3. Result from standard methods of analysis for the dominant singularity only for the $D=2$ HC SAW series.

Method	x_c	$\mu = x_c^{-1}$	γ
Padé unbiased	0.541 191 ± 0.000 010	1.847 78 ± 0.000 03	1.343 ± 0.002
Ratio unbiased	0.5412 ± 0.0001	1.8477 ± 0.0003	1.348 ± 0.005
Integral unbiased	0.541 1968 ± 0.000 0008	1.847 757 ± 0.000 003	1.3440 ± 0.0003
Padé biased by x_c	(0.541 196 1002 ... given)		1.3437 ± 0.0001
Ratio biased by x_c	(0.541 196 1002 ... given)		1.344 ± 0.001
'Exact' results	0.541 196 1002 ...	1.847 759 065 ...	1.343 75

Table 4. Summary of RGA analysis for correction terms HC SAW series.

	Unbiased		Biased
Trial Δ	y_c	γ	γ
0.70	1.000 06	1.347	1.344
0.75	1.000 05	1.347	1.344
0.80	1.000 03	1.347	1.344
0.85	1.000 02	1.346	1.344 5
0.90	1.000 015	1.346	1.344 1
0.950	1.000 002	1.3443	1.344 20
0.955	1.000 002	1.3442	1.344 14
0.960	1.000 002	1.3440	1.344 08
0.965	1.000 000	1.3439	1.344 03
0.970	1.000 000	1.3438	1.344 00
0.975	0.999 9999	1.3437	1.343 93
0.980	0.999 9999	1.3437	1.343 88
0.985	0.999 997	1.3435	1.343 83
0.990	0.999 997	1.3432	1.343 78
0.995	0.999 996	1.3431	1.343 74
1.000	0.999 995	1.3430	1.343 68
1.05	0.999 995	1.342	1.343 2
1.10	0.999 991	1.342	1.342 8
1.15	0.999 990	1.341	1.342 3
1.20	0.999 985	1.339	1.341 8
1.25	0.999 980	1.338	1.341 2
1.30	0.999 98	1.337	1.340 6
1.35	0.999 98	1.335	1.340 0
1.40	0.999 98	1.334	1.339
1.45	0.999 98	1.333	1.337
1.50	0.999 98	1.330	1.335
1.55	0.999 98	1.332	1.33
1.60	0.999 97	1.330	1.33

If we bias the estimates of γ by specifying the exact value of μ we improve our estimates from the Padé approximants and ratio analysis by one significant figure (lines 4 and 5, table 3).

With this kind of precision from methods that account for the dominant singularity only, one might predict at the outset that the correction-to-scaling effect is small. Several attempts were made to identify the important correction terms. We were particularly concerned to look for the lowest-order correction term characterized by the exponent Δ in equation (1) and if that turned out to be 1.0 (the analytic correction) to see if any evidence of a non-analytic correction could be found—particularly one close to Nienhuis's predicted value $\Delta = 1.5$.

Using the transformation method of Baker and Hunter (1973) we found no evidence of a non-analytic correction. The procedure used by Guttmann (1984) based on earlier work due to Roskies (1981) and Adler *et al* (1982) (hereinafter referred to as RGA) was quite useful but again gave no evidence of a non-analytic correction either for $\Delta < 1$ or $\Delta > 1$. One transforms the series using the exact x_c and a trial Δ using $y = 1-(1-x/x_c)^{\Delta}$. The transformed series should have a singularity at 1.000 with exponent γ/Δ. One can analyse the Dlog Padé approximants for this series for γ and, if desired, bias the results by insisting that the singularity be at 1.000. The results of the analysis for several trial Δ are summarized in table 4. For the biased estimates, the most obvious agreement with Nienhuis's γ occurs when we used $\Delta = 0.995$, suggesting that the first correction term is the analytic one. For the unbiased analysis the closest agreement to $y_c = 1.0$ and $\gamma = 1.343\,75$ occurs for Δ only slightly lower at $\Delta = 0.975$—still close enough to suggest an analytic correction. There is very little evidence at $\Delta = 1.5$ except perhaps a slight improvement in the degree of convergence (to a value other than 43/32!) to suggest that Nienhuis's non-analytic correction term is present. This suggests to us that if such a correction term is present, its amplitude must be very small indeed, in keeping with the observation of Ishinabe (1988).

