On the critical behaviour of self-avoiding walks. II

1989 J. Phys. A: Math. Gen. 22 2807

(http://iopscience.iop.org/0305-4470/22/14/027)

J. Phys. A: Math. Gen. **22** (1989) 2807-2813. Printed in the UK

On the critical behaviour of self-avoiding walks: II

A J Guttmann

Department of Mathematics, University of Melbourne, Parkville, Victoria 3052, Australia

Received 7 February 1989, in final form 30 March 1989

Abstract. For the self-avoiding walk problem, the coefficients of the chain generating function and of the generating function for the sum of square end-to-end distances have been extended to 20 terms for the triangular lattice, to 27 terms for the diamond lattice, to 21 terms for the simple cubic lattice and to 16 terms for the BCC lattice. Precise estimates of the critical points are obtained, and for the exponents we find that $\gamma = 1.161 \pm 0.002$ and $\nu = 0.592 \pm 0.003$ encompasses all the three-dimensional lattice data.

1. Introduction

In an earlier paper (Guttmann 1987a, hereafter referred to as I) we presented extended series for both the square lattice and simple cubic (SC) lattice self-avoiding walk chain generating function $C(v)$ and mean square end-to-end distance generating function $R(v)$, where

$$C(v) = \sum c_n v^n \qquad R(v) = \sum r_n^2 v^n$$

where c_n is the number of n-step self-avoiding random walks (SAW) with fixed origin and r_n^2 is the sum of the squares of the end-to-end distance of all c_n n-step SAW.

In this paper we report further extensions of the SC lattice data by an additional term, extension of the triangular lattice walk data by one term, extension of the BCC lattice data by three terms and extension of the diamond lattice data by five terms.

The computational aspects of some of these calculations are unusually interesting. The extension of the simple cubic data, which was computationally the most demanding, was performed on a two-pipe Cyber 205. The diamond lattice calculations were performed on a Cyber 990, while the triangular and BCC lattice calculations were performed on a dedicated Micro Vax II. (By the term 'dedicated' we mean that the machine did nothing else but these calculations for 168 h per week for about two months.)

The algorithm used was the dimerisation algorithm of Torrie and Whittington (1975), appropriately modified to take advantage of the vectorisation capabilities of the two Cyber machines.

The new series were analysed using the analysis protocol developed in I, based on the method of differential approximants. The numerical results for the two-dimensional triangular lattice walk exponent γ are in agreement with Nienhuis' (1982, 1984) exact exponent estimates, while the critical point estimate has been slightly refined beyond that given in I. For the three-dimensional lattices, we find consistent exponent estimates from lattice to lattice, which are in agreement with those obtained from renormalisation

0305-4470/89/142807+07$02.50

group theory and Monte Carlo analysis. The critical point estimates we believe to be the most precise that have been obtained to date.

2. Generation of series

Some manual optimisation was necessary to maximise the performance of the code on the Cyber 205. In pure scalar mode the program ran at about 14 times the speed of a Vax 11/780. Improved performance was obtained by switching from 64-bit to 32-bit precision (the latter being, in fact, the same precision as the Vax), by hand-coding Cyber 205 vector statements and by assembly coding of 'linked triad' operations. An example of a linked triad is a construction of the form $C = A + kB$, where A, B and C are vectors and k is scalar. On a sequential machine this would probably be evaluated as a sequence of pairs of operations, each pair consisting of a scalar multiplication followed by a scalar addition, with the sequence controlled by a do-loop. Without linked triads (or 'chaining') a pipelined vector machine would evaluate it as a pipelined sequence (vector) of multiplications followed by a pipelined sequence of additions. Computed as a linked triad, the output of the multiplication pipe is fed directly into the addition pipe with no storage of intermediate results. Thus, for the two-pipe Cyber 205, the time for multiplication of an n-component 32-bit vector by a 32-bit scalar or for addition of two n-component 32-bit vectors is $T(n) = 51 + n/4$ cycles, while that for a linked triad of the above form is $61 + n/4$ cycles. Hence, for large vectors a time saving approaching 50% is attainable. The denominator of 4 in these expressions is the product of a factor of 2 due to the 205 having two vector pipes and another factor of 2 due to using 32-bit precision.

