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Exact enumeration of self-avoiding walks on BCC and FCC lattices

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Abstract. Self-avoiding walks on the body-centered-cubic (BCC) and face-centered-cubic (FCC) lattices are enumerated up to lengths 28 and 24, respectively, using the length-doubling method. Analysis of the enumeration results yields values for the exponents γ and ν which are in agreement with, but less accurate than, those obtained earlier from enumeration results on the simple cubic lattice. The non-universal growth constant and amplitudes are accurately determined, yielding for the BCC lattice $\mu = 6.530\,520(20)$, $A = 1.1785(40)$, and $D = 1.0864(50)$, and for the FCC lattice $\mu = 10.037\,075(20)$, $A = 1.1736(24)$, and $D = 1.0460(50)$.

Keywords: critical exponents and amplitudes, exact results, loop models and polymers, series expansions

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Contents

1. Introduction

The enumeration of self-avoiding walks (SAWs) on regular lattices is a classical combinatorial problem in statistical physics, with a long history, see e.g. [1, 2]. Of the three-dimensional lattices, the simple cubic (SC) lattice has drawn the most effort, starting with a paper by Orr [3] from 1947, where the number of SAWs Z_N was given for all N up to $N_{\max} = 6$; these results were obtained by hand. In 1959, Fisher and Sykes [4] used a computer to enumerate all SAWs up to $N_{\max} = 9$; Sykes and collaborators extended this to 11 terms in 1961 [5], 16 terms in 1963 [6], and 19 terms in 1972 [7]. In the following decade, Guttmann [8] enumerated SAWs up to $N_{\max} = 20$ in 1987, and extended this by one step in 1989 [9]. In 1992, MacDonald *et al* [10] reached $N_{\max} = 23$, and in 2000 MacDonald *et al* [11] reached $N_{\max} = 26$. In 2007, a combination of the lace expansion and the two-step method allowed for the enumeration of SAWs up to $N_{\max} = 30$ steps [12]. Recently, the length-doubling method [13] was presented which allowed enumerations to be extended up to $N_{\max} = 36$. To date, this is the record series for the SC lattice.

The body-centered-cubic (BCC) and face-centered-cubic (FCC) lattices are in principle equally as physically relevant as the SC lattice, but enumeration is hampered by the larger lattice coordination numbers, which detriments most enumeration methods severely. It is also slightly more cumbersome to write computer programs to perform enumerations for these lattices. Consequently, the SC lattice has served as the test-bed problem for new enumeration algorithms, and the literature on enumerations for the BCC and FCC lattices is far more sparse. For the BCC lattice, Z_N was determined up to $N_{\max} = 15$ in 1972 [7], and to $N_{\max} = 16$ in 1989 [9]. The current record of $N_{\max} = 21$ was obtained in 1997 by Butera and Comi [14] as the $N \to 0$ limit of the high temperature series for the susceptibility of the N-vector model. For the FCC lattice, enumerations up to $N_{\max} = 12$ were performed in 1967 [15], and the record of $N_{\max} = 14$ was achieved way back in 1979 [16].

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Enumeration results derive their relevance from the ability to determine critical exponents, which, according to renormalization group theory, are believed to be shared between SAWs on various lattices and real-life polymers in solution [17]. Two such exponents are the entropic exponent γ and the size exponent ν. Given the number Z_N of SAWs of all lengths up to $N_{\max}$ and the sum P_N of their squared end-to-end distances, these two exponents can be extracted using the relations

$$Z_N = A\mu^N N^{\gamma-1}\left(1+\frac{a}{N^{\Delta_1}}+O\left(\frac{1}{N}\right)\right); \tag{1}$$

$$\frac{P_N}{Z_N} = \sigma D N^{2\nu}\left(1+\frac{b}{N^{\Delta_1}}+O\left(\frac{1}{N}\right)\right). \tag{2}$$

In these expressions, the growth constant μ and the amplitudes A and D are non-universal (model-dependent) quantities, while the leading correction-to-scaling exponent is a universal quantity with value $\Delta_1 = 0.528(8)$ [18]. Sub-leading corrections-to-scaling are absorbed into the $O(1/N)$ term. σ is a lattice specific constant to ensure that our amplitude 'D' is the same as in earlier work. σ corrects for the fact that with our definition each step of the walk is of length $\sqrt{2}$ for the BCC lattice (leading to $\sigma = 2$), and of length $\sqrt{3}$ for the FCC lattice (leading to $\sigma = 3$). Note that for bipartite lattices, of which the SC and BCC lattices are examples, there is an additional alternating 'anti-ferromagnetic' singularity, that is sub-leading but which still must be treated carefully as the odd-even oscillations tend to become amplified by series analysis techniques. Because of universality, the exponents are clearly more interesting from a physics perspective. However, accurate estimates for the growth constant and the amplitudes can also be very helpful for many kinds of computer simulations of lattice polymers.

