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Self-avoiding walks on the simple cubic lattice

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Abstract. We have substantially extended the series for the number of self-avoiding walks and the mean-square end-to-end distance on the simple cubic lattice. Our analysis of the series gives refined estimates for the critical point and critical exponents. Our estimates of the exponents γ and ν are in good agreement with recent high-precision Monte Carlo estimates, and also with recent renormalization group estimates. Critical amplitude estimates are also given. A new, improved rigorous upper bound for the connective constant $\mu < 4.7114$ is obtained.

1. Introduction

A self-avoiding walk (SAW) can be defined as a connected path on a lattice which has no self-intersections. Let c_n denote the number of n-step SAWs, distinct up to a translation. It is known that $c_n \sim \mu^n$, where $\mu = 1/x_c$ is known as the *connective constant* and x_c is known as the *critical point*. It is universally accepted, though not proved, that $c_n \sim \mu^n n^{\gamma-1}$.

Traditionally, interest centres on two generating functions,

$$C(x) = \sum_{n\geqslant 0} c_n x^n \sim A_0(x) + A_1(x)(1-\mu x)^{-\gamma} \tag{1}$$

and

$$R(x) = \sum_{n\geqslant 0} \rho_n x^n \sim B_0(x) + B_1(x)(1-\mu x)^{-\gamma-2\nu} \tag{2}$$

where

$$\rho_n = \sum_{i=1}^{c_n} r_i^2. \tag{3}$$

Here r_i is the Euclidean distance between the endpoints of the ith SAWs. The mean-square end-to-end distance is then defined by $\langle R^2\rangle_n = \rho_n/c_n$.

As well as its importance as the $n \to 0$ limit of an O(n) model, the enumeration of SAW on various lattices is an interesting combinatorial problem in its own right. It is nicely reviewed in [13, 16].

Despite strenuous effort over the past 50 years or so this problem has not been solved on any regular two- or three-dimensional lattice. However, for the hexagonal lattice the critical

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point, $x_c^2 = 1/(2+\sqrt{2})$ as well as the critical exponent for the related problem of self-avoiding polygons (SAPs) $\alpha = \frac{1}{2}$ are known exactly [19], though non-rigorously. Very firm evidence exists from previous numerical work that the exponents are universal for regular lattices in any dimension, so in particular $\alpha = \frac{1}{2}$ for all two-dimensional lattices [8, 11, 14]. Other exponents for the two-dimensional problem are also exactly known. The conformal invariance of the system implies that, for regular two-dimensional lattices, the critical exponents are rational, and we also know that the critical points for the two-dimensional model are algebraic.

For three-dimensional systems we still expect universality of exponents, but have no reason to believe that the critical points are algebraic or that the exponents are rational. In order to estimate the critical parameters, such as the critical point, critical exponent and amplitude(s), one traditionally resorts to numerical methods. For many problems the method of series expansions is the most powerful method of approximation. For other problems Monte Carlo methods are superior, while for critical exponents the renormalization group and other field-theoretical methods have achieved stunning precision.

However, field theoretical methods are under-pinned by an explicit belief in universality, and it is important that estimates of critical points and critical exponents from series and Monte Carlo studies, that make no such assumption, should be compared with the field theory based predictions.

2. Generation of series

Algorithm. The MacDonald algorithm [17] consists of two main parts, (a) the generation of SAWs referred to here as *base chains* and (b) a process of *double* concatenation where smaller chains are added to both ends of the base chain. There are several symmetry features used to speed up the algorithm constructing the base chains. These include the use of 6-point symmetry about the origin, mirror symmetry in the x–y and x–z planes since the first step is always along the x-axis, and two-way reverse symmetry which is considering the endpoint as the origin and noting if a new chain is thus generated. A minimum reduction by a factor from 6 to a possible 48 ($6 \times 4 \times 2$) in the number of chains to be directly computed may thus be achieved. Shorter chains are then added to both ends to obtain longer chains, all the while ensuring that the self-avoiding property is not violated. Let us assume as an example we need to enumerate walks of length 26. Base chains are of length 14 and shorter end-chains of length 6. This is done in the following manner:

(1) Precompute a list A; each item of this list corresponds to a particular SAW of length 6 which can be added to the base chain. Each item in the list A is itself a list of co-ordinates (x, y, z) of all the points in the corresponding walk of length 6.
(2) Precompute a second list B[p] which for a given point p lists which SAWs of length 6, with reference to list A, go through that point. The points p comprise the set of all points within 6 units of the origin, i.e the sum of the absolute values of its coordinates is less than or $\leqslant 6$.
(3) Then method (a) described above is used to construct SAW of length 14, but extra information is stored during the recursive construction of the base chain. This information is the number of points of intersection the 6 unit SAW, generated in A, has with the current base chain within 6 units of the origin of the base chain. This is done by using list B. If a point added to the base chain is within 6 units of the origin, then the intersection list must be updated by incrementing by one 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 chain during the recursive search. After the construction of each base chain we have

