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Universal amplitude ratios for three-dimensional self-avoiding walks

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Abstract
We have calculated exactly the number, the mean-square end-to-end distance, the mean-square radius of gyration, and the mean-square distance of a monomer from the origin for n-step self-avoiding walks on the simple cubic, diamond, body-centred cubic and face-centred cubic lattices, respectively, up to 20, 30, 16 and 13 steps by a computer. Two universal amplitude ratios are estimated.

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1. Introduction

A self-avoiding walk (SAW) is a model of a polymer [1]. We are interested in the following functions: (1) the chain generating function for SAWs $C(x) = \sum c_n x^n$, where c_n is the total number of n-step SAWs; (2) the mean-square end-to-end distance of n-step SAWs R_n^2; (3) the mean-square radius of gyration of n-step SAWs G_n^2 and (4) the mean-square distance of a monomer from the origin of n-step SAWs M_n^2.

The asymptotic forms at large n are believed to be [2]

$$c_n \approx A\mu^n n^{\gamma-1} \qquad R_n^2 \approx Bn^{2\nu} \qquad G_n^2 \approx Cn^{2\nu} \qquad M_n^2 \approx Dn^{2\nu} \tag{1}$$

where μ is called the connective constant. The exponents γ and ν depend only on the space dimensionality d but not on the particular lattice chosen. The amplitudes A, B, C, D and the connective constant μ vary from lattice to lattice. Exact values for the exponents have been derived for $d = 2$ and the results are [3, 4]

$$\gamma = 43/32 = 1.343\,75 \qquad \nu = 3/4 = 0.75. \tag{2}$$

For $d = 3$ the exact results are not available and we have

$$\gamma \approx 7/6 \qquad \nu \approx 3/5. \tag{3}$$

Although the amplitudes are lattice-dependent, Cardy and Saleur [5] used the c-theorem in conformal theory to prove that the amplitude ratios C/B and D/B are universal for two-dimensional SAWs. A minor mistake in their work was discovered [6, 7] and corrected later [8]. From exact enumeration results for SAWs on the square lattice up to 21 steps and the triangular lattice up to 15 steps, Guttmann and Yang [6] obtained for both lattices

$$C/B = 0.1396 \pm 0.001 \qquad D/B = 0.4375 \pm 0.002. \tag{4}$$

From a Monte Carlo study of SAWs on the square lattice, Caracciolo *et al* found that [8]

$$C/B = 0.140\,26 \pm 0.000\,11 \qquad D/B = 0.439\,62 \pm 0.000\,33. \tag{5}$$

Lin and Huang [9] studied SAWs on the kagome lattice up to 30 steps and found that

$$C/B = 0.140 \pm 0.001 \qquad D/B = 0.440 \pm 0.001. \tag{6}$$

The series for the number of three-dimensional SAWs and the corresponding series for the mean-square end-to-end distance have been studied extensively. However, the corresponding series for the mean-square radius of gyration and the series for the mean-square distance of a monomer from the origin have been overlooked. From the standard theory of critical phenomena based on the renormalization group, the amplitude ratios C/B and D/B are universal for SAWs on regular three-dimensional lattices [10]. We have studied numerically four lattices and estimated these two universal ratios.

2. Simple cubic (SC) lattice

In a recent paper [11], the series $C(x)$ for the number of SAWs on the simple cubic lattice has been extended from the previous maximum 23 [12] to 26 steps and the series $\sum c_n R_n^2$ for the mean-square end-to-end distance from 20 to 26 [13]. The estimated values are $\mu = 4.684\,01$, $\gamma = 1.1585$, $\nu = 0.5875$, $A = 1.205$ and $AB = 1.476$. Li *et al* [10] made a high-precision Monte Carlo study of SAWs on simple cubic lattice up to 80 000 steps and their results are $B = 1.216\,67 \pm 0.000\,50$, $C = 0.194\,55 \pm 0.000\,07$ and $C/B = 0.1599 \pm 0.0002$. Their estimate of the amplitude B is slightly smaller (about 0.7%) than the estimated value given by MacDonald *et al* [11].