Though automatic vectorisation is available, the existence of a linked triad is frequently missed by the compiler, particularly if it is not in an obvious canonical form. Investigation of the assembly code identified such occurrences, and explicit assembly coding was then performed on triadic operations. A fuller discussion of this problem is given by Ramamurthy (1987).

In this way an overall speed-up from the scalar version of a factor of nearly 8 was obtained, with the result that the program ran at 100 times the speed of a Vax 11/780. Even so, around 40 h of CPU time was required to obtain the series to 21 terms. The series to 20 terms was given in I. The additional coefficients are $c_{21} = 235\,710\,090\,502\,158 v^{21}$ and $r_{21}^2 = 9679\,153\,967\,272\,734 v^{21}$.

The diamond lattice series were generated on a Cyber 990. This is a high-speed scalar machine, capable of some degree of vectorisation. Rewriting the FORTRAN code, but not resorting to assembly language programming, gave a speed of about 25 times that of a Vax 11/780. In this way the series for both the number of walks and the sum of their mean square end-to-end lengths were obtained to 27 terms. This gives five new coefficients beyond those given by Ishinabe (1989). These are also given in table 1.

For the triangular lattice, we found the coefficient of v^{20} in the chain generating function to be $c_{20} = 7812\,439\,620\,678$. The corresponding mean square end-to-end distance coefficient was not calculated.

For the BCC lattice both the number of walks and the sum of their mean square end-to-end lengths were obtained to 16 terms. This gives three new coefficients beyond those given by Ishinabe (1989). These are also given in table 1.

Table 1. Coefficients of the chain generating function $C(v)$ and the sum of the mean square distance generating function $R(v)$ for the diamond and body-centred cubic lattice.

	Diamond lattice		Body-centred cubic lattice	
	$C(v)$	$R(v)/4$	$C(v)$	$R(v)$
0	1		1	
1	4	1	8	3
2	12	8	56	48
3	36	41	392	531
4	108	176	2 648	5 088
5	324	689	17 960	44 751
6	948	2 552	120 056	373 404
7	2 796	9 083	804 824	2 999 985
8	8 196	31 408	5 351 720	23 457 672
9	24 060	106 239	35 652 680	179 561 859
10	70 188	353 304	236 291 096	1 352 017 596
11	205 284	1 158 617	1 568 049 560	10 042 445 889
12	597 996	3 756 384	10 368 669 992	73 771 019 064
13	1 744 548	12 061 945	68 626 647 608	536 817 918 837
14	5 073 900	38 418 328	453 032 542 040	3 875 387 231 484
15	14 774 652	121 504 271	2 992 783 648 424	27 783 517 769 223
16	42 922 452	381 942 224	19 731 335 857 592	197 998 094 612 568
17	124 814 484	1 194 166 357		
18	362 267 652	3 715 993 832		
19	1 052 271 732	11 514 366 573		
20	3 051 900 516	35 543 506 848		
21	8 857 050 204	109 342 447 895		
22	25 671 988 020	335 329 803 992		
23	74 449 697 484	1 025 473 390 579		
24	215 677 847 460	3 127 923 450 864		
25	625 096 195 404	9 518 194 702 643		
26	1 810 062 340 812	28 900 497 267 032		
27	5 243 388 472 212	87 574 269 583 237		

3. Analysis of series

We have used the same analysis protocol based on differential approximants described in I and discussed further in Guttmann (1989). We will not repeat the details here, but just give the results of our analysis.