Table 1. The number, c_n, of n-step SAW and the sum of the squares of their end-to-end distances ρ_n on the simple cubic lattice.

n	c_n	ρ_n
0	1	0
1	6	6
2	30	72
3	150	582
4	726	4 032
5	3 534	25 556
6	16 926	153 528
7	81 390	886 926
8	387 966	4 983 456
9	1 853 886	27 401 502
10	8 809 878	148 157 880
11	41 934 150	790 096 950
12	198 842 742	4 166 321 184
13	943 974 510	21 760 624 254
14	4 468 911 678	11 274 379 663
15	21 175 146 054	580 052 260 230
16	100 121 875 974	2 966 294 589 312
17	473 730 252 102	15 087 996 161 382
18	2 237 723 684 094	76 384 144 381 272
19	10 576 033 219 614	385 066 579 325 550
20	49 917 327 838 734	1 933 885 653 380 544
21	235 710 090 502 158	9 679 153 967 272 734
22	1 111 781 983 442 406	48 295 148 145 655 224
23	5 245 988 215 191 414	240 292 643 254 616 694
24	24 730 180 885 580 790	1 192 504 522 283 625 600
25	116 618 841 700 433 358	5 904 015 201 226 909 614
26	549 493 796 867 100 942	29 166 829 902 019 914 840

a list of 6-unit SAWS which can be added to the beginning without self-overlap. The end of the base chain is examined in a similar way to determine how many 6-unit SAWS can be added. A check is done to make sure adding a 6-unit chain to the end does not preclude adding certain ones to the beginning. This is possible when the endpoints of the base chain are within 12 units of each other. We are now able to calculate how many SAWS of length 26 have this base as their middle 14 segments. By summing over all possible bases we obtain C_{26}. Further details of the algorithm are discussed in [17].

The end-to-end distance is calculated by using list B to see which SAWs from list A may be added to the base chain. List A tells us the coordinates of the end points, thus list A is used for adding precomputed chains to both ends of the base chain.

The number of terms in the simple cubic series has been extended from the previous maximum 23 [17] to 26 for the C_N series and from 20 to 26 for the $\sum C_N R_N^2$ series [9].

The series for both SAW and squared end-to-end distances are given in table 1.

3. Analysis of the series

We first analysed both series by the numerical method of differential approximants [10]. In table 2 we have listed estimates for the critical point x_c and exponent γ from the series for the simple cubic lattice SAW generating function. The estimates were obtained by averaging

Table 2. Estimates for the critical point x_c and exponent γ obtained from first- and second-order inhomogeneous differential approximants to the series for the simple cubic lattice SAW generating function. T is the number of non-defective approximants used with the given number of terms N.

	First-order DA			Second-order DA		
N	x_c	γ	T	x_c	γ	T
14	0.213 5150(676)	1.163 67(968)	5	0.213 5011(232)	1.161 67(435)	3
15	0.213 4858(920)	1.159 83(1376)	3	0.213 5073(172)	1.164 07(363)	4
16	0.213 5037(379)	1.162 71(692)	6	0.213 5052(333)	1.163 05(410)	4
17	0.213 5088(321)	1.163 47(648)	8	0.213 5018(28)	1.162 46(72)	2
18	0.213 4939(335)	1.160 45(544)	12	0.213 5070(246)	1.163 45(454)	6
19	0.213 4824(310)	1.157 89(732)	8	0.213 4999(224)	1.162 20(442)	8
20	0.213 4994(146)	1.161 96(369)	11	0.213 4995(60)	1.162 01(128)	6
21	0.213 4961(37)	1.161 13(108)	11	0.213 4958(40)	1.161 15(104)	8
22	0.213 4967(17)	1.161 31(51)	8	0.213 4969(12)	1.161 39(36)	7
23	0.213 4962(5)	1.161 159(18)	6	0.213 4973(45)	1.161 52(156)	6
24	0.213 4958(4)	1.161 01(13)	7	0.213 4960(11)	1.161 09(36)	6
25	0.213 4950(12)	1.160 77(41)	6	0.213 4944(28)	1.160 57(96)	3
26	0.213 4947(7)	1.160 66(30)	9	0.213 4942(7)	1.160 43(31)	3