In this paper, we used the length-doubling method [13] to calculate Z_N and P_N up to $N_{\max} = 28$ and 24, on the BCC and FCC lattices, respectively. These lattices can be easily realized as subsets of the SC lattice: the collection of sites in which x, y and z are either all even or all odd forms a BCC lattice, and the collection of sites (x, y, z) constrained to even values of $x + y + z$ forms a FCC lattice. We then analyzed these series to obtain estimates for the exponents γ and ν, the growth constant μ, and the amplitudes A and D. Our results for the two exponents γ and ν agree with the most accurate values reported in the literature which are obtained on the SC lattice, reinforcing the credibility of the literature values. Our results for the growth constant μ and the amplitudes A and D for the BCC and FCC lattices are the most accurate to date.

The manuscript is organized as follows. First, in section 2 we present a short outline of the length-doubling method, and present the enumeration data. In section 3 we describe the analysis method we use, before summarizing our results and giving a brief conclusion in section 4.

2. Length-doubling method

We first present an intuitive description of the length-doubling method; a more formal description can be found in [13]. In the length-doubling method, the number Z_{2N} of SAWs with a length of $2N$ steps, with the middle rooted in the origin, is obtained from

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the walks of length N, with one end rooted in the origin, and the number $Z_N(S)$ of times that a subset S of sites is visited by such a walk of length N. The lowest-order estimate for Z_{2N} is the number of combinations of two SAWs of length N, i.e. Z_N^2. This estimate is too large since it includes pairs of SAWs which overlap. The first correction to Z_{2N} is the lowest-order estimate for the number of pairs of overlapping SAWs, which can be obtained from the number $Z_N(\{s\})$ of SAWs of length N which pass through a single site s. The first correction is then to subtract $Z_N(\{s\})^2$, summed over all sites s. This first correction is too large, as it includes pairs of SAWs twice, if they intersect twice. The second correction corrects for this over-subtraction, by adding the numbers $Z_N(\{s,t\})^2$ corresponding to SAWs that pass through the pair of sites $\{s,t\}$. Continuing this process with groups of three sites, etc the number Z_{2N} of SAWs of length $2N$ can then be obtained by the length-doubling formula

$$Z_{2N} = Z_N^2 + \sum_{S\neq\emptyset}(-1)^{|S|} Z_N^2(S), \tag{3}$$

where $|S|$ denotes the number of sites in S.

The usefulness of this formula lies in the fact that the numbers $Z_N(S)$ can be obtained relatively efficiently:

- Generate each SAW of length N.
- Generate for each SAW each of the 2^N subsets S of lattice sites, and increment the counter for each specific subset. Multiple counters for the same subset S must be avoided; this can be achieved by sorting the sites within each subset in an unambiguous way.
- Finally, compute the sum of the squares of these counters, with a positive and negative sign for subsets with an even and odd number of sites, respectively, as in equation (3).

As there are Z_N walks of length N, each visiting 2^N subsets of sites, the computational complexity is $\mathcal{O}(2^N Z_N) \sim (2\mu)^N$ times some polynomial in N which depends on implementation details. This compares favorably to generating all $Z_{2N} \sim \mu^{2N}$ walks of length $2N$, provided $\mu > 2$. This is the case on the SC lattice, with $\mu = 4.684$, and even more so for the BCC and FCC lattices, as we will show. The length-doubling method can also compute the squared end-to-end distance, summed over all SAW configurations; for details we refer to [13]. Details on the efficient implementation of this algorithm are presented in [19].

We note that the length-doubling method could be extended to the calculation of other observables, in particular the mean-squared radius of gyration and the mean-squared distance from a monomer to its endpoints. These observables are of interest because they give an alternative means of estimating the critical exponent ν, and the ratios of the observables give universal amplitude ratios. Implementing the calculations of these observables would increase the complexity of the computer code, and was not done here, but would be a worthwhile extension for future work.

The direct results of the length-doubling method, applied to SAWs on the BCC and FCC lattices, are presented in tables 1 and 2, respectively. The BCC results for $N \leqslant 26$

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and FCC results for $N \leqslant 22$ were obtained and verified by two independent computer programs: SAWdoubler 2.0, available from www.staff.science.uu.nl/∼bisse101/SAW/, and Raoul Schram's program. The BCC results presented for the largest problems $N = 27, 28$ were obtained by SAWdoubler 2.0 only, and the FCC results for $N = 23, 24$ were obtained by Raoul Schram's program only. Thus the largest two problem instances for each lattice were not independently verified since these require a very large amount of computer time and memory. Still, based on our analysis we believe that the given values are correct.