For the HC the ultimate comparison for series results is with Nienhuis's prediction. However, we may also compare our results with previous analyses of the 34-term series by others. Adler (1983) used the exact x_c to estimate $\gamma = 1.344$ and three correction exponents $\Delta_1 = 0.93$, $\Delta_2 = 1.2$ and $\Delta_3 = 1.5$. Guttmann (1987) reanalysed the series to obtain $0.541\,1935 \pm 0.000\,0045$ and $\gamma = 1.3440 \pm 0.0003$, with no attempt to determine the Δ. Our results with the longer series improve the agreement with Nienhuis for x_c and γ but do not agree with Adler for the correction exponents.

For the SQ lattice we do not know μ or x_c exactly. However, we have analysed the series in exactly the same way as for the HC series. The results obtained for the dominant singularity using Padé (PA) and integral approximants (IA) are summarized in table 5. We have used Nienhuis's γ value to form Padés to $[f(x)]^{1/\gamma}$ and obtained biased estimates for x_c. However, the IA results are the most convincing and our value of $x_c = 0.379\,0520 \pm 0.000\,0010$ agrees well with Guttmann's (1987) value $x_c = 0.379\,0528 \pm 0.000\,0015$ from this series with three fewer terms and from the $\langle R_N^2 \rangle$ series. From their analysis of polygon series Guttmann and Enting (1988) have concluded $x_c = 0.379\,052\,28 \pm 0.000\,000\,15$. Guttmann's $\gamma = 1.343\,61$ ● $0.000\,13$ is very close to our estimate. All of this evidence seems mutually consistent and would lead us to accept the IA value for x_c as our best estimate. The Guttmann and Enting polygon result appears to be the most precise estimate for x_c and suggests that our qualitative

Table 5. Results from standard methods of analysis for the dominant singularity only for the $D = 2$ SQ SAW series.

	x_c	$\mu = x_c^{-1}$	γ
Padé unbiased	$0.379\,04 \pm 0.000\,02$	$2.638\,24 \pm 0.000\,14$	1.340 ± 0.005
Integral unbiased	$0.379\,0520 \pm 0.000\,001\,0$	$2.638\,161 \pm 0.000\,007$	1.3436 ± 0.0002
Padé biased by γ	$0.379\,06 \pm 0.000\,01$	$2.638\,10 \pm 0.000\,07$	(1.343 75 given)

confidence limits might be unnecessarily conservative when compared with their statistically based limits.

When we analyse this series to look for the correction term using the RGA transformation, we find some evidence of a non-analytic correction term with $\Delta \sim 0.85$ in at least apparent conflict with our analysis of the HC lattice. However, for the SQ lattice we do not know x_c exactly. We apply the transformation, this time scanning over a range of x_c and a range of trial Δ, looking for consistency with Nienhuis's γ and for the degree of convergence in the estimates of γ. For the HC lattice consistency with Nienhuis did not occur at the same Δ as the best overall convergence, but they did occur close together. Since x_c is now adjustable, the task is harder. Based on these two criteria alone one would conclude that $\Delta \sim 0.85$. To conclude $\Delta = 1.00$ and $\gamma = 1.343\,75$ one would have to increase x_c to 0.379 065 which is apparently inconsistent with our IA estimate of $x_c = 0.379\,052$.

3.2. 3D SAWs

We have analysed our 23-term SC series by the same methods as we used for the 2D lattices. In table 6 we show our conclusions from the analysis for the dominant singularity. The standard Padé approximant procedures—both biased and unbiased—lead to Padé tables of estimates for x_c and γ which show unprecedented convergence to the values:

$$x_c = 0.213\,4987$$

$$\gamma = 1.161\,932.$$

We present the Padé data in table 7. We show in part (*b*) of the table the biased Padé estimates for γ using three different values of x_c: the value above from the unbiased locations of the pole and values that differ from it by one in the sixth decimal place. For the upper and lower values of x_c, the convergence is not as striking as it is for the middle value (three fewer decimal places).