values obtained from first-order $[L/J; M]$ and second-order $[L/J; M; K]$ inhomogeneous differential approximants. Using the first N terms of the series, for fixed N we obtained a number of approximants, and hence the same number of estimates of the critical point and critical exponent. We then averaged over those non-defective approximants which lay within a reasonable distance of the mean—some 6 standard deviations. We used approximants such that the difference between J, M and K did not exceed 2. These are therefore 'diagonal' approximants. Some approximants were excluded from the averages because the estimates were obviously spurious. The errors quoted reflect the spread (basically one standard deviation) among the included approximants. Note that these error bounds should *not* be viewed as a measure of the true error as they cannot include systematic sources of error. We discuss further the systematic error below. If we were to accept these results at face value—and we argue below that we should not—we would conclude that $x_c = 0.213\,494(1)$ and $\gamma = 1.1604(5)$.

In an earlier paper [9], we analysed the same series but to length 20 terms. Based on that series, and the same method of analysis as above, we concluded that $x_c = 0.213\,497(10)$ and $\gamma = 1.1613(21)$. While the errors include our newer values, it is clear that the central estimates for both x_c and γ have declined. What is happening here is that we need significantly longer series to really reach the asymptotic regime. Monte Carlo studies [15] reach similar conclusions. It is pointed out in [15] that as corrections-to-scaling are much stronger in three dimensions than in two, much longer chains were needed to give believable, convergent results.

When we analyse the series using unbiased and biased Padé approximant methods we observe striking apparent convergence to $x_c = 0.213\,4987(2)$ and $\gamma = 1.161\,93(1)$. Although this is tempting to believe, the evidence that such series estimates can be very slow to truly converge is now quite substantial.

We have explicit evidence for this in the case of the simpler problem of SAP on the square lattice. The problem is simpler because there are no non-analytic corrections to scaling [7, 14], and we know the exact value of the critical exponent. In [14] we presented a new algorithm which permitted a radical extension of the series to 90 terms. A careful analysis of this very long series showed a systematic shift in estimates of critical parameters for 50, 60, 70 and 80 terms, seemingly asymptoting to unchanged estimates at around 100 terms! Given the

Table 3. Estimates for the critical point x_c and exponent γ obtained from first- and second-order inhomogeneous differential approximants to the series for the bcc lattice Ising model high-temperature susceptibility series. T is the number of non-defective approximants used with the given number of terms N.

	First-order DA			Second-order DA		
N	x_c	γ	T	x_c	γ	T
11	0.156 1014(66)	1.2456(15)	3	—	—	0
12	0.156 1241(101)	1.2488(17)	5	0.156 1258(57)	1.2490(11)	2
13	0.156 0966(438)	1.2443(73)	7	0.156 1158	1.2472	1
14	0.156 0930(124)	1.2438(38)	10	0.156 0977	1.2446	1
15	0.156 0899(129)	1.2426(30)	11	0.156 1001(99)	1.2451(26)	4
16	0.156 0952(95)	1.2438(25)	12	0.156 0991(68)	1.2448(17)	6
17	0.156 0954(49)	1.2439(15)	9	0.156 0962(32)	1.2441(10)	7
18	0.156 0950(21)	1.2437(66)	10	0.156 0938(65)	1.2431(31)	7
19	0.156 0938(15)	1.2434(52)	7	0.156 0976(66)	1.2444(14)	2
20	0.156 0919(11)	1.2427(42)	8	0.156 0945(82)	1.2432(28)	6
21	0.156 0918(8)	1.2428(37)	7	0.156 0934(78)	1.2431(36)	5

presence of non-analytic correction-to-scaling terms for the three-dimensional version of the problem, we could reasonably expect that similarly long series would be needed in that case before the asymptotic regime is reached.

A visual inspection of table 2 clearly reveals a systematic shift of critical parameters with increasing order of the series. How do we extrapolate this trend? One way is to look at the analogous series for the three-dimensional Ising model susceptibility, for which, by virtue of numerous high-precision Monte Carlo estimates, we have a rather precise estimate of the critical exponent. Furthermore, we expect similar non-analytic scaling corrections for both the Ising and SAW problem. (RG theory predicts one to be a little more than 0.5, and the other a little less.)