3. Analysis

We now proceed to analyze our series in order to extract estimates for various parameters. In addition to the expressions for Z_N and P_N/Z_N in equations (1) and (2), we also have

$$P_N = \sigma AD\mu^N N^{2\nu+\gamma-1}\left(1 + \frac{c}{N^{\Delta_1}} + O\left(\frac{1}{N}\right)\right). \tag{4}$$

As discussed earlier, we expect the critical exponents γ and ν and the leading correction-to-scaling exponent Δ_1 to be the same for self-avoiding walks on the SC, BCC, and FCC lattices. The amplitudes A and D are non-universal quantities, i.e. they are lattice dependent, while $\sigma = 2$ for the BCC lattice and $\sigma = 3$ for the FCC lattice. In the analysis below, we include a subscript to indicate the appropriate lattice.

The BCC lattice is bipartite, which introduces an additional competing correction which has a factor of $(-1)^N$, so causing odd-even oscillations. We reduce the influence of this additional sub-leading correction by treating the sequences for even and odd N separately. See section 3.3 for further details.

We now describe the method of analysis we used, which involved two stages: extrapolation of the series via a recently introduced method involving differential approximants [20], and then direct fitting of the extended series with the asymptotic forms in equations (1), (2) and (4). We then discuss in more detail some aspects of the analysis, and report our final estimates in table 5.

3.1. Extrapolation

The method of differential approximants, described in [21], is perhaps the most powerful general-purpose method for the analysis of series arising from lattice models in statistical mechanics. The basic idea is to approximate the unknown generating function F by the solution of an ordinary differential equation with polynomial coefficients. In particular if we know r coefficients $f_0, f_1, \cdots, f_{r-1}$ of our generating function F, then we can determine polynomials $Q_i(z)$ and $P(z)$ which satisfy the following Kth order differential equation order by order:

$$\sum_{i=0}^{K} Q_i(z)\left(z\frac{\mathrm{d}}{\mathrm{d}z}\right)^{\mathrm{i}} F(z) = P(z). \tag{5}$$

Table 1. Enumeration results for the number of three-dimensional self-avoiding walks Z_N and the sum of their squared end-to-end distances P_N on the BCC lattice.

N	Z_N	P_N
1	8	24
2	56	384
3	392	4 248
4	2 648	40 704
5	17 960	358 008
6	120 056	2 987 232
7	804 824	23 999 880
8	5 351 720	187 661 376
9	35 652 680	1 436 494 872
10	236 291 096	10 816 140 768
11	1 568 049 560	80 339 567 112
12	10 368 669 992	590 168 152 512
13	68 626 647 608	4 294 543 350 696
14	453 032 542 040	31 003 097 851 872
15	2 992 783 648 424	222 268 142 153 784
16	19 731 335 857 592	1 583 984 756 900 544
17	130 161 040 083 608	11 228 345 566 400 136
18	857 282 278 813 256	79 223 666 339 548 320
19	5 648 892 048 530 888	556 634 161 952 309 400
20	37 175 039 569 217 672	3 896 382 415 388 139 840
21	244 738 250 638 121 768	27 181 650 674 871 447 672
22	1 609 522 963 822 562 936	189 042 890 267 974 827 744
23	10 588 362 063 533 857 304	1 311 064 323 033 684 408 072
24	69 595 035 470 413 829 144	9 069 398 712 299 296 227 648
25	457 555 628 726 692 288 712	62 590 336 418 536 387 660 248
26	3 005 966 051 800 541 943 464	431 019 462 253 450 273 360 416
27	19 752 610 526 081 274 414 584	2 962 188 249 772 759 155 770 280
28	129 713 248 317 927 812 262 200	20 319 964 852 485 237 389 626 176

The function determined by the resulting differential equation is our approximant. The power of the method derives from the fact that such ordinary differential equations accommodate the kinds of critical behavior that are typically seen for models of interest.

Differential approximants are extremely effective at extracting information about critical exponents from the long series that have been obtained for two-dimensional lattice models, such as self-avoiding polygons [22] or walks [23] on the square lattice. However, differential approximants have been far less successful for the shorter series available for three-dimensional models such as SAWs on the simple cubic lattice [12, 13]. For short series, it seems that corrections-to-scaling due to confluent corrections are too strong at the orders that can be reached to be able to reliably determine critical exponents. (In fact, it is extremely easy to be misled by apparent convergence, while in fact estimates have not settled down to their asymptotic values.) The method that has proved most reliable is direct fitting of the asymptotic form [12], which we describe in the next section.

However, we can do better than the usual method of performing direct fits of the original series, and adopt a promising new approach recently invented by Guttmann [20], which is a hybrid of the differential approximant and direct fitting techniques. The underlying idea is to exploit the fact that differential approximants can be used to extrapolate series with high accuracy even in circumstances when the resulting estimates

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Table 2. Enumeration results for the number of three-dimensional self-avoiding walks Z_N and the sum of their squared end-to-end distances P_N on the FCC lattice.