Table 6. Results from standard methods of analysis for the dominant singularity only for the $D = 3$ SC SAW series.

	x_c	$\mu = x_c^{-1}$	γ
Padé unbiased	0.213 4987 ± 0.000 0010	4.683 869 ± 0.000 022	1.161 93 ± 0.000 10
Integral unbiased	0.213 4965 ± 0.000 0030	4.683 918 ± 0.000 065	1.1613 ± 0.0010
Padé biased by x_c	(0.213 4987 given)		1.161 9315 ± 0.000 0015

The RGA transformation analysis which we expect to locate the correction-to-scaling exponent indicates quite strongly that the correction is analytic. We have scanned over a grid of Δ values from 0.4 to 1.2 and over five values of x_c from 0.213 487 to 0.213 507. The criteria we apply in interpreting the results are consistency of the poles in the approximants with $y_c = 1.0$ exactly and the degree of convergence in the values of both the poles and the residues.

This time we have no semi-rigorous knowledge of γ as we did in two dimensions. We detect excellent convergence of poles and residues for $x_c = 0.213\,497$ for $\Delta = 1.0$ and for $x_c = 0.213\,502$ for $\Delta = 0.9$, 1.0 and 1.1. We then used $x_c = 0.213\,4987$ (our best

Table 7. (*a*) Unbiased estimates of x_c and γ for the SC lattice from roots and residues respectively to $d\{\log f(x)\}/dx$.

N/D	Root	Residue
7/8	0.213 4951	1.161 604
8/8	5544	1.173 506
9/9	4974	1.161 802
8/9	4991	975
9/8	4981	872
10/9	4963	710
9/10	4987	927
10/10	4987	926
11/10	4987	929
10/11	4987	927
11/11	4987	928

(*b*) Biased estimates for γ for the SC lattice obtained by evaluating at $x = x_c$ Padé approximants to $(x_c - x)\, d\{\log f(x)\}/dx$.

N/D	$x_c = 0.213\,4977$	$x_c = 0.213\,4987$	$x_c = 0.213\,4997$
7/8	1.161 6441	1.161 8904	1.161 9571
8/8	1 6626	1 9320	2 0325
9/8	1 6541	1 9295	2 0359
8/9	1 6585	1 9302	2 0367
9/9	1 6507	1 9309	2 0308
10/9	1 6552	1 9313	2 0479
9/10	1 6654	1 9313	2 0596
10/10	0 5346	1 9302	1 1776
11/10	1 8410	1 9318	2 2806
10/11	1 8537	1 9316	2 2595
11/11	2 4551	1 9330	3 3921

estimate from the Dlog Padé analysis) and scanned over all the Δ values. At $\Delta = 1.0$ there is once again a striking convergence of the poles to $y_c = 0.999\,9998$.

The residues are well converged to $\gamma = 1.161\,93$, although when $\Delta = 1.0$ the residues (not the poles) are completely insensitive to the choice of x_c. When we bias the transformed function to have a pole at $y_c = 1.0$ the γ we get has converged to $\gamma = 1.161\,930 \pm 0.000\,002$. For other values of x_c and Δ the roots and residues of the approximants to the transformed function are not nearly so well converged as at $x_c = 0.213\,4987$ and $\Delta = 1.0$. We illustrate this in table 8, where we present the roots and residues for the above pair of parameters and for one other pair: $x_c = 0.213\,492$ and $\Delta = 0.5$ which appears to be the best choice of x_c for a Δ of 0.5. We conclude that there is no evidence for a non-analytic singularity from the RGA analysis. Combining all the evidence and relaxing the confidence limit on γ to reflect the uncertainty on x_c we would conclude from our series

$$x_c = 0.213\,4987 \pm 0.000\,0010$$

$$\gamma = 1.161\,93 \pm 0.000\,10$$

$$\Delta = 1.00 \pm 0.02.$$

Our results for γ in three dimensions are consistent with, but much more precise than, McKenzie's (1979a) analysis of the FCC series. She found $\gamma = 1.1615 \pm 0.0005$

Table 8. Padé approximants to the RGA transformed series on SC lattice for two different choices of x_c and Δ.