Unfortunately the sc Ising susceptibility series is only known to 21 terms [3], which is well short of the 26 terms presented here for SAW. However, we also have 21 terms for the body-centred cubic (bcc) susceptibility series [3, 18], which is roughly equivalent in length to a 26 term sc series, bearing in mind the higher co-ordination number of the bcc lattice. Analysing that series in the same way, we obtain the results shown in table 3 and find the same trend as observed with the sc SAW series. The last approximants suggest $v_c = 0.156\,092$, and $\gamma = 1.242\,75$. But for the Ising model $\gamma \approx 1.238$, a downward shift of about 0.005. A plot of the estimates of the exponent versus the critical point displays considerable linearity, so this can be invoked to determine one critical parameter if the other is known. So assuming $\gamma = 1.238$, the linearity of the plot of approximants gives $v_c = 0.156\,078$, a shift of 0.000 014.

In [3] a 21 term SAW series for the bcc lattice is also given, and direct application of differential approximants also gives rise to estimates of the critical exponent and critical point which are slowly decreasing as the number of available terms increases. A more careful analysis [3] gives the estimates $\gamma = 1.1582(8)$ and $\nu = 0.5879(6)$ in that case.

For sc SAWS, similar linearity is observed. In figure 1 we show the differential approximant estimates of the critical exponent and critical point, as tabulated in table 2. The RG and field theory estimates for γ are around 1.158, a shift in γ from our direct estimate of 0.0024. Invoking linearity, as discussed above, then gives an estimate of x_c of 0.213 488, which is in fact rather less than the change found for the bcc Ising susceptibility series.

Much of the change in the critical parameters with increased series length is presumably

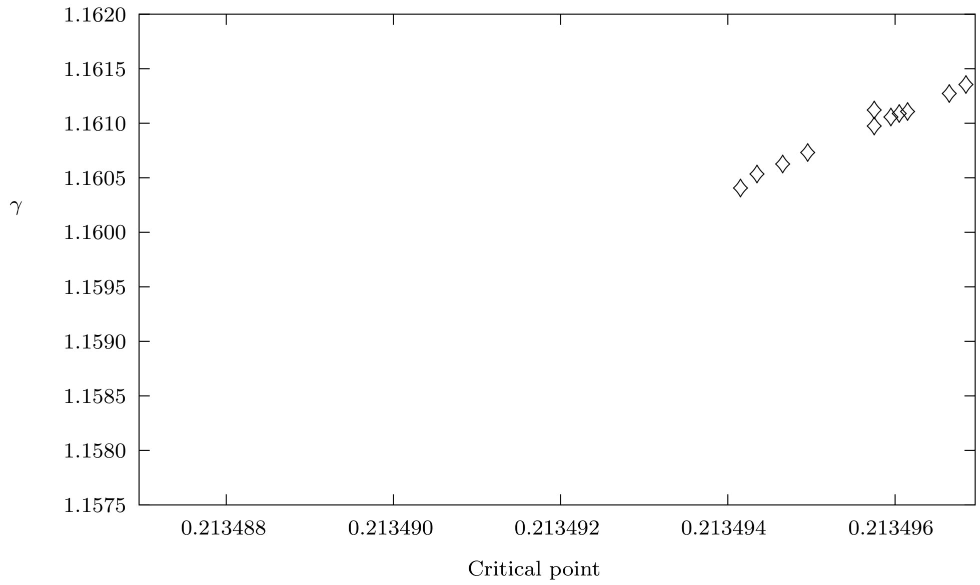

Figure 1. Estimates of γ and critical point, showing linear dependence.

due to the presence of nonlinear confluent terms. To take this into account, we have also tried to estimate the critical temperature by using two different variants of the ratio method, using only the approximate value of the confluent exponent as biasing input. The first method, due to Zinn-Justin [21, 22] relies on a sequence of nonlinear transformations to estimate the critical point. The original papers contain minor errors, but the corrected equations are available in [10]. Using this method, notably equation (2.30) of [10], one obtains a sequence of estimates of x_c with correction terms of order $O(1/n^{1+\theta})$. Here θ is the correction-to-scaling exponent, estimated variously at between 0.47 and 0.48 for the SAW model. For our purposes the value is not critical—even 0.5 would suffice—and one extrapolates the estimates of x_c against $1/n^{1+\theta}$. This results in a linear plot, with very minor odd–even oscillations characteristic of a loose packed lattice. Extrapolating alternate pairs gives estimates of $1/x_c$ of between 4.6840 and 4.6841. Taking the average gives $x_c = 0.213\,4905(23)$. Similarly, a modified linear extrapolation method can also be effectively used. In this method one first forms the ratios of coefficients $r_n = c_n/c_{n-2}$, where the ratio of alternate terms is used to minimize the effect of oscillations caused by a singularity on the negative real axis. One then forms the sequence $\sqrt{nr_n - (n-1)r_{n-1}}$ which should also approach $1/x_c$ linearly when plotted against $1/n^{1+\theta}$. Here the effect of odd and even extrapolants is more marked, but extrapolating each subsequence linearly, one again obtains $1/x_c = 4.684\,05(5)$.