N	Z_N	P_N
1	12	24
2	132	576
3	1 404	9 816
4	14 700	144 288
5	152 532	1 951 560
6	1 573 716	25 021 536
7	16 172 148	309 080 808
8	165 697 044	3 714 659 040
9	1 693 773 924	43 714 781 448
10	17 281 929 564	505 948 384 608
11	176 064 704 412	5 777 220 825 912
12	1 791 455 071 068	65 234 797 723 584
13	18 208 650 297 396	729 724 191 726 408
14	184 907 370 618 612	8 097 639 351 530 304
15	1 876 240 018 679 868	89 239 258 469 121 912
16	19 024 942 249 966 812	977 545 487 795 069 952
17	192 794 447 005 403 916	10 651 662 728 070 257 016
18	1 952 681 556 794 601 732	115 520 552 778 504 791 136
19	19 767 824 914 170 222 996	1 247 619 751 507 795 906 248
20	200 031 316 330 580 106 948	13 423 705 093 594 869 393 216
21	2 023 330 401 919 804 218 996	143 942 374 595 787 212 970 696
22	20 458 835 772 261 851 432 748	1 538 749 219 442 520 114 999 744
23	206 801 586 042 610 941 719 148	16 403 200 314 230 418 676 555 512
24	2 089 765 228 215 904 826 153 292	174 411 223 302 510 038 302 309 440

for critical exponents are not particularly accurate, or even when the asymptotic behavior is non-standard such as being of stretched exponential form. The extrapolations can be extremely useful in cases where corrections-to-scaling are large, as the few extra terms they provide may be the only evidence of a clear trend from the direct fits.

We have 28 exact terms for the BCC series, and 24 exact terms for the FCC series. We used second order inhomogeneous approximants to extrapolate the series for Z_N, P_N, and P_N/Z_N, where we allowed the multiplying polynomials to differ by degree at most 3. In each case we calculated trimmed mean values, eliminating the outlying top and bottom 10% of estimates, with the standard deviation of the remaining extrapolated coefficients providing a proxy for the confidence interval. Note that this is an assumption, and relies on the extrapolation procedure working well for our problem. In practice, this approach of inferring the confidence interval from the spread of estimates appears to be quite reliable in the cases for which it has been tested. We have also confirmed the reliability of the extrapolations by using the method to 'predict' known coefficients from truncated series. We report our extended series in tables 3 and 4.

3.2. Direct fits

We then fitted sequences of consecutive terms of the extrapolated series for Z_N and P_N/Z_N to the asymptotic forms given in equations (1) and (2), respectively. We found that fits of P_N/Z_N were superior to fits of P_N for estimates of ν and the parameter D, and hence we do not report fits of P_N here.

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Table 3. Extrapolated coefficients of the various BCC series obtained from differential approximants. The confidence intervals are the standard deviations of the central 80% of estimates.

N	Z_N	P_N	P_N/Z_N
29	$8.519\,843\,781\,50(70) \times 10^{23}$	$1.391\,489\,520\,51(11) \times 10^{26}$	163.323 360 851(42)
30	$5.592\,866\,9767(12) \times 10^{24}$	$9.513\,461\,0227(17) \times 10^{26}$	170.099 897 96(10)
31	$3.672\,098\,7764(23) \times 10^{25}$	$6.494\,430\,1898(72) \times 10^{27}$	176.858 809 53(40)
32	$2.409\,790\,7972(39) \times 10^{26}$	$4.427\,231\,8727(75) \times 10^{28}$	183.718 514 86(77)
33	$1.581\,658\,3535(44) \times 10^{27}$	$3.014\,025\,691(25) \times 10^{29}$	190.561 1070(19)
34	$1.037\,661\,297(10) \times 10^{28}$	$2.0493\,782\,03(42) \times 10^{30}$	197.499 7221(33)
35	$6.808\,628\,821(74) \times 10^{28}$	$1.391\,831\,542(69) \times 10^{31}$	204.421 7013(47)
36	$4.465\,743\,83(26) \times 10^{29}$	$9.442\,164\,66(95) \times 10^{31}$	211.435 420(11)
37	$2.929\,428\,561(97) \times 10^{30}$	$6.398\,8380(13) \times 10^{32}$	218.432 947(13)
38	$1.920\,9657(36) \times 10^{31}$	$4.332\,1295(17) \times 10^{33}$	225.518 346(32)

Table 4. Extrapolated coefficients of the various FCC series obtained from differential approximants. The confidence intervals are the standard deviations of the central 80% of estimates.