	$x_c = 0.213\,4920$, $\Delta = 0.5$		$x_c = 0.213\,4987$, $\Delta = 1.0$	
N/D	Root	Residue	Root	Residue
6/7	0.996 2851*D*+00	−0.113 6054*D*+01	0.999 8550*D*+00	−0.115 9724*D*+01
7/7	0.100 1152*D*+01	−0.117 1813*D*+01	0.999 9629*D*+00	−0.116 1247*D*+01
8/7	0.100 0552*D*+01	−0.116 5811*D*+01	0.999 9742*D*+00	−0.116 1436*D*+01
7/8	0.100 0711*D*+01	−0.116 7549*D*+01	0.999 9833*D*+00	−0.116 1605*D*+01
8/8	0.100 0907*D*+01	−0.116 9543*D*+01	0.100 0261*D*+01	−0.117 3505*D*+01
9/8	0.100 0789*D*+01	−0.116 8265*D*+01	0.999 9941*D*+00	−0.116 1802*D*+01
8/9	0.100 0814*D*+01	−0.116 8558*D*+01	0.100 0002*D*+01	−0.116 1975*D*+01
9/9	0.100 0966*D*+01	−0.117 0087*D*+01	0.999 9974*D*+00	−0.116 1872*D*+01
10/9	0.100 0467*D*+01	−0.116 4624*D*+01	0.999 9889*D*+00	−0.116 1710*D*+01
9/10	0.100 0626*D*+01	−0.116 6602*D*+01	0.999 9998*D*+00	−0.116 1927*D*+01
10/10	0.100 3258*D*+01	−0.116 7028*D*+01	0.999 9998*D*+00	−0.116 1926*D*+01
11/10	0.100 0027*D*+01	−0.115 8571*D*+01	0.999 9999*D*+00	−0.116 1929*D*+01
10/11	0.100 0236*D*+01	−0.116 1867*D*+01	0.999 9998*D*+00	−0.116 1927*D*+01
11/11	0.100 0109*D*+01	−0.115 9904*D*+01	0.999 9998*D*+00	−0.116 1928*D*+01

and consistency with the RG prediction of a correction exponent $\Delta = 0.465$ (LeGuillou and Zinn-Justin 1977, Baker *et al* 1978). Guttmann (1987) reanalysed McKenzie's series and obtained $\gamma = 1.1629 \pm 0.0018$ and for his 20-terms SC series concluded $\gamma = 1.1613 \pm 0.0021$ and $x_c = 0.213\,497 \pm 0.000\,010$. Our results indicate a greater degree of convergence to apparently more precise values for x_c and γ which are consistent with Guttmann.

3.3. 4D SAWs

At $D = 4$, the upper critical dimension, we expect mean field exponents with a logarithmic correction factor $f(x) \approx A(1 - x/x_c)^{-1} |\ln(1 - x/x_c)|^{\delta}$ (Larkin and Khmel'nitskii 1969). Table 2 shows the extended series for the number of distinct chains for $N \leqslant 18$. As expected, we find for our $d = 4$ hypercubic series that the methods which do not account for the logarithmic correction are extremely slow to converge to the expected mean field values. Both direct and Dlog Padé approximants should have poles at x_c, while the residues of the Dlog Padés are unbiased estimates of γ. For our series we found slowly increasing poles in the direct Padé approximants which had reached $x = 0.147\,39$. For the Dlog Padés, however, the poles were slowly decreasing and had reached $x = 0.147\,68$. We would regard these as bounds on x_c. The residues of the Dlog Padés had decreased to about 1.065—still a long way from 1.0. Euler transformations did little to improve these estimates. Using first-order non-homogeneous IAs we see poles and residues near 0.147 66 and 1.060 respectively. Confidence limits are very difficult to estimate because of the slow convergence.