A variation of the method of differential approximants that specifically biases approximants with the assumed value of the confluent exponent has been devised by Butera and Comi [3]. In this method one constructs first-order inhomogeneous differential approximants, which are biased to have a confluent exponent at the chosen value of θ and a singularity at a chosen value of x_c. By plotting estimates of the critical exponent γ, against x_c, the effect of the uncertainty in both x_c and θ can be estimated. This particular analysis gives [4] $\gamma = 1.1585(5)$.

Thus all methods that carefully take into account corrections-to-scaling, and the approach to the asymptotic limit, give good agreement.

We turn now to the asymptotic form of the coefficients. We expect that the asymptotic form for the coefficients of the SAW generating function will consist of two parts. These are the dominant ferromagnetic contribution, and a sub-dominant contribution from the antiferromagnetic singularity. The ferromagnetic singularity is characterized by the exponent γ while the antiferromagnetic exponent is characterized by the same exponent as the internal energy, which is usually denoted $1 - \alpha$. Both the ferromagnetic and antiferromagnetic parts have sub-dominant terms with exponent given by the correction-to-scaling exponent θ. Hence the expected asymptotic form of the coefficients is

$$c_n x_c^n \sim n^{\gamma-1}[a_0 + a_1/n^\theta + a_2/n + a_3/n^{\theta+1} + a_4/n^2 + \cdots] \\ +(-1)^n n^{\alpha-2}[b_0 + b_1/n^\theta + b_2/n + \cdots] \tag{4}$$

where the RG estimate of α is 0.235. While we have used this estimate in our analysis, we could have made use of the hyperscaling relation $d\nu = 2 - \alpha$. Together with the estimate of $\nu = 0.5875$ which we subsequently obtain, this gives $\alpha = 0.2375$. Use of this value would give almost indistinguishable results in our subsequent analysis. There should also be correction terms with exponent 2θ and so on, but as θ is close to 0.5, these will be indistinguishable in our analysis from analytic corrections. That is to say, a term $\mathrm{O}(n^{-2\theta})$ behaves very similarly to a term of $\mathrm{O}(1/n)$.

We have fitted the available data to the above form for a range of values of the critical exponent $1.160 \leqslant \gamma \leqslant 1.155$. In each case we tuned the critical point to yield the most stable estimates of the amplitudes. The results are shown in table 4. In all cases very stable fits are achieved, which suggests that our assumed asymptotic form is basically correct. It also shows that good results can be achieved for a range of values of the critical parameters by varying them to stabilise the amplitude sequences. This approach was shown to be appropriate for the much longer two-dimensional SAP series [14]. That is to say, we look for maximum stability among the last five estimates, and that is found for $\gamma = 1.1585$, and $x_c = 0.213\,492$. However, we cannot, on the basis of this analysis completely rule out other values of γ in the range studied. The leading amplitudes $a_0 = 1.205$, and $b_0 = 0.080$ also follow from this analysis, but the estimate of a_0 is seen to depend on the estimate of γ, though that of b_0 is relatively insensitive to small shifts in γ. Writing the walk generating function as

$$C(x) = \sum c_n x^n \sim A_0(x) + A_1(1 - \mu x)^{-\gamma} + D_0(1 + \mu x)^{1-\alpha} \tag{5}$$

it follows that $A_1 = a_0\Gamma(\gamma) \approx 1.121$ and $D_0 = b_0\Gamma(\alpha - 1) \approx -0.40$.

We also analysed the series for the squared end-to-end distance by the method of (unbiased) differential approximants, but found that almost all approximants making use of our newly found coefficients were defective. A biased analysis, using the above estimate of the critical point, also produced defective approximants from almost all entries using the new coefficients. A coefficient by coefficient quotient of the two series, that is an analysis of the series whose coefficients are given by ρ_n/c_n, which will have critical point exactly 1.0, and exponent 2ν was also carried out. The differential approximants were again almost all defective. However, we can use our estimate of the critical point obtained from the above analysis of the SAW generating function in an analysis of the asymptotic form of the coefficients, bypassing the differential approximant analysis. So, tentatively accepting the estimates of the critical parameters found in our SAW analysis, we repeated the above analysis *mutatis mutandis* of the series for the sum of the squared end-to-end distances. In this way, we obtained exponent estimates in satisfying agreement with recent high-precision Monte Carlo estimates [15]. The appropriate asymptotic form in this case is

$$\rho_n x_c^n \sim n^{\gamma+2\nu-1}[d_0 + d_1/n^\theta + d_2/n + d_3/n^{\theta+1} + d_4/n^2 + \cdots] \\ +(-1)^n n^{\alpha-2}[e_0 + e_1/n^\theta + e_2/n + \cdots]. \tag{6}$$

Table 4. Sequences of amplitudes for different assumed values of the critical exponent γ and connective constant μ for the SAW series. N is the maximum order of the series used in the analysis.