N	Z_N	P_N	P_N/Z_N
25	$2.111\,165\,270\,9103(46) \times 10^{25}$	$1.850\,104\,492\,114\,73(82) \times 10^{27}$	87.634 280 348 06(26)
26	$2.132\,245\,848\,773(38) \times 10^{26}$	$1.958\,277\,810\,1818(72) \times 10^{28}$	91.841 089 1195(22)
27	$2.153\,033\,629\,72(17) \times 10^{27}$	$2.068\,615\,279\,889(35) \times 10^{29}$	96.079 097 491(11)
28	$2.173\,552\,5326(10) \times 10^{28}$	$2.181\,101\,876\,19(13) \times 10^{30}$	100.347 327 420(41)
29	$2.193\,824\,0975(32) \times 10^{29}$	$2.295\,724\,275\,39(38) \times 10^{31}$	104.644 865 52(13)
30	$2.213\,867\,7922(93) \times 10^{30}$	$2.412\,470\,697\,49(92) \times 10^{32}$	108.970 856 72(37)
31	$2.233\,701\,285(63) \times 10^{31}$	$2.531\,330\,7684(21) \times 10^{33}$	113.324 498 76(98)
32	$2.253\,340\,58(14) \times 10^{32}$	$2.652\,295\,3987(45) \times 10^{34}$	117.705 0374(24)
33	$2.272\,8013(51) \times 10^{33}$	$2.775\,356\,6769(86) \times 10^{35}$	122.111 7622(56)

To convert the fitting problem to a linear equation, we took the logarithm of the coefficients, which from equations (1) and (2) we expect to have the following asymptotic forms:

$$\log Z_N = N \log \mu + (\gamma - 1) \log N + \log A + \frac{a}{N^{\Delta_1}} + O\left(\frac{1}{N}\right); \tag{6}$$

$$\log \frac{P_N}{Z_N} = 2\nu \log N + \log \sigma D + \frac{b}{N^{\Delta_1}} + O\left(\frac{1}{N}\right). \tag{7}$$

We used the linear fitting routine 'lm' in the statistical programming language R to perform the fits.

In all of the fits, we biased the exponent Δ_1 of the leading correction-to-scaling term, performing the fits for three different choices of $\Delta_1 = 0.520, 0.528, 0.536$ which correspond to the best Monte Carlo estimate of $\Delta_1 = 0.528(8)$. We approximated the next-to-leading correction-to-scaling term with a term of order $1/N$, which we expect to behave as an effective term which takes into account three competing corrections with exponents $-2\Delta_1, -1, -\Delta_2 \approx -1$. For $\log Z_N$, we fitted $\log A$, $\log \mu$, γ, the amplitude a, and the amplitude of the $1/N$ effective term. For $\log(P_N/Z_N)$, we fitted $\log D$, ν, the

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amplitude b, and the amplitude of the $1/N$ term. For the BCC lattice, we minimized the impact of the odd-even oscillations by fitting even and odd subsequences separately. We included the extrapolated coefficients in our fits, repeating the calculation for the central estimates and for values which are one standard deviation above and below them.

This procedure gave us up to nine estimates for each sequence of coefficients (from the three choices of Δ_1, and the three choices of extrapolated coefficient values). For the central parameter estimates we used the case where $\Delta_1 = 0.528$ (the central value) in combination with the central value of the extrapolated coefficients. We also calculated the maximum and minimum parameter estimates over the remaining 8 cases.

Our criterion for truncation of the extrapolated series was as follows. We performed fits using the additional terms from the Z_N series, and truncated the series at the point where the additional spread due to the range of extrapolated coefficients meant that they were no help in determining the trend in figures 1, 3 and 4. We truncated the extrapolated P_N series at the same point. For the BCC lattice, we found that five of the extrapolated coefficients gave a spread which was only moderately greater than the spread arising from varying Δ_1, effectively extending the series to 33 terms. For the FCC lattice, we found we could use three additional coefficients, extending the series to 27 terms. Further extrapolated coefficients resulted in increasingly divergent fits.

For each of the parameter estimates, we plotted them against the expected relative magnitude of the first neglected correction-to-scaling term. This should result in approximately linear convergence as we approach the $N \to \infty$ limit which corresponds to approaching the y-axis from the right in the following figures. In equations (6) and (7) we expect that the next term, which is not included in the fits, is $O(N^{-1-\Delta_1})$; given that $\Delta_1 \approx 0.5$, we take the neglected term to be $O(N^{-3/2})$. The value of N that is used in the plot is the maximum value of N in the sequence of fitted coefficients, which we denote $N_{\max}$ in the plots.

We plot our fitted values in figures 1–8. For ease of interpretation we converted estimates of $\log \mu$, $\log A$, and $\log D$ to estimates of μ, A, and D. We note that the parameter estimates arising from the odd subsequence of the BCC series for Z_N benefited dramatically from the extrapolated sequence. Examining estimates for γ in figure 1, $\mu_{\rm bcc}$ in figure 3, and $A_{\rm bcc}$ in figure 5 we see in each case that the trend of the odd subsequence would be dramatically different were it not for the three additional odd terms in the extrapolated sequence. In other cases the additional coefficients are useful, and certainly make the trend for the estimates clearer, but they are not as crucial.