We have calculated the mean-square radius of gyration, and the mean-square distance of a monomer from the origin for n-step self-avoiding walks on the simple cubic lattice up to 20 steps by a computer. The results are given in table 1. For the convenience of readers we also list the number of n-step SAWs and $c_n R_n^2$.

Since the exponent ν has been estimated already from a series which contains six more terms than ours, we made biased estimates [14] of C and D with $\nu = 0.5875$ from the data of table 1 using the method of Padé approximants and found that

$$C = 0.192 \pm 0.005 \qquad D = 0.58 \pm 0.01. \tag{7}$$

From the estimated values of B, C and D, we can obtain the ratios C/B and D/B. However, these two ratios can be estimated directly with greater precision and we shall explain this method in section 6.

3. Diamond (DA) lattice

The series for the number of SAWs and the series for the mean-square end-to-end distance on the diamond lattice were computed by Guttmann [15] up to 27 steps and the estimated values are $\gamma = 1.161 \pm 0.002$, $\nu = 0.592 \pm 0.003$ and $x_c = \mu^{-1} = 0.347\,34 \pm 0.000\,02$. We

Table 1. Exact enumeration results for the number, the mean-square end-to-end distance, the mean-square distance of a monomer from the origin and the mean-square radius of gyration for self-avoiding walks on the simple cubic lattice.

n	$c_n/6$	$c_n R_n^2/6$	$(n+1)c_n M_n^2/6$	$(n+1)^2 c_n G_n^2/6$
1	1	1	1	1
2	5	12	17	22
3	25	97	182	292
4	121	672	1 566	2 994
5	589	4 261	11 931	26 613
6	2 821	25 588	83 479	212 532
7	13 565	147 821	552 108	1 583 808
8	64 661	830 576	3 489 548	11 126 940
9	308 981	4 566 917	21 351 857	75 021 053
10	1 468 313	24 692 980	127 023 801	487 286 330
11	6 989 025	131 682 825	739 923 498	3 079 847 364
12	33 140 457	694 386 864	4 228 390 218	18 971 359 374
13	157 329 085	3 626 770 709	23 809 194 967	114 611 086 221
14	744 818 613	18 790 632 772	132 218 649 171	679 491 899 320
15	3 529 191 009	96 675 376 705	726 256 580 504	3 970 337 752 176
16	16 686 979 329	494 382 431 552	3 947 530 263 656	22 868 496 906 360
17	78 955 042 017	2 514 666 026 897	21 276 669 105 001	130 240 792 686 993
18	372 953 947 349	12 730 690 730 212	113 738 242 204 065	733 407 393 089 174
19	1762 672 203 269	64 177 763 220 925	603 959 174 412 606	4 092 890 484 164 740
20	8319 554 639 789	322 314 275 563 424	3185 894 424 423 422	22 633 188 890 656 962

extended his results to three more steps and calculated the mean-square radius of gyration, and the mean-square distance of a monomer from the origin up to 30 steps. The results are given in table 2.

We made biased estimates of amplitudes by using the method of Padé approximants with $\gamma = 1.1585$ and $\nu = 0.5875$. The results are

$$A = 1.24 \pm 0.01 \qquad B = 1.42 \pm 0.01 \qquad C = 0.226 \pm 0.002 \qquad D = 0.678 \pm 0.005. \tag{8}$$

The amplitude ratios C/B and D/B are estimated directly and the results are discussed in section 6.