N	a_0	a_1	a_2	a_3	a_4	b_0	b_1	b_2
$x_c = 0.213\,493$								
$\gamma = 1.160$								
13	1.187 41	0.0670	−0.2876	0.7084	−0.4417	−0.0756	−0.0508	0.1523
14	1.195 96	−0.0295	0.1950	−0.2681	0.3048	−0.0703	−0.0812	0.2002
15	1.205 27	−0.1395	0.7743	−1.4969	1.2939	−0.0760	−0.0467	0.1429
16	1.194 85	−0.0111	0.0662	0.0710	−0.0288	−0.0824	−0.0065	0.0732
17	1.192 65	0.0171	−0.0958	0.4441	−0.3574	−0.0810	−0.0153	0.0891
18	1.193 15	0.0104	−0.0554	0.3477	−0.2690	−0.0807	−0.0174	0.0930
19	1.192 31	0.0220	−0.1277	0.5260	−0.4385	−0.0802	−0.0210	0.1000
20	1.192 96	0.0128	−0.0682	0.3745	−0.2895	−0.0798	−0.0238	0.1058
21	1.193 17	0.0097	−0.0477	0.3208	−0.2350	−0.0799	−0.0229	0.1038
22	1.192 76	0.0158	−0.0894	0.4333	−0.3527	−0.0802	−0.0210	0.0998
23	1.192 82	0.0149	−0.0835	0.4169	−0.3351	−0.0802	−0.0207	0.0992
24	1.192 72	0.0165	−0.0946	0.4484	−0.3699	−0.0803	−0.0203	0.0982
25	1.192 71	0.0166	−0.0956	0.4512	−0.3731	−0.0803	−0.0203	0.0983
26	1.192 67	0.0174	−0.1013	0.4684	−0.3930	−0.0803	−0.0201	0.0977
$x_c = 0.213\,492$								
$\gamma = 1.1585$								
13	1.198 69	0.0289	−0.2030	0.5998	−0.3840	−0.0756	−0.0506	0.1519
14	1.207 41	−0.0695	0.2895	−0.3967	0.3777	−0.0702	−0.0815	0.2006
15	1.216 89	−0.1815	0.8790	−1.6471	1.3842	−0.0760	−0.0465	0.1426
16	1.206 55	−0.0540	0.1764	−0.0915	0.0719	−0.0823	−0.0068	0.0736
17	1.204 44	−0.0270	0.0211	0.2662	−0.2431	−0.0810	−0.0151	0.0888
18	1.205 04	−0.0350	0.0690	0.1519	−0.1384	−0.0807	−0.0176	0.0935
19	1.204 27	−0.0244	0.0032	0.3143	−0.2927	−0.0802	−0.0209	0.0998
20	1.205 00	−0.0348	0.0698	0.1446	−0.1259	−0.0798	−0.0240	0.1062
21	1.205 28	−0.0388	0.0966	0.0741	−0.0543	−0.0799	−0.0228	0.1037
22	1.204 93	−0.0336	0.0612	0.1698	−0.1544	−0.0801	−0.0212	0.1003
23	1.205 04	−0.0353	0.0730	0.1372	−0.1193	−0.0802	−0.0207	0.0991
24	1.205 00	−0.0346	0.0678	0.1518	−0.1354	−0.0802	−0.0205	0.0987
25	1.205 03	−0.0352	0.0722	0.1392	−0.1211	−0.0803	−0.0203	0.0982
26	1.205 03	−0.0352	0.0719	0.1399	−0.1219	−0.0803	−0.0203	0.0982
$x_c = 0.213\,491$								
$\gamma = 1.1570$								
13	1.209 68	−0.0068	−0.1269	0.5051	−0.3349	−0.0756	−0.0504	0.1517
14	1.218 55	−0.1068	0.3734	−0.5073	0.4389	−0.0702	−0.0818	0.2010
15	1.228 15	−0.2203	0.9706	−1.7742	1.4587	−0.0760	−0.0464	0.1424
16	1.217 85	−0.0934	0.2712	−0.2254	0.1521	−0.0823	−0.0070	0.0740
17	1.215 79	−0.0670	0.1196	0.1236	−0.1552	−0.0810	−0.0152	0.0888
18	1.216 45	−0.0758	0.1720	−0.0016	−0.0405	−0.0806	−0.0179	0.0939
19	1.215 72	−0.0657	0.1094	0.1531	−0.1875	−0.0802	−0.0210	0.0999
20	1.216 49	−0.0766	0.1797	−0.0261	−0.0113	−0.0797	−0.0243	0.1067
21	1.216 80	−0.0811	0.2091	−0.1031	0.0669	−0.0799	−0.0230	0.1038
22	1.216 47	−0.0762	0.1761	−0.0142	−0.0261	−0.0801	−0.0215	0.1007
23	1.216 60	−0.0781	0.1893	−0.0508	0.0132	−0.0802	−0.0209	0.0994
24	1.216 57	−0.0776	0.1859	−0.0411	0.0025	−0.0802	−0.0208	0.0991
25	1.216 61	−0.0783	0.1907	−0.0550	0.0183	−0.0802	−0.0206	0.0987
26	1.216 61	−0.0784	0.1913	−0.0568	0.0205	−0.0802	−0.0206	0.0987