Our final parameter estimates are plotted on the y-axes.

3.3. Further details

We now briefly discuss two further aspects of the analysis.

Firstly, the influence of the anti-ferromagnetic singularity, which is observed for bipartite lattices such as the BCC lattice, can be discerned from the series. As discussed in more detail in [12], in the asymptotic expression for Z_N the leading contribution of the anti-ferromagnetic singularity is of the form const.$\mu^N(-1)^N N^{\alpha-2}$, where α is the critical exponent associated with self-avoiding polygons. We have performed an analysis of the Z_N series for the BCC lattice via first order inhomogeneous differential

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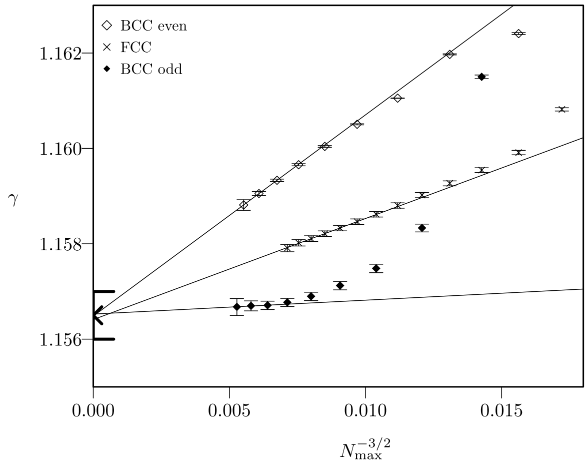

Figure 1. Variation of fitted value of γ with $N_{\max}$. The line of best fit to the final six values is shown for the FCC lattice and to the final three values for the BCC lattice, separately for the odd and even values. Our final estimate is plotted on the y-axis.

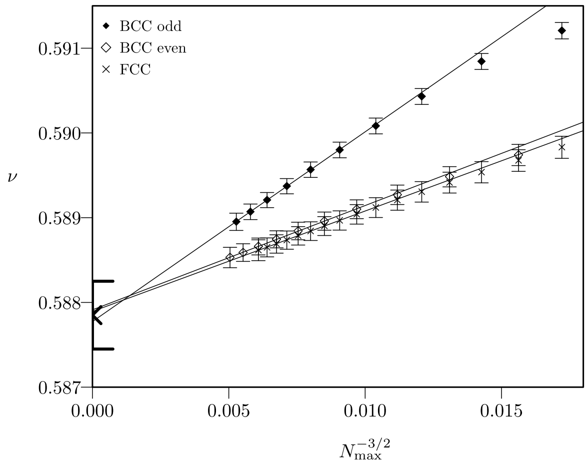

Figure 2. Variation of fitted value of ν with $N_{\max}$. The line of best fit to the final six values is shown for the FCC lattice and to the final three values for the BCC lattice, separately for the odd and even values. Our final estimate is plotted on the y-axis.

approximants. We found a strong signal of a singularity at $z = -1/\mu_{\mathrm{bcc}}$; the resulting estimate of μ_{bcc} is less accurate than that coming from our direct fits and we do not report it here. The associated exponent of the singularity of the generating function, which corresponds to $1 - \alpha$, is in the vicinity of 0.76–0.78, where this range represents the spread of differential approximant estimates and should not be regarded as a confidence interval. This is consistent with a value of α in the range of 0.22–0.24, which may be compared with the expected value of $\alpha = 0.237\,2090(12)$ obtained from the hyperscaling relation $d\nu = 2 - \alpha$, with $\nu = 0.587\,597\,00(40)$ [18]. One could extract further information from the series for Z_N and P_N, such as the amplitudes of the anti-ferromagnetic terms, but we choose not to do so here because to be able to perform the fits we would need to bias the value of α, and even then the resulting estimates would be quite inaccurate.

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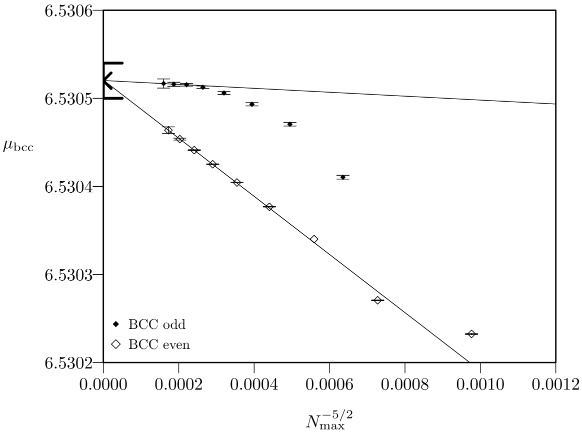

Figure 3. Variation of fitted value of μ_{bcc} with N_{max}. The line of best fit to the final three values is shown, separately for the odd and even values. Our final estimate is plotted on the y-axis.