4. Body-centred cubic (BCC) lattice

High-temperature series expansions for the susceptibility and the second correlation moment of the N-vector spin model on the body-centred cubic lattice were obtained by Butera and Comi [16] of order β^{21}. The special case of $N = 0$ corresponds to a self-avoiding walk [1] such that the series for the susceptibility corresponds to the $C(x)$ series and the series for the correlation moment to the $\sum c_n R_n^2$ series. The critical point and the exponents are estimated as follows [16]:

$$x_c = 0.153\,131(2) \qquad \gamma = 1.1612(8) \qquad \nu = 0.591(2). \tag{9}$$

From these two series, we made biased estimations for the amplitudes A and B using the method of Padé approximants with $x_c = \mu^{-1} = 0.153\,131$, $\gamma = 1.1585$ and $\nu = 0.5875$. The results are

$$A = 1.16 \pm 0.01 \qquad B = 1.06 \pm 0.01. \tag{10}$$

Table 2. Exact enumeration results for the number, the mean-square end-to-end distance, the mean-square distance of a monomer from the origin and the mean-square radius of gyration for self-avoiding walks on the diamond lattice.

n	$c_n/4$	$c_n R_n^2/4$	$(n+1)c_n M_n^2/4$	$(n+1)^2 c_n G_n^2/4$
1	1	1	1	1
2	3	8	11	14
3	9	41	74	116
4	27	176	398	746
5	81	689	1 883	4 121
6	237	2 552	8 135	20 300
7	699	9 083	33 212	93 440
8	2 049	31 408	129 524	405 636
9	6 015	106 239	488 507	1 687 383
10	17 547	353 304	1 789 583	6 753 810
11	51 321	1 158 617	6 418 654	26 307 092
12	149 499	3 756 384	22 576 698	99 817 558
13	436 137	12 061 945	78 233 431	371 382 217
14	1 268 475	38 418 328	267 277 949	1 355 404 008
15	3 693 663	121 504 271	903 165 352	4 875 193 600
16	10 730 613	381 942 224	3 019 423 720	17 280 369 496
17	31 203 621	1 194 166 357	10 009 581 021	60 563 128 677
18	90 566 913	3 715 993 832	32 905 022 321	209 818 417 170
19	263 067 933	11 514 366 573	107 450 446 394	720 394 458 228
20	762 975 129	35 543 506 848	348 518 726 594	2 450 455 002 870
21	2 214 262 551	109 342 447 895	1 124 320 164 949	8 274 346 086 703
22	6 417 997 005	335 329 803 992	3 607 005 563 535	27 725 447 501 828
23	18 612 424 371	1 025 473 390 579	11 520 096 050 100	92 336 430 942 304
24	53 919 461 865	3 127 923 450 864	36 622 950 904 364	305 538 317 619 516
25	156 274 048 851	9 518 194 702 643	115 987 794 015 815	1 005 820 707 404 091
26	452 515 585 203	28 900 497 267 032	365 901 078 312 447	3 292 998 912 340 922
27	1 310 847 118 053	87 574 269 583 237	1 150 583 520 143 406	10 733 678 967 247 668
28	3 794 281 468 641	264 871 770 584 528	3 605 833 053 175 462	34 821 964 967 801 834
29	10 986 440 189 271	799 718 478 318 855	11 269 062 818 629 937	112 538 766 555 627 767
30	31 789 702 212 633	2410 654 958 503 592	35 115 264 324 405 463	362 214 141 414 158 224

We calculated the mean-square radius of gyration and the mean-square distance of a monomer from the origin up to 16 steps. The results are given in table 3. We made biased estimations for the amplitudes C and D with $\nu = 0.5875$ and the results are

$$C = 0.166 \pm 0.002 \qquad D = 0.505 \pm 0.005. \tag{11}$$

The amplitude ratios C/B and D/B are estimated directly and the results are discussed in section 6.

5. Face-centred cubic (FCC) lattice

The coordination number of the face-centred cubic lattice is 12, which means that at each successive step, there are about ten times as many SAWs as in the preceding step. The first 12 terms of the chain generating function were obtained by Martin *et al* [17]. This series was later extended to 14 terms [18]. Guttmann [19] studied this series and concluded that $x_c = 0.099\,637 \pm 0.000\,006$ and $\gamma = 1.163 \pm 0.002$. We made a biased estimation using the

Table 3. Exact enumeration results for the number, the mean-square end-to-end distance, the mean-square distance of a monomer from the origin and the mean-square radius of gyration for self-avoiding walks on the body-centred cubic lattice.