To account for the logarithmic factor we transform the series by dividing out $(x - x_c^*)^{-1}$, raise the series to the power $1/\delta$, differentiate to make the log a simple pole and then evalute direct Padés and look for consistency with the initial x_c^* all for a range of trial x_c^* and δ. We find the best convergence and self-consistency at $x_c = 0.147\,60$ and $\delta = 0.25$ but $\delta = 0.27$ was almost as good. (The results were not particularly sensitive to δ.) Thus our results are entirely consistent with the expected logarithmic behaviour if we use $x_c = 0.147\,60$. This value for x_c is between the values we obtained for direct and Dlog Padés and we assume they are each converging slowly to this value from either side. Hence we would conclude that

$$x_c = 0.147\,60 \pm 0.000\,10$$

$$\delta = 0.25 \pm 0.02.$$

Guttmann (1978) found $\delta = 0.23 \pm 0.04$ for this lattice and McKenzie (1979b) on the hyper-face-centred cubic lattice found $\delta = 0.24 \pm 0.03$.

3.4. 5D SAWs

At $D = 5$ we expect pure mean-field behaviour. With our 13-terms series we observe slow convergence which has reached the following:

Direct Padés:	$x_c = 0.113\,05$
Dlog Padés:	$x_c = 0.113\,17$
	$\gamma = 1.025$
Integral approximants:	$x_c = 0.1132$
	$\gamma = 1.025.$

However, if we use direct Padé approximants, multiply by $x - x_c^*$ and test for the degree of convergence to an amplitude we find the best convergence when $x_c^* = 0.113\,03$. On the other hand, if we take Dlog Padés, multiply by $x - x_c^*$ and test for convergence to $\gamma = 1.00$ we find the best results for $x_c^* = 0.113\,07$. Hence we conclude that the $D = 5$ series analysis is consistent with the expected mean field behaviour and that

$$x_c = 0.113\,05 \pm 0.000\,05.$$

We plan to extend this series even further and to investigate the correction-to-scaling behaviour (Guttmann 1981).

4. Conclusion

We have used an efficient method for enumerating chains on various lattices. The method is dependent on the storage of information which has to be recalculated many times during the generation of long chains. This technique may be extended to the enumeration of *all* graphs, but this task is at best non-trivial. We have with modest computing power (VAX 11/780 and SUN 386i) extended the existing series in two to five dimensions. It would be possible to extend the $D = 3$ and the $D = 2$ SQ results by an additional one or two terms and the $D = 2$ HC SAWs by at least eight terms. This may be done by subdividing the enumeration into disjoint subsets. We are in the process of doing this.

We have confirmed Nienhius's predictions in two dimensions for the SAW exponents and critical fugacity of the HC lattice, but apart from the analytic term have found no evidence for the presence of a correction-to-scaling term of 1.5 with the extended series. This is disconcerting but may reflect the fact that the amplitude of this correction term is extremely small. The indication of a possible non-analytic $\Delta < 1.0$ for the SQ lattice is perplexing. We will investigate this further when we have extended the series on both $D = 2$ lattices and we will also look for other appropriate methods of analysis for the correction terms. The $D = 3$ analysis has shown a striking degree of convergence. That consistency and the lack of any evidence for a non-analytic correction again lead us to conclude that the amplitude for such correction terms is very small or perhaps even zero. We also confirm the presence of the logarithmic correction with mean-field exponents in four-dimensions and thus are in agreement with the predictions and general facets of the renormalization group. In five dimensions, although the series is still short, we observe the expected classical behaviour. The renormalization scenario with the concept of an upper critical dimensionality is strongly supported by our results.

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Note added in proof. We have since extended the HC to 50 terms, the SQ to 32 terms, SC to 24, and the 4D hypercubic to 21 terms. A recent preprint from Boston University has extended the SQ to 34 terms and is in agreement with our values.

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