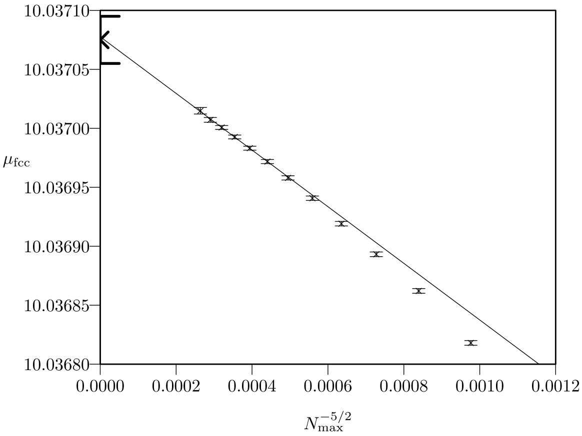

Figure 4. Variation of fitted value of μ_{fcc} with N_{max}. The line of best fit to the final six values is shown. Our final estimate is plotted on the y-axis.

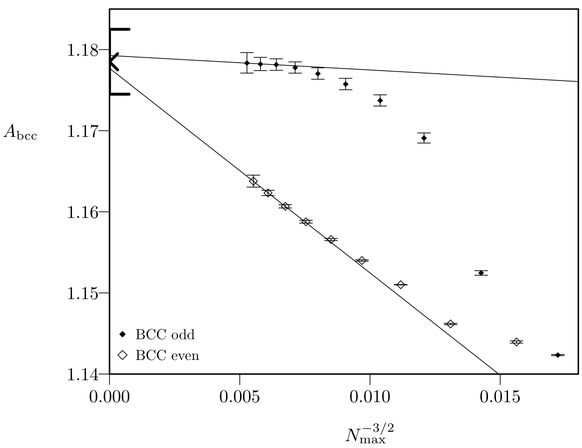

Figure 5. Variation of fitted value of D_{bcc} with N_{max}. The line of best fit to the final three values is shown, separately for the odd and even values. Our final estimate is plotted on the y-axis.

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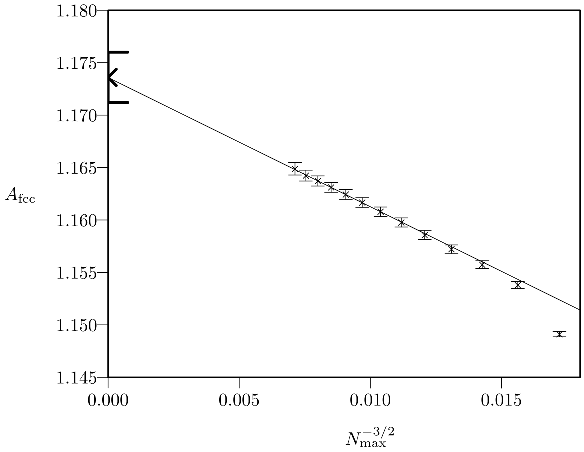

Figure 6. Variation of fitted value of A_{fcc} with N_{max}. The line of best fit to the final six values is shown. Our final estimate is plotted on the y-axis.

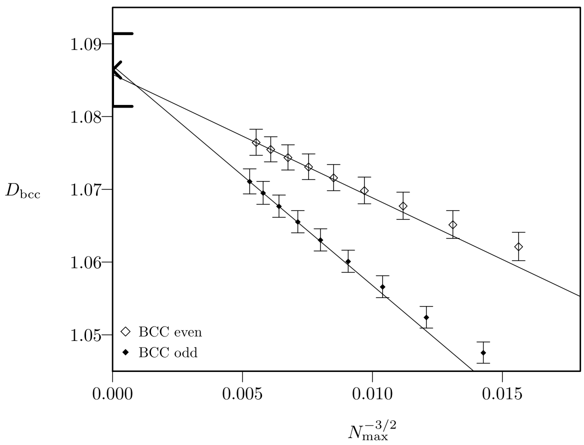

Figure 7. Variation of fitted value of D_{bcc} with N_{max}. The line of best fit to the final three values is shown, separately for the odd and even values. Our final estimate is plotted on the y-axis.

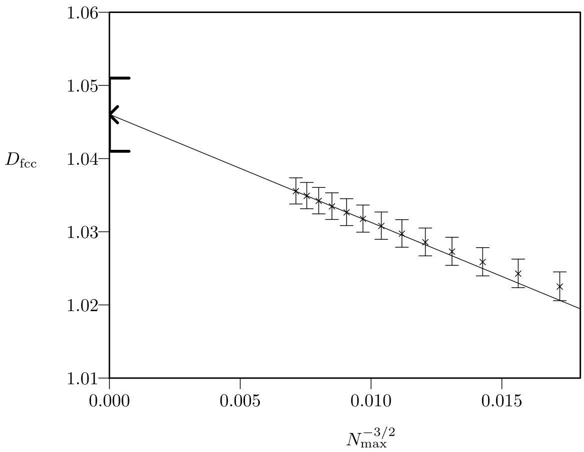

Figure 8. Variation of fitted value of D_{fcc} with N_{max}. The line of best fit to the final six values is shown. Our final estimate is plotted on the y-axis.