n	$c_n/8$	$c_n R_n^2/8$	$(n+1)c_n M_n^2/8$	$(n+1)^2 c_n G_n^2/8$
1	1	1	1	1
2	7	16	23	30
3	49	177	338	548
4	331	1 696	4 018	7 766
5	2 245	14 917	42 395	95 581
6	15 007	124 468	411 637	1 059 212
7	100 603	999 995	3 781 364	10 958 400
8	668 965	7 819 224	33 228 340	107 000 732
9	4 456 585	59 853 953	282 787 949	1 002 919 433
10	29 536 387	450 672 532	2 341 138 243	9 061 897 542
11	196 006 195	3 347 481 963	18 981 640 182	79 685 665 460
12	1 296 083 749	24 590 339 688	151 031 542 138	683 195 865 502
13	8 578 330 951	178 939 306 279	1 184 221 616 405	5 745 246 546 679
14	56 629 067 755	1 291 795 743 828	9 159 456 815 933	47 426 867 197 944
15	374 097 956 053	9 261 172 589 741	70 078 671 934 528	385 878 427 423 912
16	2 466 416 982 199	65 999 364 870 856	530 646 513 107 928	3 095 508 365 057 224

Table 4. Exact enumeration results for the number, the mean-square end-to-end distance, the mean-square distance of a monomer from the origin and the mean-square radius of gyration for self-avoiding walks on the face-centred cubic lattice.

n	$c_n/12$	$c_n R_n^2/12$	$(n+1)c_n M_n^2/12$	$(n+1)^2 c_n G_n^2/12$
1	1	1	1	1
2	11	24	35	46
3	117	409	786	1 280
4	1 225	6 012	14 354	27 930
5	12 711	81 315	232 165	526 007
6	131 143	1 042 564	3 465 621	8 967 144
7	1 347 679	12 878 367	48 863 948	142 226 388
8	13 808 087	154 777 460	660 172 360	2 135 591 332
9	141 147 827	1 821 449 227	8 628 332 223	30 716 312 051
10	1 440 160 797	21 081 182 692	109 821 362 909	426 723 115 802
11	14 672 058 701	240 717 534 413	1 367 840 196 838	5 761 084 490 984
12	149 287 922 589	2 718 116 571 816	16 731 864 664 214	75 936 755 874 222
13	1 517 387 524 783	30 405 174 655 267	201 568 203 476 849	980 723 557 080 247

method of Padé approximants for the amplitude A with $x_c = 0.099\,637$ and $\gamma = 1.1585$ and found that

$$A = 1.16 \pm 0.02. \tag{12}$$

Majid *et al* [20] studied the first 12 terms of the series $\sum c_n R_n^2$ and concluded that

$$B = 1.05 \pm 0.03 \qquad \nu = 0.5875 \pm 0.0015. \tag{13}$$

We extended their result to one more term and calculated the mean-square radius of gyration, and the mean-square distance of a monomer from the origin up to 13 steps. The results are

Table 5. The ratios r_n for the SC, DA, BCC and FCC lattices.

n	SC	BCC	FCC	DA
1	0.250 000	0.250 000	0.250 000	0.250 000
2	0.203 704	0.208 333	0.212 963	0.194 444
3	0.188 144	0.193 503	0.195 599	0.176 829
4	0.178 214	0.183 160	0.185 828	0.169 545
5	0.173 492	0.177 987	0.179 688	0.166 143
6	0.169 509	0.173 672	0.175 532	0.162 338
7	0.167 412	0.171 226	0.172 560	0.160 740
8	0.165 391	0.168 942	0.170 343	0.159 445
9	0.164 271	0.167 561	0.168 637	0.158 829
10	0.163 089	0.166 178	0.167 288	0.157 985
11	0.162 419	0.165 310	0.166 201	0.157 678
12	0.161 663	0.164 397	0.165 309	0.157 235
13	0.161 232	0.163 812	0.164 567	0.157 090
14	0.160 716	0.163 173		0.156 801
15	0.160 425	0.162 759		0.156 733
16	0.160 058	0.162 291		0.156 552
17	0.159 853			0.156 530
18	0.159 583			0.156 409
19	0.159 436			0.156 412
20	0.159 231			0.156 332
21				0.156 351
22				0.156 297
23				0.156 324
24				0.156 289
25				0.156 322
26				0.156 300
27				0.156 335
28				0.156 323
29				0.156 359
30				0.156 353