For the triangular lattice data, the additional coefficient gives 10 non-defective first-order approximants ($K = 1$) and 7 second-order approximants ($K = 2$) which combine together to give the estimates

$$\left.\begin{aligned}\gamma &= 1.343\,41 \pm 0.000\,49\\ v_c &= 0.240\,9173 \pm 0.000\,0016\end{aligned}\right\} \quad K = 1$$

$$\left.\begin{aligned}\gamma &= 1.3452 \pm 0.0077\\ v_c &= 0.240\,921 \pm 0.000\,016\end{aligned}\right\} \quad K = 2.$$

These results are entirely consistent with the exact value $\gamma = \frac{43}{32} = 1.343\,75$. Imposing this value, linear regression among the approximants that gave rise to the above values gives

$$v_c = 0.240\,9193 \qquad K = 1$$

$$v_c = 0.240\,918 \qquad K = 2.$$

These are consistent with, but slightly more precise than, our earlier estimate based on first-order differential approximants of $0.240\,920 \pm 0.000\,003$.

For the SC lattice data, the additional coefficient gives 11 non-defective first-order approximants ($K = 1$) and 8 second-order approximants ($K = 2$) which combine together to give the estimates

$$\left.\begin{aligned} \gamma &= 1.1610 \pm 0.0008 \\ v_c &= 0.213\,496 \pm 0.000\,003 \end{aligned}\right\} \quad K = 1$$

$$\left.\begin{aligned} \gamma &= 1.1611 \pm 0.0010 \\ v_c &= 0.213\,496 \pm 0.000\,004 \end{aligned}\right\} \quad K = 2.$$

These results are entirely consistent with, but apparently more precise than, our earlier estimates $\gamma = 1.1613 \pm 0.0021$ and $v_c = 0.213\,497 \pm 0.000\,010$.

We have also analysed the generating function for $\langle R_n^2 \rangle = r_n^2 / c_n$, biased at 1.0. The estimate of $1 + 2\nu$ based on all 21 terms was 2.1890 ± 0.0041. (This adds an extra row to table 8 of I.) This additional entry does not alter our previous estimate of $\nu = 0.592 \pm 0.004$, though it does suggest that our upper bound is very conservative. We remark that an additional analysis biasing the series both at $+1.0$ and -1.0, which is appropriate for loose-packed lattices, does not appear to improve the quality of the approximants. Thus the $\langle R_n^2 \rangle$ series continue to display poorer convergence than the chain generating function series, presumably due to the more complicated confluent singularity structure, as explained in I.

For the diamond lattice data, we show the results of the analysis of the chain generating function in table 2. As explained in I, each row gives the mean and twice the standard deviation of the critical point and critical exponent estimates of the L approximants obtained from a Kth-order inhomogeneous differential approximant using n series coefficients, where L, K and n are given in table 2.

These data may be combined, as in I, and yield the overall estimates

$$\left.\begin{aligned} \gamma &= 1.1600 \pm 0.0036 \\ v_c &= 0.347\,34 \pm 0.000\,02 \end{aligned}\right\} \quad K = 1$$

$$\left.\begin{aligned} \gamma &= 1.1627 \pm 0.0021 \\ v_c &= 0.347\,37 \pm 0.000\,01 \end{aligned}\right\} \quad K = 2.$$

In table 3 we give the results of the corresponding analysis of the $\langle R_n^2 \rangle$ series, biased at 1.0. Combining these results gives $1 + 2\nu = 2.184 \pm 0.006$, where the general downward trend of the estimates has been taken into account as for the SC lattice, so that $\nu = 0.592 \pm 0.003$.

For the BCC data our series are still comparatively short. For the corresponding Ising susceptibility series we have five further terms (Nickel 1982), and as our analysis (Guttmann 1987b) showed, these five extra terms moved the estimate of the exponent γ downward by about 0.001. Repetition of the analysis performed on the diamond lattice data above gave the overall results

$$\left.\begin{aligned} \gamma &= 1.1626 \pm 0.0011 \\ v_c &= 0.153\,136 \pm 0.000\,004 \end{aligned}\right\} \quad K = 1$$

$$\left.\begin{aligned} \gamma &= 1.1631 \pm 0.0012 \\ v_c &= 0.153\,138 \pm 0.000\,004 \end{aligned}\right\} \quad K = 2.$$

Table 2. Diamond lattice $C(v)$ series. Summary of critical point and exponent estimates from first- and second-order differential approximants.