Table 4. (Continued)

N	a_0	a_1	a_2	a_3	a_4	b_0	b_1	b_2
$x_c = 0.213\,490$								
$\gamma = 1.1550$								
13	1.224 35	−0.0543	−0.0268	0.3813	−0.2712	−0.0756	−0.0503	0.1514
14	1.233 40	−0.1563	0.4835	−0.6513	0.5181	−0.0701	−0.0821	0.2015
15	1.243 16	−0.2716	1.0903	−1.9387	1.5543	−0.0760	−0.0463	0.1422
16	1.232 91	−0.1453	0.3943	−0.3975	0.2542	−0.0822	−0.0074	0.0745
17	1.230 91	−0.1197	0.2469	−0.0581	−0.0446	−0.0810	−0.0152	0.0888
18	1.231 63	−0.1293	0.3046	−0.1959	0.0816	−0.0806	−0.0182	0.0944
19	1.230 93	−0.1197	0.2450	−0.0487	−0.0583	−0.0801	−0.0211	0.1001
20	1.231 75	−0.1313	0.3194	−0.2381	0.1280	−0.0797	−0.0246	0.1072
21	1.232 08	−0.1360	0.3508	−0.3206	0.2118	−0.0799	−0.0232	0.1042
22	1.231 78	−0.1315	0.3200	−0.2374	0.1247	−0.0800	−0.0218	0.1013
23	1.231 90	−0.1335	0.3337	−0.2754	0.1656	−0.0801	−0.0212	0.1000
24	1.231 88	−0.1331	0.3312	−0.2684	0.1579	−0.0801	−0.0211	0.0997
25	1.231 91	−0.1336	0.3350	−0.2794	0.1704	−0.0801	−0.0210	0.0994
26	1.231 91	−0.1337	0.3353	−0.2802	0.1713	−0.0801	−0.0210	0.0994

We expect on universality grounds that the correction-to-scaling exponent θ is the same as for SAWs. The behaviour of the antiferromagnetic singularity has not, as far as we know, been considered for this problem. Our differential approximant analysis of this series allows us to estimate this exponent, and we find it to be in agreement with the corresponding quantity for SAWs. Accordingly, we have assumed this to be the case. As the analysis is not sensitive to a small variation in this exponent, this is not a vital assumption. In this analysis we have fixed the value of the connective constant to that found in the analysis of the SAW series.

Using our estimate of x_c quoted above, we show in table 5 the estimates of the amplitudes $d_0, \ldots, d_3$, and e_0, e_1, e_2 obtained with $\mu = 4.684\,01$ and $\gamma + 2\nu = 2.3334$. We find $d_0 = 1.476$, $d_1 = 0.520$, $d_2 = 0.580$, $d_3 = 0.27$ and $e_0 = 0.05$, $e_1 = 0.00$ and $e_2 = -0.08$, where we expect errors to be confined to the last quoted digit. Using the value of $\gamma = 1.1585$ estimated above, we find $\nu = 0.5875$. This is in unexpectedly good agreement with the recent high-precision Monte Carlo estimate [15] $\nu = 0.5877 \pm 0.0006$, and also agrees with recent renormalization group ϵ-expansion and $d = 3$ expansion results, which have central estimates in the range 0.5875–0.5882. It is also in good agreement with the estimates obtained from the bcc series [3] of 0.5879(6).