Table 5. Summary of our parameter estimates for γ and ν, with comparison to values from the literature. Except where noted, the series estimates for γ and ν from the literature come from the simple cubic lattice.

Source[a]	γ	ν
This work	1.156 50(50)	0.587 85(40)
[26] MC (2017)	1.156 953 00(95)	
[18] MC (2016)		0.587 597 00(40)
[27] CB (2016)	1.1588(25)	0.5877(12)
[13] Series $N \leqslant 36$ (2011)	1.156 98(34)	0.587 72(17)
[28] MC (2010)		0.587 597(7)
[12][b] Series $N \leqslant 30$ (2007)	1.1569(6)	0.587 74(22)
[29] MC (2004)	1.1573(2)	
[30] MC (2001)		0.5874(2)
[11] Series $N \leqslant 26$ (2000)	1.1585	0.5875
[31] MC (1998)	1.1575(6)	
[32] FT $d = 3$ (1998)	1.1596(20)	0.5882(11)
[32] FT ϵ bc (1998)	1.1571(30)	0.5878(11)
[14] Series $N \leqslant 21$ (1997)	1.161(2)	0.592(2)
[14] Series $N \leqslant 21$, biased (1997)	1.1594(8)	0.5878(6)
[14] BCC series $N \leqslant 21$ (1997)	1.1612(8)	0.591(2)
[14] BCC series $N \leqslant 21$, biased (1997)	1.1582(8)	0.5879(6)
[33] MCRG (1997)		0.587 56(5)
[34] MC (1995)		0.5877(6)
[10] Series $N \leqslant 23$ (1992)	1.161 93(10)	
[9] Series $N \leqslant 21$ (1989)	1.161(2)	0.592(3)

[a] Abbreviations: MC ≡ Monte Carlo, CB ≡ conformal bootstrap, FT ≡ field theory, MCRG ≡ Monte Carlo renormalization group.
[b] Using equations (74) and (75) with $0.516 \leqslant \Delta_1 \leqslant 0.54$.

Secondly, we have performed one additional analysis of the Z_N series for the BCC lattice, using the method of Zinn-Justin [24], together with the enhancement described by Butera and Comi [25] (starting at Equation (23) of that paper) which involves performing an additional extrapolation. We found that this enhanced method is significantly better than the original method of Zinn–Justin, and is quite powerful in obtaining estimates of μ_{bcc}. The resulting estimates are consistent with those from the direct fitting procedure, and of roughly comparable accuracy; we find that μ_{bcc} is in the vicinity of $6.530\,525 - 6.530\,535$. Note that we did not attempt to combine the enhanced Zinn-Justin method with the differential approximant extrapolation procedure, which would have reduced the spread somewhat.

4. Summary and conclusion

We give our estimates for γ and ν in table 5, where we also include estimates coming from the literature. We observe that our estimates are consistent with the literature values, but that the recent Monte Carlo estimates of γ and ν, using the pivot algorithm, are far more accurate than the estimates from series. The estimates coming from our enumerations on the BCC and FCC lattices are not quite as precise as the estimates coming from the SC lattice only, but the fact that they are coming from two independent sources, with different systematic errors, makes these new estimates more robust.

In addition, our estimates of the non-universal quantities for the BCC lattice are $A_{\mathrm{bcc}} = 1.1785(40)$, $D_{\mathrm{bcc}} = 1.0864(50)$, and $\mu_{\mathrm{bcc}} = 6.530\,520(20)$, which should be compared with earlier estimates of 6.5304(13) [9] from 1989, and unbiased and biased estimates respectively of 6.530 36(9) and 6.530 48(12) [14] from 1997. Our estimates of the non-universal quantities for the FCC lattice are $A_{\mathrm{fcc}} = 1.1736(24)$, $D_{\mathrm{fcc}} = 1.0460(50)$, and $\mu_{\mathrm{fcc}} = 10.037\,075(20)$, which should be compared with earlier estimates of 10.036 55 [16] from 1979, and 10.0364(6) [8] from 1987 (where these estimates come from different analyses of the same $N \leqslant 14$ term series).

In conclusion, the length-doubling algorithm has resulted in significant extensions of the BCC and FCC series. The application of a recently invented series analysis technique [20], which combines series extrapolation from differential approximants with direct fitting of the extrapolated series, has given excellent estimates of the various critical parameters. In particular, estimates of the growth constants for the BCC and FCC lattices are far more accurate than the previous literature values.

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