	$K=1$				
n	Critical point		Critical exponent		L
16	0.347 5135	0.000 3068	−1.176 8275	0.022 9056	4
17	0.347 3996	0.000 3015	−1.166 9021	0.030 5992	10
18	0.347 4040	0.000 2634	−1.166 3807	0.028 7292	11
19	0.312 7142	0.219 7531	−1.055 6630	0.741 9848	10
20	0.308 7767	0.231 5826	−1.033 5407	0.775 2823	9
21	0.284 1819	0.281 0066	−0.947 5911	0.937 0825	11
22	0.315 7481	0.209 4436	−1.051 8605	0.697 7571	11
23	0.347 3337	0.000 0732	−1.157 4595	0.011 2242	11
24	0.347 3499	0.000 0952	−1.159 5264	0.015 0142	11
25	0.347 3408	0.000 0858	−1.158 4533	0.014 4188	11
26	0.347 3197	0.000 2103	−1.154 7071	0.036 8470	11
27	0.347 3454	0.000 0242	−1.159 3832	0.004 5143	9
	$K=2$				
n	Critical point		Critical exponent		L
16	0.000 0000	—	0.000 0000	—	1×
17	0.000 0000	—	0.000 0000	—	1×
18	0.347 2804	0.000 0418	−1.154 2270	0.005 4374	2×
19	0.347 3235	0.000 3150	−1.161 0528	0.024 5923	2×
20	0.347 4094	—	−1.167 6784	—	1×
21	0.347 3958	0.000 0354	−1.165 9049	0.004 1696	5
22	0.347 4049	0.000 0394	−1.167 2672	0.005 9761	4
23	0.260 5036	0.347 3382	−0.869 1550	1.158 8800	4
24	0.347 3633	0.000 0429	−1.162 2211	0.006 4901	4
25	0.347 3506	0.000 0190	−1.160 3824	0.003 2035	8
26	0.347 3496	0.000 0395	−1.160 4947	0.008 1326	6
27	0.347 3483	0.000 0300	−1.160 0153	0.005 7920	7

Decreasing the estimate of γ by around 0.001 then brings it into good agreement with the SC estimate, and linear regression adequately takes account of the dependence of the estimates of γ on the estimates of v_c. In this way, we estimate $v_c = 0.153\,129 \pm 0.000\,010$.

Analysis of the BCC $\langle R_n^2 \rangle$ series as above displays the same dependence on order. That is, the exponent estimates decrease as the number of series coefficients used in the analysis increases. The last entry using all 16 terms gives $\nu = 0.595$, and so the decreasing trend implies excellent agreement with our earlier quoted estimate, $\nu = 0.592 \pm 0.004$. Taking the diamond and SC results into account, a sharpening of the confidence limits to ± 0.003 would seem to be acceptable.

4. Conclusion

Our results for critical points and critical exponents are summarised in table 4. The critical point estimates are believed accurate to within a few parts in the last quoted

Table 3. Diamond lattice (R_n^2) series. Summary of biased (at 1.0) exponent estimates from first- and second-order differential approximants. Table entries are $-1-2\nu$.

	$K=1$				$K=2$		
n	Critical exponent		L	n	Critical exponent		L
15	−2.193 3674	0.009 1402	4	15	—	—	0×
16	−2.191 1632	0.006 7646	4	16	−2.194 1835	—	1×
17	−2.191 2702	0.015 7813	10	17	—	—	0×
18	−2.190 6014	0.000 7349	11	18	−2.187 1552	—	1×
19	−2.190 9763	0.003 9679	12	19	−2.192 6328	0.004 1694	2×
20	−2.190 1439	0.000 6538	5	20	−2.192 1337	0.005 9837	2×
21	—	—	0×	21	−2.189 3255	0.000 8717	2×
22	−2.188 2741	0.003 0812	2×	22	−2.190 6224	0.002 7715	5
23	−2.191 2046	0.009 6639	5	23	−2.190 3151	0.001 7517	3×
24	−2.189 2058	0.001 4958	5	24	−2.190 2652	—	1×
25	−2.189 6137	0.003 3479	3×	25	−2.187 4493	—	1×
26	−2.185 6371	0.006 1528	5	26	−2.185 4883	0.001 3660	3×
27	−2.185 9705	0.000 7148	3×	27	−2.185 9416	—	1×

Table 4. Summary of critical point and critical exponent estimates obtained in this work. For completeness we also quote results for other lattices treated in previous work.