given in table 4. We made biased estimations for the amplitudes with $\nu = 0.5875$ and the results are

$$B = 1.03 \pm 0.03 \qquad C = 0.161 \pm 0.003 \qquad D = 0.49 \pm 0.02. \tag{14}$$

The amplitude ratios C/B and D/B are estimated directly and the results are discussed in section 6.

6. Discussion and conclusion

Meir [21] pointed out that the amplitude ratio can be calculated both more accurately and with less effort as a direct ratio than by making individual estimates and taking their quotient. The generating function for the series whose coefficients are these ratios has a simple pole at $x = 1$ (where x is the dummy variable of the generating function). The residue at the pole is the required amplitude ratio.

We define two ratios such that

$$r_n = G_n^2 \big/ R_n^2 \qquad s_n = M_n^2 \big/ R_n^2 \,. \tag{15}$$

Table 6. The ratios s_n for the SC, DA, BCC and FCC lattices.

n	SC	BCC	FCC	DA
1	0.500 000	0.500 000	0.500 000	0.500 000
2	0.472 222	0.479 167	0.486 111	0.458 333
3	0.469 072	0.477 401	0.480 440	0.451 220
4	0.466 071	0.473 821	0.477 512	0.452 273
5	0.466 674	0.473 677	0.475 855	0.455 491
6	0.466 061	0.472 453	0.474 876	0.455 385
7	0.466 872	0.472 673	0.474 283	0.457 063
8	0.466 818	0.472 174	0.473 922	0.458 213
9	0.467 533	0.472 463	0.473 707	0.459 819
10	0.467 648	0.472 251	0.473 586	0.460 480
11	0.468 249	0.472 535	0.473 529	0.461 661
12	0.468 414	0.472 454	0.473 514	0.462 325
13	0.468 918	0.472 715	0.473 529	0.463 284
14	0.469 094	0.472 699		0.463 803
15	0.469 520	0.472 933		0.464 575
16	0.469 692	0.472 952		0.465 026
17	0.470 057			0.465 670
18	0.470 220			0.466 051
19	0.470 536			0.466 593
20	0.470 687			0.466 924
21				0.467 389
22				0.467 678
23				0.468 080
24				0.468 336
25				0.468 689
26				0.468 916
27				0.469 228
28				0.469 431
29				0.469 710
30				0.469 893

These ratios are given in tables 5 and 6, respectively, for the simple cubic lattice, the diamond lattice, the body-centred cubic lattice and the face-centred cubic lattice.

Among the four lattices, the diamond lattice has the smallest coordination number (four) which means that it is relatively easy to count SAWs on the diamond lattice. We made biased estimations using the method of Padé approximants. For the simple cubic lattice, we found that

$$C/B = 0.158 \pm 0.002 \qquad D/B = 0.477 \pm 0.002. \tag{16}$$

For the body-centred cubic lattice, we found that

$$C/B = 0.158 \pm 0.003 \qquad D/B = 0.477 \pm 0.003. \tag{17}$$

For the face-centred cubic lattice, we found that

$$C/B = 0.158 \pm 0.004 \qquad D/B = 0.477 \pm 0.004. \tag{18}$$

For the diamond lattice, we found that

$$C/B = 0.158 \pm 0.002 \qquad D/B = 0.477 \pm 0.002. \tag{19}$$

We did not consider corrections to the scaling, which may be the reason that our estimated value of the universal amplitude ratio C/B is slightly smaller than the corresponding value given by Li *et al* [10].

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