This estimate of ν is rather stable to the assumed value of γ. For example, if we shift the critical exponent γ to 1.155, then the connective constant μ shifts to 4.8406 as shown above. Repeating our immediately preceding analysis of the squared end-to-end distance series gives stability of amplitude estimates for $\gamma + 2\nu = 2.3311$, or $\nu = 0.5881$. So a 3% shift in γ produces a shift in ν of less than 0.1%.

4. Rigorous upper bound on μ

Many workers have developed techniques for the establishment of rigorous upper and lower bounds on the connective constant for SAW on various lattices. The main techniques are reviewed in [20]. For the simple cubic lattice the best bounds are $4.572\,14 < \mu < 4.756$ [2,12]. Based on the extended enumerations we have given, it is possible to obtain an improved upper bound using the method of Ahlberg and Janson [1].

Table 5. Sequences of amplitudes for the square endtoend distance generating function. x_c is fixed at 0.213 492. This sequence is produced with $\gamma + 2\nu = 2.3334$.

N	d_0	d_1	d_2	d_3	e_0	e_1	e_2
13	1.475 93	−0.5204	0.5786	−0.2712	0.0303	0.1034	−0.2339
14	1.475 81	−0.5193	0.5749	−0.2673	0.0188	0.1711	−0.3425
15	1.475 73	−0.5185	0.5722	−0.2642	0.0284	0.1122	−0.2433
16	1.475 92	−0.5204	0.5790	−0.2723	0.0552	−0.0595	0.0598
17	1.475 92	−0.5203	0.5789	−0.2721	0.0559	−0.0641	0.0682
18	1.475 94	−0.5206	0.5800	−0.2735	0.0612	−0.1009	0.1386
19	1.475 98	−0.5210	0.5815	−0.2755	0.0537	−0.0471	0.0320
20	1.475 96	−0.5208	0.5808	−0.2745	0.0497	−0.0184	−0.0268
21	1.475 97	−0.5209	0.5812	−0.2751	0.0472	0.0007	−0.0672
22	1.475 97	−0.5208	0.5809	−0.2747	0.0454	0.0150	−0.0985
23	1.475 96	−0.5208	0.5807	−0.2744	0.0467	0.0045	−0.0749
24	1.475 96	−0.5208	0.5806	−0.2742	0.0457	0.0124	−0.0931
25	1.475 96	−0.5207	0.5804	−0.2739	0.0473	−0.0007	−0.0622
26	1.475 95	−0.5207	0.5803	−0.2737	0.0464	0.0068	−0.0803

They prove the result that, if $n > 2$, the connective constant is less than the positive root of

$$c_1 x^{n-1} = (c_n - (c_1 - 2)c_{n-1})x + (c_1 - 2)((c_1 - 1)c_{n-1} - c_n).$$

From the coefficients in the table below, setting $n = 26$, one immediately obtains the bound $\mu < 4.7114$. This is a worthwhile improvement on the previous best bound, cited above.

5. Conclusion

We have presented substantially extended series for the SAW and squared end-to-end distance series, and given a detailed analysis using ratio methods, differential approximants and asymptotic fitting. Together these three methods provide convincing evidence of agreement with exponent estimates obtained by other methods. While our preferred estimate of γ at 1.1585 is about 1% higher than the most recent ϵ-expansion estimates, it is about 1% lower than corresponding $d = 3$ expansion estimates. A recent high quality Monte Carlo study [5] gave $\gamma = 1.1575 \pm 0.0006$. For the exponent ν our estimates are much more precise, being encompassed within the range $0.5870 \leqslant \nu \leqslant 0.5881$ which is in agreement with almost all recent MC and RG and series studies. Our estimates are also entirely consistent with those obtained for the bcc lattice SAW series [3]. The connective constant is much less amenable to study by other methods, and we estimate $x_c = 0.213\,491 \pm 0.000\,004$, or, equivalently, $\mu = 4.684\,04 \pm 0.000\,09$. This is perhaps a less precise estimate than some quoted previously, but the more reliable as a consequence! We note in passing that the traditional methods used in the past (Padé, direct application of differential approximants and transformations to extract the correction terms) would have led to consistently misleadingly precise but *slightly inaccurate* critical points, exponents and correction to scaling terms [17]. We have also estimated the critical amplitudes for the ferromagnetic and antiferromagnetic singularities, and these are found to be $A_0 \approx 1.121$ and $B_0 \approx -0.40$ where no confidence limit is quoted, for, as explained in detail above, our estimates depend on the value of γ chosen. These amplitude estimates should, however, have errors confined to the last quoted digit if γ is close to 1.1585, as suggested by our analysis above.

Finally, the extended enumeration data allows us to calculate an improved upper bound on the connective constant, $\mu < 4.7114$.

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