Lattice	Critical point	Exponent γ	Exponent ν
Square	0.379 0523	1.343 75†	0.750 00†
Triangular	0.240 919	1.343 75†	0.750 00†
Diamond	0.347 36	1.161 ± 0.003	0.592 ± 0.003
Simple cubic	0.213 496	1.161 ± 0.001	0.592 ± 0.004
Body-centred cubic	0.153 13	1.162 ± 0.002	0.592 ± 0.004
Face-centred cubic‡	0.099 637	1.163 ± 0.002	0.592

† Exact value.
‡ Result given in I.

digit. The exponent γ is entirely consistent with the recent field theoretical results of Le Guillou and Zinn-Justin (1985) of $\gamma = 1.160 \pm 0.004$, as well as an analysis by Ishinabe (1989) using shorter series.

The overall estimate of the exponent $\nu = 0.592 \pm 0.003$ is in agreement with earlier Monte Carlo work (Rapaport 1985, Madras and Sokal 1988), though it is slightly higher than the field theory estimate of Le Guillou and Zinn-Justin of 0.588 ± 0.001, a result also obtained by Ishinabe recently on the basis of a ratio-type analysis of shorter series. The formula of Flory, $\nu = 3(d+2)$, is seen to be exact for $d = 1$, 2 and 4, but not for $d = 3$. As shown by de Gennes (1979), the Flory formula depends on the cancellation of two competing approximations. It is remarkable that it is correct for three distinct dimensionalities.

Our second-order differential approximants give no evidence of a confluent singularity. Other methods we have tried in order to detect confluent singularities are also inconsistent. We conclude by remarking that we believe that there has as yet been no unequivocal evidence of a *universal* non-analytic correction-to-scaling exponent for the SAW problem in two or three dimensions. As the series are extended, the effect of the confluent term in the new coefficients diminishes. Hence, while longer series (or

Monte Carlo work on long walks) are desirable to sharpen estimates of the physically important leading singularity, they are less obviously useful in detecting confluent exponents. Earlier work on this question is reviewed in I. More recent discussion has been given by Ishinabe (1989) and Enting and Guttmann (1989).

Acknowledgments

I would like to thank Glenn Torrie for the use of his dimerisation program on which the enumerations are based. I would also like to thank Darryl Chivers and Roger Brown for helping to optimise the program on the Cyber 990 and Cyber 205, respectively, and Peter Price for useful suggestions regarding the optimisation description. This work was supported by a grant from the Australian Research Grants Committee.

References

de Gennes P G 1979 *Scaling Concepts in Polymer Physics* (Ithaca, NY: Cornell University Press)
Enting I G and Guttmann A J 1989 *J. Phys. A: Math. Gen.* **22** 1371
Guttmann A J 1987a *J. Phys. A: Math. Gen.* **20** 1839
—— 1987b *J. Phys. A: Math. Gen.* **20** 1855
—— 1989 *Phase Transitions and Critical Phenomena* vol 13, ed C Domb and J Lebowitz (New York: Academic) to appear
Ishinabe T 1989 *J. Phys. A: Math. Gen.* **22** in press
Le Guillou J C and Zinn-Justin J 1985 *J. Physique Lett.* **46** L137
Madras N and Sokal A D 1988 *J. Stat. Phys.* **50** 109
Nickel B G 1982 *Phase Transitions-Cargese 1980* ed M Levy, J C Le Guillou and J Zinn-Justin (New York: Plenum) p 291
Nienhuis B 1982 *Phys. Rev. Lett.* **49** 1062
—— 1984 *J. Stat. Phys.* **34** 731
Ramamurthy M 1987 *Supercomputer* **22** 41
Rapaport D C 1985 *J. Phys. A: Math. Gen.* **18** 113
Torrie G and Whittington S G 1975 *J. Phys. A: Math. Gen.* **8** 1178